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Supporting Information

# Barrier to Proton Transfer in the Dimer of Formic Acid: A Pure Rotational Study

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# Supporting Information:

## Content:

1) Experimental part
2) Completion of Ref. [17].
3) Tables of measured transition frequencies.
4) Material on the flexible model
    a. *Notes by Rolf Meyer*
    b. *Fortran computer program for the flexible model*
    c. *Input File*
    d. *Output file*

1) **Experimental Section** In the experiments all samples were obtained from Aldrich and used without further purification, except the species containing OD, which were prepared by direct exchange of the OH species with $D_2O$. The rotational spectra in the 6-18.5 GHz frequency region were measured on a COBRA-type[26] pulsed supersonic-jet Fourier-transform microwave (FTMW) spectrometer,[27] described elsewhere.[28] We needed to substitute the ALC MW power amplifier normally used in our spectrometer (ALS06, Max output power 0.1 W) with a TriQuint RM022020 MW power amplifier (Max output power 20 W. In addition, we needed to change the excitation time (π/2 pulse length) usual for polar molecules (1.1 μs) to ca. 6 μs. To observe the rotational transitions of the asymmetrically deuterated dimers of FA, we needed 10,000-30,000 accumulation cycles for of each spectrum: Helium at a total pressure of 0.3 MPa was streamed over the various samples, in such a way to have ca. 1% concentration of the species of interest. The obtained mixtures were expanded through the solenoid valve (General Valve, Series 9, nozzle diameter 0.5 mm) into the Fabry-Pérot-type cavity. The rest frequency was calculated as the arithmetic mean of the frequencies of the two Doppler components. The estimated accuracy of the frequency measurements is better than 3 kHz, resolution is better than 7 kHz.

2) **Completion of Reference [17]**.

Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

3) Tables of measured transition frequencies.

**Table S1.** Experimental transition frequencies of DCOOH-HCOOH.

| *J'* | *Ka'* | *Kc'* | *F'* | *J"* | *Ka"* | *Kc"* | *F"* | $0^+$ | | $0^-$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | *ν*/MHz | *Δν*/kHz | *ν*/MHz | *Δν*/kHz |
| 2 | 0 | 2 | 3 | 1 | 0 | 1 | 2 | 7569.4916 | 1.3 | 7560.5639 | 2.3 |
| 2 | 0 | 2 | 2 | 1 | 0 | 1 | 1 | 7569.4916 | -1.9 | 7560.5639 | -0.8 |
| 2 | 0 | 2 | 1 | 1 | 0 | 1 | 0 | 7569.5266 | -8.1 | 7560.6091 | 3.4 |
| 2 | 0 | 2 | 1 | 1 | 0 | 1 | 1 | 7569.4069 | -5.8 | 7560.4862 | 2.0 |
| 2 | 0 | 2 | 2 | 1 | 0 | 1 | 2 | 7569.534 | -8.2 | 7560.6091 | -4.2 |
| 3 | 0 | 3 | 4 | 2 | 0 | 2 | 3 | 11205.2798 | 1.3 | 11190.1039 | -0.6 |
| 3 | 0 | 3 | 3 | 2 | 0 | 2 | 2 | 11205.2798 | -0.1 | 11190.1039 | -2.0 |
| 3 | 0 | 3 | 2 | 2 | 0 | 2 | 1 | 11205.288 | -0.7 | 11190.1173 | 2.6 |
| 3 | 0 | 3 | 2 | 2 | 0 | 2 | 2 | 11205.2006 | -7.3 | 11190.0321 | -2.1 |
| 3 | 0 | 3 | 3 | 2 | 0 | 2 | 3 | 11205.3346 | 2.8 | 11190.1607 | 3.1 |
| 5 | 0 | 5 | 6 | 4 | 0 | 4 | 5 | 18011.0709 | -1.9 | 17978.7483 | 3.8 |
| 5 | 0 | 5 | 5 | 4 | 0 | 4 | 4 | 18011.0709 | -2.2 | 17978.7483 | 3.5 |
| 5 | 0 | 5 | 4 | 4 | 0 | 4 | 3 | 18011.0709 | -4.7 | 17978.7483 | 1.0 |
| 2 | 1 | 2 | 3 | 1 | 1 | 1 | 2 | 7048.459 | -0.6 | 7036.3504 | -0.2 |
| 2 | 1 | 2 | 2 | 1 | 1 | 1 | 1 | 7048.5134 | 3.3 | 7036.4052 | 4.2 |
| 2 | 1 | 2 | 1 | 1 | 1 | 1 | 0 | 7048.4088 | -0.1 | 7036.297 | -2.7 |
| 2 | 1 | 2 | 1 | 1 | 1 | 1 | 1 | 7048.4756 | 6.7 | 7036.37 | 9.8 |
| 2 | 1 | 2 | 2 | 1 | 1 | 1 | 2 | 7048.4881 | 2.1 | 7036.3806 | 3.8 |
| 2 | 1 | 1 | 3 | 1 | 1 | 0 | 2 | 8214.0053 | -0.6 | 8209.9011 | -0.1 |
| 2 | 1 | 1 | 2 | 1 | 1 | 0 | 1 | 8214.0559 | -0.5 | 8209.954 | 2.4 |
| 2 | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 8213.9541 | -0.6 | 8209.853 | 3.0 |
| 2 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 8214.0238 | 7.7 | 8209.9166 | 5.1 |
| 2 | 1 | 1 | 2 | 1 | 1 | 0 | 2 | 8214.0315 | -0.3 | 8209.9275 | 0.4 |
| 3 | 1 | 3 | 4 | 2 | 1 | 2 | 3 | 10536.5331 | 1.7 | 10518.1067 | 2.4 |
| 3 | 1 | 3 | 3 | 2 | 1 | 2 | 2 | 10536.5469 | 1.1 | 10518.1169 | -1.8 |
| 3 | 1 | 3 | 2 | 2 | 1 | 2 | 1 | 10536.5331 | 1.4 | 10518.1067 | 2.1 |
| 3 | 1 | 3 | 2 | 2 | 1 | 2 | 2 | 10536.4867 | -3.9 | 10518.0626 | -1.2 |
| 3 | 1 | 3 | 3 | 2 | 1 | 2 | 3 | 10536.5677 | -4.5 | 10518.141 | -3.9 |
| 3 | 1 | 2 | 4 | 2 | 1 | 1 | 3 | 12280.4784 | -1.6 | 12273.84 | 1.3 |
| 3 | 1 | 2 | 3 | 2 | 1 | 1 | 2 | 12280.4944 | 0.1 | 12273.8551 | 2.1 |
| 3 | 1 | 2 | 2 | 2 | 1 | 1 | 1 | 12280.4784 | -1.9 | 12273.84 | 1.0 |
| 3 | 1 | 2 | 3 | 2 | 1 | 1 | 3 | 12280.5209 | 0.7 | 12273.8839 | 5.1 |
| 3 | 1 | 2 | 2 | 2 | 1 | 1 | 2 | 12280.4449 | 4.9 | 12273.798 | -0.8 |
| 4 | 1 | 4 | 5 | 3 | 1 | 3 | 4 | 13986.877 | 4.5 | 13961.7774 | 1.3 |
| 4 | 1 | 4 | 4 | 3 | 1 | 3 | 3 | 13986.877 | -1.9 | 13961.7774 | -5.0 |
| 4 | 1 | 4 | 3 | 3 | 1 | 3 | 2 | 13986.877 | 2.3 | 13961.7774 | -0.9 |
| 4 | 1 | 3 | 5 | 3 | 1 | 2 | 4 | 16292.5417 | -2.3 | 16282.7008 | -0.6 |
| 4 | 1 | 3 | 4 | 3 | 1 | 2 | 3 | 16292.5417 | -8.6 | 16282.7008 | -6.8 |
| 4 | 1 | 3 | 3 | 3 | 1 | 2 | 2 | 16292.5417 | -4.5 | 16282.7008 | -2.7 |
| 5 | 1 | 5 | 6 | 4 | 1 | 4 | 5 | 17395.7562 | 2.3 | 17363.2262 | 1.1 |
| 5 | 1 | 5 | 5 | 4 | 1 | 4 | 4 | 17395.7562 | -1.2 | 17363.2262 | -2.3 |
| 5 | 1 | 5 | 4 | 4 | 1 | 4 | 3 | 17395.7562 | 0.4 | 17363.2262 | -0.7 |
| 3 | 2 | 1 | 4 | 2 | 2 | 0 | 3 | 11686.6183 | -4.9 | 11677.7099 | -7.2 |
| 3 | 2 | 1 | 3 | 2 | 2 | 0 | 2 | 11686.6699 | -6.0 | 11677.764 | -5.8 |
| 3 | 2 | 2 | 4 | 2 | 2 | 1 | 3 | 11446.5098 | 16.9 | 11434.4172 | -6.3 |
| 3 | 2 | 2 | 3 | 2 | 2 | 1 | 2 | 11446.5394 | -5.7 | 11434.4672 | -8.5 |
| 4 | 2 | 3 | 5 | 3 | 2 | 2 | 4 | 15214.1277 | 4.1 | 15197.7048 | 0.1 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 2 | 3 | 4 | 3 | 2 | 2 | 3 | 15214.152 | 6.4 | 15197.7264 | -0.4 |
| 4 | 2 | 2 | 5 | 3 | 2 | 1 | 4 | 15788.5385 | 0.9 | 15779.2378 | 4.0 |
| 4 | 2 | 2 | 4 | 3 | 2 | 1 | 3 | 15788.5624 | 2.2 | 15779.2562 | -0.3 |

**Table S2.** Experimental transition frequencies of DCOOH-HCOOD.

| *J'* | *Ka'* | *Kc'* | $F_1$' | $F_2$' | *J"* | *Ka"* | *Kc"* | $F_1$" | $F_2$" | *ν*/MHz | *Δν*/kHz |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 2 | 2 | 3 | 1 | 0 | 1 | 1 | 2 | 7524.8159 | 5.1 |
| 2 | 0 | 2 | 3 | 4 | 1 | 0 | 1 | 2 | 3 | 7524.8159 | 0.3 |
| 2 | 0 | 2 | 3 | 3 | 1 | 0 | 1 | 2 | 2 | 7524.8298 | 2.0 |
| 2 | 0 | 2 | 2 | 2 | 1 | 0 | 1 | 1 | 1 | 7524.8474 | -1.1 |
| 3 | 0 | 3 | 4 | 5 | 2 | 0 | 2 | 3 | 4 | 11133.9002 | -0.7 |
| 3 | 0 | 3 | 2 | 3 | 2 | 0 | 2 | 1 | 2 | 11133.9156 | 1.4 |
| 2 | 1 | 1 | 3 | 2 | 1 | 1 | 0 | 2 | 1 | 8175.2474 | 5.2 |
| 2 | 1 | 1 | 3 | 4 | 1 | 1 | 0 | 2 | 3 | 8175.2692 | 1.9 |
| 2 | 1 | 1 | 3 | 3 | 1 | 1 | 0 | 2 | 2 | 8175.3017 | -1.2 |
| 2 | 1 | 1 | 2 | 3 | 1 | 1 | 0 | 1 | 2 | 8175.3471 | -6.1 |
| 3 | 1 | 2 | 4 | 5 | 2 | 1 | 1 | 3 | 4 | 12221.0113 | 1.6 |
| 3 | 1 | 2 | 4 | 4 | 2 | 1 | 1 | 3 | 3 | 12221.023 | -2.3 |
| 3 | 1 | 2 | 3 | 3 | 2 | 1 | 1 | 2 | 2 | 12221.044 | -2.0 |
| 4 | 1 | 3 | 5 | 6 | 3 | 1 | 2 | 4 | 5 | 16210.3557 | 0.6 |
| 5 | 0 | 5 | 6 | 7 | 4 | 0 | 4 | 5 | 6 | 17879.6499 | 1.2 |
| 2 | 1 | 2 | 3 | 4 | 1 | 1 | 1 | 2 | 3 | 7000.7093 | 1.8 |
| 2 | 1 | 2 | 3 | 3 | 1 | 1 | 1 | 2 | 2 | 7000.7414 | -1.6 |
| 3 | 1 | 3 | 4 | 5 | 2 | 1 | 2 | 3 | 4 | 10463.478 | 2.6 |
| 3 | 1 | 3 | 4 | 4 | 2 | 1 | 2 | 3 | 3 | 10463.49 | -0.9 |
| 3 | 1 | 3 | 3 | 3 | 2 | 1 | 2 | 2 | 2 | 10463.5089 | -2.7 |
| 4 | 1 | 4 | 5 | 6 | 3 | 1 | 3 | 4 | 5 | 13886.8072 | 4.6 |
| 4 | 1 | 4 | 5 | 5 | 3 | 1 | 3 | 4 | 4 | 13886.8072 | -3.9 |
| 5 | 1 | 5 | 6 | 7 | 4 | 1 | 4 | 5 | 6 | 17266.1406 | -1.3 |
| 3 | 2 | 2 | 4 | 5 | 2 | 2 | 1 | 3 | 4 | 11381.8793 | 6.7 |
| 3 | 2 | 2 | 4 | 4 | 2 | 2 | 1 | 3 | 3 | 11381.9134 | -1.0 |
| 3 | 2 | 2 | 3 | 4 | 2 | 2 | 1 | 2 | 3 | 11381.9567 | 0.3 |
| 3 | 2 | 1 | 4 | 5 | 2 | 2 | 0 | 3 | 4 | 11629.9628 | -4.3 |
| 3 | 2 | 1 | 4 | 4 | 2 | 2 | 0 | 3 | 3 | 11630.0097 | 0.2 |
| 1 | 1 | 1 | 1 | 2 | 0 | 0 | 0 | 1 | 2 | 7577.263 | 5.4 |
| 1 | 1 | 1 | 2 | 2 | 0 | 0 | 0 | 1 | 1 | 7577.2884 | 1.4 |
| 1 | 1 | 1 | 2 | 3 | 0 | 0 | 0 | 1 | 2 | 7577.3009 | -0.7 |
| 2 | 1 | 2 | 2 | 3 | 1 | 0 | 1 | 1 | 2 | 10783.9659 | 5.5 |
| 2 | 1 | 2 | 2 | 2 | 1 | 0 | 1 | 1 | 1 | 10783.9795 | -4.3 |
| 2 | 1 | 2 | 3 | 3 | 1 | 0 | 1 | 2 | 2 | 10783.9932 | -4.9 |
| 2 | 1 | 2 | 3 | 4 | 1 | 0 | 1 | 2 | 3 | 10784.007 | 0.5 |
| 2 | 1 | 2 | 3 | 2 | 1 | 0 | 1 | 2 | 1 | 10784.0218 | -3.5 |

**Table S3.** Experimental transition frequencies of DCOOD-HCOOH.

| *J'* | *Ka'* | *Kc'* | $F_1$' | $F_2$' | *J"* | *Ka"* | *Kc"* | $F_1$" | $F_2$" | *ν*/MHz | *Δν*/kHz |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 2 | 2 | 3 | 1 | 0 | 1 | 1 | 2 | 7526.4223 | -5.0 |
| 2 | 0 | 2 | 3 | 4 | 1 | 0 | 1 | 2 | 3 | 7526.4223 | -9.8 |
| 2 | 0 | 2 | 3 | 3 | 1 | 0 | 1 | 2 | 2 | 7526.444 | -0.4 |
| 2 | 0 | 2 | 2 | 2 | 1 | 0 | 1 | 1 | 1 | 7526.4565 | -8.6 |
| 3 | 0 | 3 | 4 | 5 | 2 | 0 | 2 | 3 | 4 | 11136.1151 | 12.1 |
| 3 | 0 | 3 | 2 | 3 | 2 | 0 | 2 | 1 | 2 | 11136.1249 | 8.6 |
| 2 | 1 | 1 | 3 | 2 | 1 | 1 | 0 | 2 | 1 | 8177.3217 | 6.0 |
| 2 | 1 | 1 | 3 | 4 | 1 | 1 | 0 | 2 | 3 | 8177.3429 | 2.1 |
| 2 | 1 | 1 | 3 | 3 | 1 | 1 | 0 | 2 | 2 | 8177.3739 | -2.5 |
| 2 | 1 | 1 | 2 | 3 | 1 | 1 | 0 | 1 | 2 | 8177.4302 | 3.4 |
| 3 | 1 | 2 | 4 | 5 | 2 | 1 | 1 | 3 | 4 | 12224.0541 | -0.5 |
| 3 | 1 | 2 | 4 | 4 | 2 | 1 | 1 | 3 | 3 | 12224.0663 | -3.8 |
| 3 | 1 | 2 | 3 | 3 | 2 | 1 | 1 | 2 | 2 | 12224.0851 | -5.7 |
| 4 | 1 | 3 | 5 | 6 | 3 | 1 | 2 | 4 | 5 | 16214.2777 | -1.2 |
| 5 | 0 | 5 | 6 | 7 | 4 | 0 | 4 | 5 | 6 | 17882.5532 | 3.1 |
| 2 | 1 | 2 | 3 | 4 | 1 | 1 | 1 | 2 | 3 | 7002.0797 | 0.8 |
| 2 | 1 | 2 | 3 | 3 | 1 | 1 | 1 | 2 | 2 | 7002.1087 | -5.8 |
| 3 | 1 | 3 | 4 | 5 | 2 | 1 | 2 | 3 | 4 | 10465.4774 | -0.7 |
| 3 | 1 | 3 | 4 | 4 | 2 | 1 | 2 | 3 | 3 | 10465.4957 | 2.0 |
| 3 | 1 | 3 | 3 | 3 | 2 | 1 | 2 | 2 | 2 | 10465.514 | -0.4 |
| 3 | 1 | 3 | 3 | 3 | 2 | 1 | 2 | 2 | 3 | 10465.5284 | -0.6 |
| 4 | 1 | 4 | 5 | 6 | 3 | 1 | 3 | 4 | 5 | 13889.3828 | -2.9 |
| 4 | 1 | 4 | 5 | 5 | 3 | 1 | 3 | 4 | 4 | 13889.3932 | -1.0 |
| 5 | 1 | 5 | 6 | 7 | 4 | 1 | 4 | 5 | 6 | 17269.2547 | -3.0 |
| 3 | 2 | 2 | 4 | 5 | 2 | 2 | 1 | 3 | 4 | 11384.498 | -3.2 |
| 3 | 2 | 2 | 4 | 4 | 2 | 2 | 1 | 3 | 3 | 11384.5393 | -3.8 |
| 3 | 2 | 2 | 3 | 4 | 2 | 2 | 1 | 2 | 3 | 11384.5871 | 2.0 |
| 3 | 2 | 1 | 4 | 5 | 2 | 2 | 0 | 3 | 4 | 11632.9674 | 4.0 |
| 3 | 2 | 1 | 4 | 4 | 2 | 2 | 0 | 3 | 3 | 11633.0092 | 3.4 |
| 3 | 2 | 1 | 3 | 4 | 2 | 2 | 0 | 2 | 3 | 11633.0493 | 1.2 |
| 1 | 1 | 1 | 1 | 2 | 0 | 0 | 0 | 1 | 2 | 7576.5844 | 6.5 |
| 1 | 1 | 1 | 2 | 2 | 0 | 0 | 0 | 1 | 1 | 7576.604 | -3.3 |
| 1 | 1 | 1 | 2 | 3 | 0 | 0 | 0 | 1 | 2 | 7576.6177 | -4.3 |
| 2 | 1 | 2 | 2 | 3 | 1 | 0 | 1 | 1 | 2 | 10783.7972 | 1.2 |
| 2 | 1 | 2 | 2 | 2 | 1 | 0 | 1 | 1 | 1 | 10783.8184 | -0.9 |
| 2 | 1 | 2 | 3 | 3 | 1 | 0 | 1 | 2 | 2 | 10783.8374 | 3.7 |
| 2 | 1 | 2 | 3 | 4 | 1 | 0 | 1 | 2 | 3 | 10783.8374 | -4.7 |
| 2 | 1 | 2 | 3 | 2 | 1 | 0 | 1 | 2 | 1 | 10783.8615 | 0.6 |

## 4) Material on the flexible model

*a) Notes by R. Meyer, June 2017 – November 2018*

# Formic Acid Dimer
## Flexible Model Calculations

based on:

| | | |
|---|---|---|
| program | FF.prog.f | (to be opened with Text Wrangler or TextEdit) |
| input file | FFin | (to be opened with TextEdit or Text Wrangler) |
| output file | FFout | (to be opened with TextEdit or Text Wrangler) |

Table I. Energy levels from model calculations for formic acid dimer[a]

| isotopic species | | HCOOH...HOOCD | | HCOOH...HOOCH | |
|---|---|---|---|---|---|
| | | model 1 | model 2 | model 1 | model 2 |
| $\mathcal{E}_{00s}$ | $cm^{-1}$ | 1355.84 | 1455.44 | 1355.84 | 1455.44 |
| $(\mathcal{E}_{01s} - \mathcal{E}_{00s})$ | $cm^{-1}$ | 357.19 | 371.76 | 357.19 | 371.76 |
| $(\mathcal{E}_{10s} - \mathcal{E}_{00s})$[b] | $cm^{-1}$ | 2354.49 | 2539.12 | 2354.49 | 2539.12 |
| $E_{0s}$ | $cm^{-1}$ | 66.69 | 77.73 | 67.12 | 78.19 |
| $E_{1s} - E_{0s}$ | $cm^{-1}$ | 140.71 | 155.84 | 141.53 | 156.75 |
| $E_{0a} - E_{0s}$ | MHz | 331.28[c] | 331.30[c] | 334.89 | 334.85 |
| isotopic species | | HCOOD...DOOCD | | HCOOH...DOOCH | |
| | | model 1 | model 2 | model 1 | model 2 |
| $\mathcal{E}_{00s}$ | $cm^{-1}$ | 1046.92 | 1123.42 | 1164.35 | 1250.03 |
| $(\mathcal{E}_{01s} - \mathcal{E}_{00s})$ | $cm^{-1}$ | 355.54 | 375.23 | 357.59 | 375.19 |
| $(\mathcal{E}_{10s} - \mathcal{E}_{00s})$[b] | $cm^{-1}$ | 1738.30 | 1871.61 | 1971.11 | 2124.87 |
| $E_{0s}$ | $cm^{-1}$ | 71.19 | 80.29 | 69.93 | 79.80 |
| $E_{1s} - E_{0s}$ | $cm^{-1}$ | 146.10 | 160.13 | 144.94 | 159.48 |
| $E_{0a} - E_{0s}$ | MHz | 10.08 | 7.44 | 49.81 | 41.74 |

| parameters | | model 1 | model 2 |
|---|---|---|---|
| $B_e$ | $cm^{-1}$ | 2559 | 2559 |
| $D_e$ | $cm^{-1}$ | 5267 | 5267 |
| $f_1$ | $cm^{-1}$ | 5292 | 5292 |
| $a_1$ | 1 | 0.6019[d] | 0.5296[d] |
| $w$ | 1 | 0[e] | -0.80[e] |

[a] Levels denoted by $\mathcal{E}$ refer to the 2D subsystem at fixed $y_2 = 1$; their indices are the vibrational quantum numbers $v_x$, $v_1$ and the symmetry label *s* or *a* of the respective tunneling sublevel. Levels denoted by $E$ are relative to the value of $\mathcal{E}_{00s}(y_2=1)$. They refer to $v_x$, = 0, $v_1 = 0$ and $v_2 = 0$ or 1.
[b] Estimated as $2\times \mathcal{E}_{00s} - (\mathcal{E}_{01s} - \mathcal{E}_{00s})$.
[c] In the above spectroscopic description this splitting is denoted as $E_1$-$E_0$ = $\Delta E_{01}$. Its observed value is 331.6 MHz.
[d] Adjusted.
[e] Assumed

Table used to study the data published for the formic acid dimer (symmetry $C_{2h}$) by J. O. Richardson, *Phys.Chem.Chem.Phys.*, **2017**, *19*, 966-970 (Tables 1 and 2).

| *f* | Mode | | $\Delta E$ / $cm^{-1}$ | $\omega_{min}$ / $cm^{-1}$ | $\Delta\omega$ / $cm^{-1}$ | $\Delta E_f$ / $\Delta E_{f-1}$ | $\sum\Delta\omega$ / $cm^{-1}$ |
|---|---|---|---|---|---|---|---|
| 1 $A_g$ | $\nu_{OH}$ | *x* | 0.47 | 3232 | | | |
| 2 $A_g$ | $\nu_R$ | $y_2$ | 0.17 | 209 | 305 | 0.36 | |
| 3 $A_g$ | $\beta_R$ | $y_1$ | 0.037 | 167 | 52 | 0.22 | |
| 4 $A_g$ | $\beta_{OCO}$ | $y_2$ | 0.047 | 693 | 81 | **1.27** | |
| 5 $A_g$ | $\nu_{CO}(+)$ | $y_2$ | 0.048 | 1255 | 53 | 1.00 | |
| 6 $A_g$ | $\beta_{OH}$ | $y_2$ | 0.031 | 1481 | 210 | 0.65[a] | |
| 7 $A_g$ | $\nu_{CO}(-)$ | $y_1$ | 0.019 | 1715 | 34 | 0.61 | |
| 8 $A_g$ | $\beta_{CH}$ | $y_1$ | 0.018 | 1408 | -11 | 0.95 | |
| 9 $A_g$ | $\nu_{CH}$ | $y_2$ | 0.018 | 3095 | 6 | 1.00 | 730 |
| 10 $B_u$ | $\nu_{OH}$ | | 0.28 | 3326 | -2085 | **15.6**[b] | |
| 11 $A_u$ | $\perp\ \delta_{OH}$ | | 0.12 | 970 | 430 | 0.43[a] | |
| 12 $B_g$ | $\perp\ \delta_{OH}$ | | 0.055 | 956 | 385 | 0.46[a] | |
| 13 $B_u$ | $\beta_R$ | | 0.033 | 275 | 317 | 0.60 | |
| 14 $B_u$ | $\beta_{OH}$ | | 0.024 | 1448 | 156 | 0.73[a] | |
| 15 $B_u$ | $\nu_{CO}(+)$ | | 0.033 | 1258 | 146 | **1.38** | |
| 16 $B_u$ | $\beta_{OCO}$ | | 0.030 | 716 | 98 | 0.91 | |
| 17 $B_g$ | $\perp\ \delta_R$ | | 0.026 | 254 | 63 | 0.87 | |
| 18 $A_u$ | $\perp\ \delta_R$ | | 0.023 | 170 | 56 | 0.88 | |
| 19 $B_u$ | $\nu_{CO}(-)$ | | 0.016 | 1780 | -37 | 0.70 | |
| 20 $A_u$ | $\perp\ \delta_{CH}$ | | 0.015 | 1100 | -21 | 0.94 | |
| 21 $B_g$ | $\perp\ \delta_{CH}$ | | 0.016 | 1084 | -19 | 1.07 | |
| 22 $B_u$ | $\beta_{CH}$ | | 0.014 | 1406 | -11 | 0.88 | |
| 23 $A_u$ | $\perp\ \tau_R$ | | 0.014 | 70 | 12 | 1.00 | |
| 24 $B_u$ | $\nu_{CH}$ | | 0.013 | 3097 | 9 | 0.93 | 229 |

[a] $\Delta E_f/\Delta E_{f-1} = \exp[-\Delta E_{ZP} / 245\ cm^{-1}]$, $\Delta E_{ZP} = \Delta\omega/2$ (Increment to zero point energy).
[b] $\Delta E_f/\Delta E_{f-1} = \exp[-\Delta E_{ZP} / 380\ cm^{-1}]$.

*b) Fortran computer program for the flexible model*

```
C-----------------------------------------------------------------------
C ...... The program FMXYPZ is a Flexible Model Treatment for .........
C ...... molecular systems with three noncyclic degrees of freedom. ....
C ...... It decomposes a 3D problem with a potential function .........
C ...... V(x,y,z) into a series of 2D subproblems and a 1D problem .....
C ...... by treating the variable z as a parameter. ...................
C ...... For a set of equidistant values of z the 2D system ...........
C ......... [T(x,y;z) + V(x,y;z) - E(z)] psi(x,y;z) = 0 ...............
C ...... is solved for (at least) the lowest state to obtain ..........
C ...... the function E0(z) as the potential function for the z-mode ...
C ...... Similar in concept to the Born-Oppenheimer approximation ......
C ...... the method is expected to be the more accurate ...............
C ...... the slower the z-motion relative to the x- and y-motions .....
C .....................................................................
C ...... As application is intended to symmetric double minimum ........
C ...... hydrogen transfer systems, the program allows one to use ......
C ...... both  tunneling sublevels of the vibrationsl ground state .....
C ...... yielding two potential energy functions E0s(z) and E0a(z) .....
C ...... and after solution of the two respective 1D problems the ......
C ...... tunneling doublet for the overall vibrational ground state. ...
C .....................................................................
C ...... This version ( March 2017) is an application to treat .........
C ...... tunnel splittings in the FORMIC ACID DIMER ...................
C-----------------------------------------------------------------------
      PROGRAM FMXYPZ
      IMPLICIT REAL*8 (A-H, O-Z)
      COMMON  NDX,NDY,NDZ,NX,NY,NZ,NDDX,NDDY,NDDZ,NCX,NCY,NCZ,NXY,NV,
     &        NA,JABC(25,3),RTP(25,3),AM(25),
     &        DX,DY,DZ, DRX,DRY,DRZ, DDX(2*91),DDY(2*91),DDZ(2*91),
     &        RGT(91*91,15),GDET(91*91),V(91*91),GXXE,GXYE,GYYE,
     &        E0(24+8),PSI0(91*91*(24+8)),PSI1(91*91,3)
      DIMENSION PARAM(20),U0(101*101),U1(101*101),
     &          EXS(90),WS(90),PHI(101*90),VZ(91,2),
     &          VYY(91,2,3),CHI(91,4,2,2),EV(4,2,2)
      CHARACTER*80 TIT
C .....................................................................
C .......... The Flexible Model Treatment of Intramolecular Motion .....
C .......... has been described in ....................................
C                R. Meyer, J. Mol. Spectrosc. 76, 266 (1979)
C .......... It uses a meh point method described in ..................
C                R. Meyer, J. Chem. Phys. 52, 2053 (1970)
C .....................................................................
C .......... This program treats the concerted double hydrogen .........
C .......... transfer (varaiable x) and its coupling with two ..........
C .......... heavy atom motions (y1 and y2) of different symmetries ....
C .......... based on a Born-Oppenheimer-type decoupling of fast .......
C .......... motions (x and y1) from the relatively slow motion (y2) ...
C .......... The first approach of this type has been presented ........
C .......... for a prototype system in ................................
C                J. Manz, R. Meyer, E. Pollak, and J. Römelt,
C                Chem. Phys. Lett. 93, 184 (1982)
C .....................................................................
C .......... For application to a specific molecular system, the .......
C .......... program reads from an input file a standard ..............
C .......... configuration and the nuclear masses .....................
C .....................................................................
C ...... input: .......................................................
C ............. TIT = title, one row of text ..........................
C ............. NA  = number of atoms ................................
C .............       including dummies, if any, with mass 0 ..........
C .............       NA should currently not exceed 25 ...............
C .....................................................................
C ...... input (see explanations in SUBROUTINE CARTO): ................
C .......... L,JA,JB,JC,VR,VT,VP,AM  .................................
C .......... (AM = atomic masses in u = 'unified' atomic mass units) ...
C .......... The program will use only the masses supplied in AM and ...
C .......... the labels of atoms and their reference atoms. It will ....
C .......... overwrite the spherical coordinates in array VR,VT,VP .....
```

```
C .......... Nevertheless it is recommended to supply the respective ...
C .......... data in order to facilitate checking .....................
C ......................................................................
      DO 100 ISOT = 1,4
      READ 901,TIT,NA
  901 FORMAT(A,/,6I5)
      PRINT*,"Standard configuration as read from input"
      PRINT 902,TIT,NA
  902 FORMAT(1X,79(1H*),/,1X,A,/,1X,79(1H*),/,5H NA =,I3)
      DO 8 K=1,NA
      READ 903, L,(JABC(K,I),I=1,3), (RTP(K,I),I=1,3),AM(K)
    8 PRINT 903,L,(JABC(K,I),I=1,3), (RTP(K,I),I=1,3),AM(K)
  903 FORMAT(4I5,F10.5,2F10.3,F20.7)
C ......................................................................
C .......... Further properties of the system are defined by ..........
C .......... two subroutines: ..........................................
C .......... SUBROUTINE MOVE calculates the spherical coordinates ......
C .......... for a given set of reduced variables x, y1, y2 ...........
C .......... SUBROUTINE POTEN defines the respective potential energy ..
C .......... V(x,y1,y2). ...............................................
C ......................................................................
C .......... NDX, NDY = NDY1, NDZ = NDY2 are dimension numbers .........
C .......... that define the number of mesh points 2*NDX +1 etc. .......
C .......... DRX, DRY = DY1, DRZ = DY2 are the grid point spacings .....
C .......... that refer to the REDUCED COORDINATES ....................
C .......... They may be linked to integers JXE0, J1E0, J2E0 in order ..
C .......... to place mesh points at the stationary points of the ......
C .......... overall potential energy function V(x,y1,y2). ............
C .......... (x,y1,y2) = (0,0,0), (1,1,1), and (-1,-1,1) ..............
C ......................................................................
C .......... To handle derivatives of wavefunctions we link the ........
C .......... REDUCED COORDINATES RX, RY, RZ to .......................
C .......... STANDARD COORDINATES X, Y, Z that are always in the .......
C .......... range (-pi,+pi) and are spaced by DX=2*PI/(2*NDX+1) etc. ..
C .......... From a standard coordinate X the reduced one is obtained ..
C .......... as RX = (DRX/DX) X. In some of the procedures below, ......
C .......... the notation "X" may refer to a reduced coordinate .......
C .......... rather than to a standard one. This may be recognized .....
C .......... from its assignment, e.g. X = DRX*FLOAT(J-NDX-1) where ....
C .......... DRX always refers to a reduced coordinate. The same .......
C .......... applies to DRY and DRZ. Derivatives taken with respect ....
C .......... to standard coordinates must be multiplied by DX/DRX ......
C .......... to obtain the derivatives with respect to reduced .........
C .......... coordinates that are the ones needed here. ................
C ......................................................................
                              PI = 3.14159265358979
                              CL = 29979.25
            NDX = 18
            NDY = 18
            NDZ = 18
          NX = 2*NDX+1
          NY = 2*NDY+1
          NZ = 2*NDZ+1
            NCX = 1
            NCY = 1
            NCZ = 1
         NDDX = 2*NX
         NDDY = 2*NY
         NDDZ = 2*NZ
            NXY = NX*NY
         DX = 2.*PI/DFLOAT(NX)
         DY = 2.*PI/DFLOAT(NY)
         DZ = 2.*PI/DFLOAT(NZ)
C            JX01 =  6
C            JY01 =  6
C            JZ01 =  6
C         DRX = 1./DFLOAT(JX01)
C         DRY = 1./DFLOAT(JY01)
C         DRZ = 1./DFLOAT(JZ01)
C ............ range of reduced variables RRV = (2*18+1)/6 ............
```

```
         RRV = DFLOAT(37)/DFLOAT(6)
         DRX = RRV/DFLOAT(NX)
         DRY = RRV/DFLOAT(NY)
         DRZ = RRV/DFLOAT(NZ)
            NV = 16
C ......................................................................
C .......... NV = number of (lowest) eigenstates wanted ................
C .......... NCX=NCY=NCZ = 1 for non-cyclic motions ....................
C .......... NOPR = 0 to enable and NOPR = 1 to suppress printing ......
C .......... NIT = number of iteration cycles for the refinement .......
C ..........       of 2D wavefunctions psi(x,y1; y2) that depend .......
C ..........       parametrically on y2 ................................
C ......................................................................
      PRINT*
      PRINT*,"  ----------- grid properties -----------"
      PRINT*,"  NDX   NDY   NDZ     DRX     DRY     DRZ    NV"
      PRINT 904, NDX,NDY,NDZ,DRX,DRY,DRZ, NV
  904 FORMAT(3I6,3F8.3,I6)
      PRINT*
      PRINT*,"       mobility constants (MHz)"
      PRINT*,"     GXXE        GXYE        GYYE"
      READ*, GXXE, GXYE, GYYE
      PRINT 905, GXXE, GXYE, GYYE
  905 FORMAT(3F12.0)
      CALL DIFFCO(NDX,DDX)
      CALL DIFFCO(NDY,DDY)
          NIT = 13
          NOPR = 1
      DO 20 JZ = 1,NZ
         RZ = DRZ*DFLOAT(JZ-(NZ+1)/2)
          Y2 = 1. + RZ
          PARAM(12) = Y2
            NOPR = 1
C ......................................................................
C ..... Enable the following statement to inspect the functions ........
C ..... GXX(X,Y), GXY(X,Y), GYY(X,Y) [preferably with NDX=NDY = 18] ....
C ..... To approximate these functions by constants choose values ......
C ..... GXXE, GXYE, GYYE at or near equilibrium and include them .......
C ..... in the input file FFin.txt ....................................
C ......................................................................
              IF(JZ.EQ.(NZ+1)/2) NOPR = 0
            IPRI = 0
              IF(JZ.EQ.(NZ+1)/2) IPRI = 1
      CALL FMXY0(PARAM,NIT,NOPR,IPRI)
      VZ(JZ,1) = E0(1)
   20 VZ(JZ,2) = E0(2)
        JZM = NDZ+1
      VZREF = VZ(JZM,1)
      PRINT 907, JZM, VZREF/CL
      PRINT*
      PRINT*," effective potentials for A-type dimer stretching"
      PRINT*,"   JZ   VZ1/cm^-1   VZ2/cm^-1  splitting / MHz"
      DO 22 JZ = 1,NZ
      VZ(JZ,1) = VZ(JZ,1) - VZREF
      VZ(JZ,2) = VZ(JZ,2) - VZREF
      J0 = JZ-(NZ+1)/2
   22 PRINT 908, J0, VZ(JZ,1)/CL, VZ(JZ,2)/CL, VZ(JZ,2)-VZ(JZ,1)
  907 FORMAT(/,17H reference at J =,I3,11H  VZ(J,1) =,F10.2,6H cm^-1)
  908 FORMAT(I6,2F12.2,F15.2)
      NV = 4
      NOPR = 0
      CALL FMZ1D(PARAM,VZ,NPER,NOPR)
  100 CONTINUE
  999 CONTINUE
      END
C ----------------------------------------------------------------------
      SUBROUTINE FMXY0(PARAM,NIT,NOPR,IPRI)
C ......................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON  NDX,NDY,NDZ,NX,NY,NZ,NDDX,NDDY,NDDZ,NCX,NCY,NCZ,NXY,NV,
```

```
     &        NA,JABC(25,3),RTP(25,3),AM(25),
     &        DX,DY,DZ, DRX,DRY,DRZ, DDX(2*91),DDY(2*91),DDZ(2*91),
     &        RGT(91*91,15),GDET(91*91),V(91*91),GXXE,GXYE,GYYE,
     &        E0(24+8),PSI0(91*91*(24+8)),PSI1(91*91,3)
      DIMENSION PARAM(20),FC(100)
      CALL KINET(PARAM,NOPR)
      CALL VPSEU2(NX,NY,NCX,NCY,DRX,DRY,DDX,DDY, RGT(1,13),RGT(1,14),
     &            RGT(1,15),GDET,PSI1(1,1),PSI1(1,2),PSI1(1,3),NOPR)
      CALL FMOBC(NX,NY,RGT(1,13),RGT(1,14),RGT(1,15),GXXE,GXYE,GYYE)
      CALL POTEN(NX,NY,DRX,DRY,PARAM,GDET,V)
      IF(NOPR.EQ.0) THEN
        PRINT *
        PRINT *,"pseudopotential + potential energy (cm^-1)"
        SC = 1./29979.25
        CALL FPRINT(NX,NY,SC,V,0)
      ENDIF
      CALL SELEST(NIT,NOPR,IPRI)
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE KINET(PARAM,NOPR)
C .....................................................................
C ........ calculate kinetic energy matrix `RGT` referring to angular ..
C ........ momentum components and internal motional momenta ..........
C ........ and determinant GDET = 1/|RGT| as functions of .............
C ........ REDUCED coordinates x and y (related to DRX and DRY) ........
C .....................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON  NDX,NDY,NDZ,NX,NY,NZ,NDDX,NDDY,NDDZ,NCX,NCY,NCZ,NXY,NV,
     &        NA,JABC(25,3),RTP(25,3),AM(25),
     &        DX,DY,DZ, DRX,DRY,DRZ, DDX(2*91),DDY(2*91),DDZ(2*91),
     &        RGT(91*91,15),GDET(91*91)
      DIMENSION PARAM(20), C(3,35), RP(3,35), RM(3,35),
     &          EV(5), DR(3,5,35),GTEN(5,5),U(5,5)
      M = 0
      DO 100 JY=1,NY
        Y = DRY*DFLOAT(JY-(NY+1)/2)
      DO 100 JX=1,NX
        X = DRX*DFLOAT(JX-(NX+1)/2)
      M = M + 1
        CALL ATPOS( 0,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      DO 20 K=1,NA
        DR(1,1,K) =  0.
        DR(1,2,K) =  RP(3,K)
        DR(1,3,K) = -RP(2,K)
        DR(2,1,K) = -RP(3,K)
        DR(2,2,K) =  0.
        DR(2,3,K) =  RP(1,K)
        DR(3,1,K) =  RP(2,K)
        DR(3,2,K) = -RP(1,K)
   20   DR(3,3,K) =  0.
      X=X+DRX/6.
        CALL ATPOS( 1,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      X=X-2.*DRX/6.
        CALL ATPOS(-1,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      DO 22 K=1,NA
      DO 22 I=1,3
   22 DR(I,4,K) = (RP(I,K)-RM(I,K))*4./DRX
      X=X-DRX/6.
        CALL ATPOS( 1,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      X=X+4.*DRX/6.
        CALL ATPOS(-1,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      X=X-2.*DRX/6.
         DO 30 K=1,NA
         DO 30 I=1,3
   30 DR(I,4,K)=DR(I,4,K)+(RP(I,K)-RM(I,K))/2./DRX
      Y=Y+DRY/6.
        CALL ATPOS( 1,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      Y=Y-2.*DRY/6.
        CALL ATPOS(-1,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
```

```
      DO 32 K=1,NA
      DO 32 I=1,3
   32 DR(I,5,K)=(RP(I,K)-RM(I,K))*4./DRY
      Y=Y-DRY/6.
        CALL ATPOS( 1,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      Y=Y+4.*DRY/6.
        CALL ATPOS(-1,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      Y=Y-2.*DRY/6.
      DO 40 K=1,NA
      DO 40 I=1,3
   40 DR(I,5,K)=DR(I,5,K)+(RP(I,K)-RM(I,K))/2./DRY
      DO 60 I=1,5
      DO 60 J=I,5
        S=0.
      DO 50 K=1,NA
   50 S=S+AM(K)*(DR(1,I,K)*DR(1,J,K)+ DR(2,I,K)*DR(2,J,K)
     &  +DR(3,I,K)*DR(3,J,K))
      GTEN(I,J)=S
   60 GTEN(J,I)=S
      CALL JACOB(5,0,GTEN,U,5)
        DET=1.
      DO 70 I=1,5
      EV(I)=505379.05/GTEN(I,I)
   70 DET = DET*GTEN(I,I)
C ......................................................................
C
C   G11=G(M,1)    G12=G(M,2)    G13=G(M,3)    G1X=G(M,4)    G1Y=G(M,5)
C                 G22=G(M,6)    G23=G(M,7)    G2X=G(M,8)    G2Y=G(M,9)
C                               G33=G(M,10)   G3X=G(M,11)   G3Y=G(M,12)
C    [ RGT(M,L) = G(M,L) ]                    GXX=G(M,13)   GXY=G(M,14)
C                                                           GYY=G(M,15)
C ......................................................................
      L = 0
      DO 90 I=1,5
      DO 90 J=I,5
      L = L + 1
      S=0.
      DO 80 K=1,5
   80 S = S + U(I,K)*EV(K)*U(J,K)
   90 RGT(M,L) = S
  100 GDET(M) = DET
      IF(NOPR.EQ.0) THEN
        JX=(NX+1)/2
        JY=(NY+1)/2
        M = (JY-1)*NX + JX
        PRINT 903, (RGT(M,L),L=13,15), GDET(M)
         SC = 1./1000.
        CALL FPRINT(NX,NY,SC,RGT(1,13),0)
        CALL FPRINT(NX,NY,SC,RGT(1,14),0)
        CALL FPRINT(NX,NY,SC,RGT(1,15),0)
         SC = 10000./GDET(M)
        CALL FPRINT(NX,NY,SC,GDET,0)
      ENDIF
  903 FORMAT(/,6H X=Y=0,/,10X,3HGXX,F15.3,2X,3HMHZ,/,10X,3HGXY,F15.3,
     &  /,10X,3HGYY,F15.3,/,10X,1HG,E17.8,15H  (AMU*A**2)**5,////,
     &  50H TABLES: GXX, GXY, GYY (GHZ),  G/G(0,0), VG (GHZ) ,/)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE VPSEU2(NX,NY,NCX,NCY,DRX,DRY,DDX,DDY,
     &                  GXX,GXY,GYY,G,GX,GY,VG,NOPR)
C ......................................................................
C ............ calculating the 2D pseudopotential function .............
C ......................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION GXX(NX,NY),GXY(NX,NY),GYY(NX,NY),G(NX,NY),
     &          DDX(2*NX),DDY(2*NY),GX(NX,NY),GY(NX,NY),VG(NX,NY)
      NXY=NX*NY
      DX=2.*3.1415926535898/DFLOAT(NX)
      DY=2.*3.1415926535898/DFLOAT(NY)
```

```
C ......................................................................
C ... Derivatives with respect to standard vaiables (-pi<=x,y<=pi) .....
C ... are transformed to reduced variables ............................
C ... by factors DX/DRX and DY/DRY ....................................
C ......................................................................
      DO 30 JPX=1,NX
      DO 30 JPY=1,NY
        LPX1=1+NX*(JPY-1)
      CALL DFNCXY(NX,NY,G,JPX,JPY,DX,DY,SX,SY)
      IF(NCX.EQ.0) CALL DFXY(NX,DDX,NXY,G,LPX1,1,JPX,SX)
      IF(NCY.EQ.0) CALL DFXY(NY,DDY,NXY,G,JPX,NX,JPY,SY)
      SX = SX*DX/DRX
      SY = SY*DY/DRY
       S = G(JPX,JPY)
       SX = SX/4./S
       SY = SY/4./S
       SXX = GXX(JPX,JPY)
       SXY = GXY(JPX,JPY)
       SYY = GYY(JPX,JPY)
       S = SXX*SX*SX + 2.*SXY*SX*SY + SYY*SY*SY
      VG(JPX,JPY) = S
      GX(JPX,JPY) = SXX*SX+SXY*SY
   30 GY(JPX,JPY) = SXY*SX+SYY*SY
      DO 60 JPX=1,NX
      DO 60 JPY=1,NY
        LPX1=1+NX*(JPY-1)
      CALL DFNCXY(NX,NY,GX,JPX,JPY,DX,DY,SX,S)
      CALL DFNCXY(NX,NY,GY,JPX,JPY,DX,DY,S,SY)
      IF(NCX.EQ.0) CALL DFXY(NX,DDX,NXY,GX,LPX1,1,JPX,SX)
      IF(NCY.EQ.0) CALL DFXY(NY,DDY,NXY,GY,JPX,NX,JPY,SY)
   60 G(JPX,JPY) = VG(JPX,JPY) + SX*DX/DRX +SY*DY/DRY
C ........ pseudopotential function (MHz) is now in G ...........
        SC = 1./1000.
      IF(NOPR.EQ.0) THEN
      PRINT*
      PRINT*," pseudopotential function in GHz"
       CALL FPRINT(NX,NY,SC,G,0)
      ENDIF
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE FMOBC(NX,NY,GXX,GXY,GYY,GXXE,GXYE,GYYE)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION GXX(NX,NY),GXY(NX,NY),GYY(NX,NY)
C ......................................................................
C ...... assuming fixed moblity coefficients with ......................
C ...... values obtained at equilibrium with NDX=NDY=NDZ = 18 ..........
C ......................................................................
      DO 10 JX = 1,NX
      DO 10 JY = 1,NY
        GXX(JX,JY) = GXXE
        GXY(JX,JY) = GXYE
        GYY(JX,JY) = GYYE
   10 CONTINUE
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE ATPOS(L,NA,X,Y,JABC,RTP,C,RP,RM,AM,PARAM)
      IMPLICIT REAL*8 (A-H,O-Z)
C ......................................................................
C ........ from JABC and RTP at reduced coordinates (x,y) calculate ....
C ........ atomic cartesian coordinates relative to center of mass .....
C ........ store in RP for L >= 0 and in RM for L < 0 .................
C ......................................................................
      DIMENSION JABC(25,3),RTP(25,3),C(3,25),PARAM(20),
     &          RP(3,NA),RM(3,NA),AM(NA),RCM(3)
      CALL MOVE(NA,X,Y, RTP(1,1),RTP(1,2),RTP(1,3),PARAM)
      CALL CARTO(NA, JABC(1,1),JABC(1,2),JABC(1,3),
     &               RTP(1,1),RTP(1,2),RTP(1,3), C )
      CALL ERASE(3,RCM)
```

```
      S=0.
      DO 10 K=1,NA
      RCM(1)=RCM(1)+C(1,K)*AM(K)
      RCM(2)=RCM(2)+C(2,K)*AM(K)
      RCM(3)=RCM(3)+C(3,K)*AM(K)
   10 S = S+AM(K)
      RCM(1)=RCM(1)/S
      RCM(2)=RCM(2)/S
      RCM(3)=RCM(3)/S
      IF(L.GE.0) THEN
        DO 20 K=1,NA
        RP(1,K)=C(1,K)-RCM(1)
        RP(2,K)=C(2,K)-RCM(2)
   20   RP(3,K)=C(3,K)-RCM(3)
      ELSE
        DO 30 K=1,NA
        RM(1,K)=C(1,K)-RCM(1)
        RM(2,K)=C(2,K)-RCM(2)
   30   RM(3,K)=C(3,K)-RCM(3)
      ENDIF
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE MOVE(NA,X,Y,VR,VT,VP,PARAM)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION VR(NA),VT(NA),VP(NA),PARAM(20)
C .....................................................................
C .... application: ---- formic acid dimer, HCOOH..HOOCD ---- 2017 .....
C .....................................................................
C ....... X is the reduced hydrogen transfer coordinate ...............
C ....... Y is the reduced B-type C-O stretching coordinate Y1 .........
C ....... Z is the reduced A-type dimer stretching coordinate Y2 .......
C .......   treated as a parameter ....................................
C .... => Do not change X, Y and Z within this subroutine <= ..........
C .....................................................................
                   PI1 = 3.141595358979/180.
        Y1 = Y
       Z = PARAM(12)
       Y2 = Z
C ... concerted transfer of hydrogens H11 and H12 ...
        X1H11  = -0.4215*X
C .....................................................................
C .......... with limited distance from CC axis .......................
C         Y1H11  = 1.1161 + 0.0729*X**2*2./(1.+X**2)
C .... assumed below: straight path of H between equilibrium sites .....
C .....................................................................
        Y1H11  = 1.1161 + 0.0729
        R1H11  = SQRT(X1H11**2+Y1H11**2)
        X1H12  = -X1H11
        VR(11) = R1H11
        VT(11) = ACOS(X1H11/R1H11)/PI1
        VP(11) = 0.
           VR(12) = R1H11
           VT(12) = ACOS(X1H12/R1H11)/PI1
           VP(12) = 180.
C ... heavy atom motions y1 & y2 .............
             RCC  = 3.5515 + 0.2749*Y2
                VR(3) = RCC/2.
                VT(3) = 90.
                VP(3) = 0.
                VR(4) = VR(3)
                VT(4) = VT(3)
                VP(4) = 180.
        RCO5 = 1.2612 + 0.0048*Y2 + 0.0474*Y1
        RCO6 = 1.2612 + 0.0048*Y2 - 0.0474*Y1
        T135 = 63.3 - 0.2*Y2 + 4.8*Y1
        T136 = 63.3 - 0.2*Y2 - 4.8*Y1
           VR(5) = RCO5
           VT(5) = T135
           VP(5) = 0.
```

```
          VR(6) = RCO6
          VT(6) = T136
          VP(6) = 180.
          VR(7) = VR(6)
          VT(7) = VT(6)
          VP(7) = 0.
          VR(8) = VR(5)
          VT(8) = VT(5)
          VP(8) = 180.
       RCH  = 1.0952 + 0.0011*Y2
       T539 = 116.7 + 0.2*Y2 - 5.2*Y1
       T639 = 116.7 + 0.2*Y2 + 5.2*Y1
          VR( 9) = RCH
          VT( 9) = T539
          VP( 9) = 180.
          VR(10) = VR(9)
          VT(10) = T639
          VP(10) = 180.
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE POTEN(NX,NY,DRX,DRY,PARAM,G,V)
C ......................................................................
C ........ Calculate the potential energy function V(x,y) .............
C ........ on the grid dimensioned by NX and NY .......................
C ......................................................................
C ........    Application: ---- formic acid dimer ----- 2017 ..........
C ......................................................................
C ........ In this application the mesh sizes DRX and DRY and the ......
C ........ the variables X and Y1 = Y are reduced coordinates to be ....
C ........ obtained when using the increments DRX and DRY supplied .....
C ........ by the calling program. The reduced variable Y2 is ..........
C ........ treated as a parameter to be found as Y2=1.+Z = PARAM(12) ...
C ........ The calling program also supplies, in the array G, the ......
C ........ pseudopotential function in MHz units ......................
C ........ The sum (pseudopotential + potential) in MHz is ............
C ........ returned in the array V ....................................
C ......................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION PARAM(20),G(NX,NY),V(NX,NY)
         PI = 3.14159265358979E0
         CL = 29979.25E0
C  .............. parameters ...........................................
                           BE = 2559.
                           DE = 5267.
                           FC1 = 5292.
                           BWP = -0.80
                           A1 = 0.5296
c                           BWP = 0.
c                           A1 = 0.6019
      Y2 = PARAM(12)
C ......................................................................
C        RCC(y2=0) = 3.5515  ; RCC(y2=1) = RCCE = 3.5515 + 0.2749
C ......................................................................
C ...... minimum energy path: Y1E(X), Y2E(X) ..........................
C ...... and potential energy parts VMEP(X), V1(X,Y1) and V2(X,Y2) .....
C ......................................................................
C ... For |x| > xcrit we postulate a linear increase of y2e with |x| ...
C ... such that dRCC/dx = dRCC/dy2 * dy2e/dx = 2*dYH11/dx .............
C ......................................................................
C ... As suggested by ab initio results we assume a Lennard-Jones ......
C ... type potential depending on the distance RCC(y2) and based .......
C ... on the local dissociation energy DE - VMEP and local ............
C ... equilibrium distance RCC[y2e(x)] ................................
C ......................................................................
      DO 10 JX = 1,NX
       X = DRX*DFLOAT(JX-(NX+1)/2)
        VMEP = BE*(1.-X**2)**2 * FSHAPE(X,BE,DE,BWP)
        Y1E = (1.+A1)*X**3/(1.+A1*ABS(X)**3)
        Y2E = X**2
```

```
          XCRIT = 0.4215/0.2749
          IF(ABS(X).GT.XCRIT)  Y2E = XCRIT*(2.*ABS(X)-XCRIT)
          R = (3.5515 + 0.2749*Y2)/(3.5515 + 0.2749*Y2E)
            V2 = (DE - VMEP) * (1./R**12 - 2./R**6 + 1.)
      DO 10 JY = 1,NY
       Y = DRY*DFLOAT(JY-(NY+1)/2)
       Y1 = Y
            V1 = FC1*(Y1-Y1E)**2
   10 V(JX,JY) = VMEP + V1 + V2
C ..................................................................
C .. convert to MHz and add pseudopotential function (do not change): ..
C ..................................................................
      DO 40 JX = 1,NX
      DO 40 JY = 1,NY
   40 V(JX,JY) = CL*V(JX,JY) + G(JX,JY)
C ..................................................................
C .... downsize very large V-values to enhance the efficiency ..........
C .....of the iterative refinement of the wavefunctions ................
C ..................................................................
      VLIM = CL*24000.
C ..................................................................
C ....         R     0.203  0.255  0.347  0.550    .....................
C ....      TANH(R)  0.200  0.250  0.334  0.501    .....................
C ..................................................................
      DO 44 JX = 1,NX
      DO 44 JY = 1,NY
      R = V(JX,JY)/VLIM
        V(JX,JY) = VLIM*TANH(R)
C-        IF(V(JX,JY).GT.VLIM) V(JX,JY) = VLIM
   44 CONTINUE
      RETURN
      END
C -------------------------------------------------------------------
      FUNCTION FSHAPE(X,B0,D0,BWP)
C ................................ called from POTEN
C ..................................................................
C ...... application:            FORMIC ACID DIMER --- 2016 ............
C ...... Shape factor for potential function V(X,Y1,Y2) ................
C ...... BWP is a parameter that influences the barrier thickness; .....
C ...... Make sure that the denominator remains > 0. ...................
C ..................................................................
      IMPLICIT REAL*8 (A-H, O-Z)
      R = SQRT(B0/D0)
      FSHAPE = 1./(1. + BWP*R*X**2 + R**2*X**4)
      RETURN
      END
C -------------------------------------------------------------------
      SUBROUTINE DFNCXY(NX,NY,F,JPX,JPY,DX,DY,DFX,DFY)
C ..................................................................
C ......... derivatives DFX = dF/dx and DFY = dF/dy  of F(x,y)  ........
C ......... evaluated, locally, at (x`,y`) given by JPX, JPY ...........
C ..................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION F(NX,NY)
      J=JPX
        IF(J.EQ.1) J=2
        IF(J.EQ.NX) J=NX-1
      K=JPY
        IF(K.EQ.1) K=2
        IF(K.EQ.NY) K=NY-1
      DFX=(F(J+1,JPY)-F(J-1,JPY))/(2.*DX)
      DFY=(F(JPX,K+1)-F(JPX,K-1))/(2.*DY)
      RETURN
      END
C -------------------------------------------------------------------
      SUBROUTINE DFXY(N,DD,NF,F,JF,LSTP,JP,DF)
C ..................................................................
C ......... Derivative DF = dF/dz (z = x or y) of F(x,y)  .............
C ......... based on true or approximate periodicity of F along z ......
C ......... using the coefficients for trigonometric interpolation .....
```

```
C ......... The variables x,y are in the range (-pi,pi) ................
C ......... The function F is given on the grid by the elements ........
C ......... of the matrix dimensioned as F(NX,NY), represented in ......
C ......... this subroutine by the vector F(NF) where NF = NX*NY .......
C .....................................................................
C ......... For z = x subsequent grid points in the x-direction ........
C ......... are spaced in F(NF) by LSTP = 1 ...........................
C ......... The value of dF/dx is returned (in DF) at .................
C ......... the JP`th gridpoint in the x-direction ....................
C ......... The first (leftmost) gridpoint at constant y ..............
C ......... is found in F(NF) at the index JF = 1 + NX*(JPY-1) .........
C ......... where JPY locates the given value of y on the grid .........
C .....................................................................
C ......... For z = y subsequent grid points in the y-direction ........
C ......... are spaced in F(NF) by LSTP = NX ..........................
C ......... The value of dF/dx is returned (in DF) at .................
C ......... the JP`th gridpoint in the y-direction ....................
C ......... The first (leftmost) gridpoint at constant x ..............
C ......... is found in F(NF) at the index JF = JPX ...................
C ......... where JPX locates the given value of x on the grid .........
C .....................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION DD(2*N),F(NF)
      DZ=2.E0*3.14159265358979E0/DFLOAT(2*N+1)
      DF=0.
        K=N-JP
        J=JF-LSTP
      DO 10 I=1,N
       K=K+1
       J=J+LSTP
   10 DF=DF+DD(K)*F(J)
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE DIFFCO(ND,D)
C ............................................ called from MAIN, FMZ1D
C ..... Coefficients of numerical differentiation based on
C ..... trigonometric interpolation, to be applied to .........
C ..... functions f(x) with x in the range (-pi,pi) ..........
C ..... that can be represented by a trigonometric basis ......
C ..... see R. Meyer, J. Chem. Phys. Vol. 52, p. 2053 (1970)
C ...........................................................
C ..... The coefficients are stored on a two-period range .....
C ...........................................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION D(4*ND+2)
      DX=2.E0*3.14159265358979E0/DFLOAT(2*ND+1)
      DO 20 J=1,ND
        D(J)=0.
        XJ=DX*DFLOAT(J)
      DO 10 K=1,ND
      AK=DFLOAT(K)
   10 D(J)=D(J)+AK*SIN(AK*XJ)
      D(J)=D(J)*2./DFLOAT(2*ND+1)
        J1=2*ND+1-J
        J2=2*ND+1+J
        J3=J1+2*ND+1
      D(J1)=-D(J)
      D(J2)=D(J)
   20 D(J3)=-D(J)
      D(2*ND+1)=0.
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE SELEST(NIT,NOPR,IPRI)
C .....................................................................
C ......... refining wavefunctions by NIT iteration cycles .............
C .....................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON  NDX,NDY,NDZ,NX,NY,NZ,NDDX,NDDY,NDDZ,NCX,NCY,NCZ,NXY,NV,
```

```
     &        NA,JABC(25,3),RTP(25,3),AM(25),
     &        DX,DY,DZ, DRX,DRY,DRZ, DDX(2*91),DDY(2*91),DDZ(2*91),
     &        RGT(91*91,15),GDET(91*91),V(91*91),GXXE,GXYE,GYYE,
     &        E0(24+8),PS(91*91,(24+8)),PS0(91*91,(24+8))
      DIMENSION PX(91*91),PY(91*91),HP(91*91),
     &          H(24+8,24+8),U(24+8,24+8)
C ......................................................................
C                GXX = RGT(.,13)   GXY = RGT(.,14)
C                                  GYY = RGT(.,15)
C ......................................................................
C ......... estimate highest possible eigenvalue EMAX .................
C ......................................................................
      VMAX = 0.
      GXXMAX = 0.
      GXYMAX = 0.
      GYYMAX = 0.
      DO 10 J = 1,NXY
      IF(VMAX.LT.V(J)) VMAX = V(J)
      IF(GXXMAX.LT.RGT(J,13))      GXXMAX = RGT(J,13)
      IF(GXYMAX.LT.ABS(RGT(J,14))) GXYMAX = ABS(RGT(J,14))
   10 IF(GYYMAX.LT.RGT(J,15))      GYYMAX = RGT(J,15)
      EMAX = VMAX + DFLOAT(NDX**2)*GXXMAX + DFLOAT(NDY**2)*GYYMAX
     &            + DFLOAT(NDX*NDY)*GXYMAX
      IF((NOPR.EQ.0).OR.(IPRI.EQ.1)) THEN
          PRINT*
          PRINT *, "Emax / cm^-1 = ", EMAX/29979.25
      ENDIF
C ......................................................................
C ......... initialize NV+8 basis functions ...........................
C ......... the 8 additional functions are used in the first 10 ........
C ......... iteration cycles ..........................................
C ......... they are intended to help selecting the NV lowest states ...
C ......................................................................
        NV0 = NV
        NV  = NV+8
      CALL COPYA(NXY,V,HP)
      CALL PSINIT(NX,NY,NV,VBH,VMAX,HP,PS)
      SC = 100000.
        EL = EMAX + VBH - VMAX
        IF(IPRI.EQ.1) PRINT 901
C ......................................................................
C ......... iterate: attenuate high energy components in basis set .....
C .........          and solve eigenvalue problem with improved basis ..
C ......................................................................
      DO 20 IT = 1,NIT
        IF(IT.GT.10) NV = NV0
      CALL ATTHEC(EL,EMAX)
      DO 12 K = 1,NV
      CALL HPSI(NX,NY,NXY,DDX,DDY,DRX,DRY,
     &          RGT(1,13),RGT(1,14),RGT(1,15),V,PX,PY,PS(1,K),HP)
      CALL COPYA(NXY,PS(1,K),PS0(1,K))
      DO 12 I = K,NV
      H(I,K) = SCALPR(NXY,PS(1,I),HP)
   12 H(K,I) = H(I,K)
      CALL JACOB(NV,0,H,U,24+8)
      DO 16 IV=1,NV
      E0(IV) = H(IV,IV)
      DO 16 JXY = 1,NXY
        PS(JXY,IV) = 0.
      DO 16  K = 1,NV
   16 PS(JXY,IV) = PS(JXY,IV) + PS0(JXY,K)*U(K,IV)
      EL = E0(NV)
      IF(((NOPR.EQ.0).OR.(IPRI.EQ.1)).AND.(IT.GT.NIT-3)) THEN
        PRINT*,"  iteration cycle ",IT
        PRINT 902, (E0(L),L=1,NV)
        PRINT*
        PRINT 905, E0(2)-E0(1)
        PRINT*
      ENDIF
   20 CONTINUE
```

```
      IF(NOPR.EQ.0) THEN
        PRINT 903
        SC = 100000.
        DO 30 L=1,NV/2
        PRINT *, L
        PRINT 904, E0(L)/29979.25
   30   CALL FPRINT(NX,NY,SC,PS(1,L),0)
      ENDIF
      IF(IPRI.EQ.1) THEN
      PRINT*
      PRINT*," SELEST: lowest four energy levels in cm^-1"
      PRINT*,"         at Y2 = 1 (JZ = NDZ+1)"
      PRINT 906, (E0(L)/29979.25,L=1,4)
      PRINT 906, ((E0(L)-E0(1))/29979.25,L=1,4)
      ENDIF
  901 FORMAT(//,20X,21H  energy levels (MHz),/)
  902 FORMAT(6F13.2,/,2X,6F13.2)
  903 FORMAT(//,45H    energy levels (cm^-1) and wavefunctions: )
  904 FORMAT(8F10.3)
  905 FORMAT(32H Tunnel splitting, E0(2)-E0(1) =,F13.2,4H MHz)
  906 FORMAT(2X,4F12.2)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE ATTHEC(EL,EM)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON  NDX,NDY,NDZ,NX,NY,NZ,NDDX,NDDY,NDDZ,NCX,NCY,NCZ,NXY,NV,
     &        NA,JABC(25,3),RTP(25,3),AM(25),
     &        DX,DY,DZ, DRX,DRY,DRZ, DDX(2*91),DDY(2*91),DDZ(2*91),
     &        RGT(91*91,15),GDET(91*91),V(91*91),GXXE,GXYE,GYYE,
     &        E0(24+8),PS(91*91,(24+8))
      DIMENSION PX(91*91),PY(91*91),HP(91*91)
C ......................................................................
C ....... attenuate high energy components in psi ......................
C ....... using roots of Tchebycheff polynomial of degree NPOL .........
C ......................................................................
      C1 = 1.
      PI = 3.14159265358979
        NPOL = 8
      IF(1.05*EL.LT.EM) EL = 1.05*EL
      DO 10 IV = 1,NV
      DO 10 J = 1,NPOL
      EZ = 0.5*(EL+EM)+0.5*(EM-EL)*COS(DFLOAT(2*J-1)*PI/DFLOAT(2*NPOL))
      CALL HPSI(NX,NY,NXY,DDX,DDY,DRX,DRY,
     &          RGT(1,13),RGT(1,14),RGT(1,15),V,PX,PY,PS(1,IV),HP)
      CALL COPYA(NXY,PS(1,IV),PX)
      CALL COMBIN(NXY,C1,PX,-C1/EZ,HP,PS(1,IV))
   10 CONTINUE
      CALL ORTHON(NXY,NV,PS)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE HPSI(NX,NY,NXY,DDX,DDY,DRX,DRY,
     &                GXX,GXY,GYY,V,PX,PY,P,HP)
C ......................................................................
C ....... using the Hamiltonian and the basis vector psi ...............
C ....... calculate H*psi ..............................................
C ....... psi is supplied as P and H*psi is returned as HP .............
C ......................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION DDX(2*91),DDY(2*91),GXX(91*91),GXY(91*91),GYY(91*91),
     &          V(91*91), PX(91*91),PY(91*91),P(91*91),HP(91*91)
                PI = 3.14159265358979
                DX = 2.*PI/DFLOAT(NX)
                DY = 2.*PI/DFLOAT(NY)
      DO 10 JPX=1,NX
      DO 10 JPY=1,NY
       LP=JPX+NX*(JPY-1)
       LPX1=LP+1-JPX
      CALL DFXY(NX,DDX,NXY,P,LPX1,1,JPX,DXP)
```

```
      CALL DFXY(NY,DDY,NXY,P,JPX,NX,JPY,DYP)
      PX(LP)=GXX(LP)*DXP*DX/DRX + GXY(LP)*DYP*DY/DRY
   10 PY(LP)=GXY(LP)*DXP*DX/DRX + GYY(LP)*DYP*DY/DRY
      DO 20 JPX=1,NX
      DO 20 JPY=1,NY
       LP=JPX+NX*(JPY-1)
       LPX1=LP+1-JPX
      CALL DFXY(NX,DDX,NXY,PX,LPX1,1,JPX,DXP)
      CALL DFXY(NY,DDY,NXY,PY,JPX,NX,JPY,DYP)
   20 HP(LP) = P(LP)*V(LP) - DXP*DX/DRX - DYP*DY/DRY
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE PSINIT(NX,NY,NV,VBH,VMAX,V,PS)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION V(91*91),PS(91*91,NV)
C ......................................................................
C ...................... initial baasis, using a copy of V ............
C ......................................................................
c      PRINT*
c      PRINT*," INITIAL BASIS, PS(JX,JY,IV) = 1 : IV, JX-NDX, JY-NDY"
      DO 20 IV = 1,NV
      CALL ERASE(NXY,PS(1,IV))
      VMIN = VMAX+1.
      J = 0
      DO 10 JY =1,NY
      DO 10 JX = 1,NX
      J = J+1
      IF(V(J).LT.VMIN) THEN
        VMIN = V(J)
        JMIN = J
        JXMIN = JX
        JYMIN = JY
      ENDIF
   10 CONTINUE
      V(JMIN) = VMAX+1.
      PS(JMIN,IV) = 1.
c      PRINT 90, IV, JXMIN-(NX+1)/2,JYMIN-(NY+1)/2
   20 CONTINUE
      VBH = VMIN
   90 FORMAT(12X,3I8)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE FPRINT(NX,NY,SC,G,NOPR)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION     G(NX,NY), IG(91)
      IF (NOPR.EQ.0) THEN
        LYSTEP = 1
         IF(NY.GT.33) LYSTEP = 2
        PRINT *
        DO 20 JX=1,NX
        DO 10 JY=1,NY
   10   IG(JY) = INT(G(JX,JY)*SC)
   20   PRINT 901, (IG(L),L=1,NY,LYSTEP)
        PRINT *
      ENDIF
  901 FORMAT(47I6)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE ERASE(N,A)
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION A(N)
      DO 10 I = 1,N
   10 A(I) = 0.
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE COPYA(N,A,B)
```

```
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(N),B(N)
      DO 10 I=1,N
   10 B(I) = A(I)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE COMBIN(N,A1,V1,A2,V2,R)
      IMPLICIT REAL*8 (A-H,O-Z)
C ........ superposition of two vectors .....
      DIMENSION V1(N),V2(N),R(N)
      DO 10 J=1,N
   10 R(J) = A1*V1(J)+A2*V2(J)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE UNITV(N,U,S)
C ........ normalize the vector U .....
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION U(N)
      S=0.
      DO 10 J=1,N
   10 S=S+U(J)**2
      S=SQRT(S)
      IF(S.GT.0.) THEN
       DO 20 J=1,N
   20  U(J)=U(J)/S
      ELSE
       PRINT *, " UNITV: S = 0"
      ENDIF
      RETURN
      END
C ----------------------------------------------------------------------
      FUNCTION SCALPR(N,A,B)
C ........ scalar product .....
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(N),B(N)
      S=0.
      DO 10 J=1,N
   10 S=S+A(J)*B(J)
      SCALPR = S
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE ORTHON(N,NC,U)
C ......................................................................
C ..... orthonormalize the first NC columns of the matrix U ...........
C ......................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION U(91*91,NC),R(91*91)
      C1 = 1.
      CALL UNITV(N,U(1,1),S)
      DO 30 K=2,NC
      DO 20 L=1,K-1
        CLK = SCALPR(N,U(1,L),U(1,K))
        CALL COMBIN(N,C1,U(1,K),-CLK,U(1,L),R)
        CALL COPYA(N,R,U(1,K))
   20 CONTINUE
      CALL UNITV(N,U(1,K),S)
   30 CONTINUE
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE JACOB(N,IV,H,U,MD)
C .................................... called from EPSI0, GTENJ
C ......................................................................
C ...... Diagonalization of a symmetric matrix H, HU = UE
C ...... N = dimension of subblock H(1..N,1..N) to be diagonalized
C ...... MD = dimension of matrix H supplied by input,
C ......     currently limited as  MD.LE.101
```

```
C ...... IV = 0 : U-matrix will be calculated
C ......................................................................
C ...... The original version of this subroutine was written
C ...... by Rutishauser, ETH Zürich, ca. 1960
C ......................................................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION H(MD,MD),U(MD,MD),X(101),IQ(101)
      IF (IV.NE.0) GOTO 4
    1 DO 3 I=1,N
         DO 2 K=1,N
    2 U(I,K)=0.
    3 U(I,I)=1.
    4 N1=N-1
         IF (N1.LT.1) GOTO 49
    5 IR=0
         DO 6 I=1,N
         IQ(I)=I
    6 X(I)=0.
      DO 34 L=1,50
         SS=0.
      DO 7 I=1,N1
         I1=I+1
         DO 7 K=I1,N
    7 SS=ABS(H(I,K))+SS
      IF (SS.EQ.0) GOTO 35
    8 TR=0.
         IF (L.GE.4) GOTO 10
    9 TR=SS*2./N/N
   10 DO 33 I=1,N1
         I1=I+1
         DO 33 K=I1,N
      E=H(I,I)+X(I)
         F=H(I,K)
         G=H(K,K)+X(K)
      EA=ABS(E)
         FA=ABS(F)*10.
         GA=ABS(G)
      IF (EA+FA.NE.EA.OR.GA+FA.NE.GA) GOTO 12
   11 H(I,K)=0.
         GOTO 33
   12 IF (FA.LT.TR) GOTO 33
   13 E=G-E
         G=ABS(E)
         IF (E+FA.NE.E) GOTO 15
   14 T=F/E
         GOTO 20
   15 TH=E*.5/F
         T=1./(SQRT(TH*TH+1.)+ABS(TH))
      IF (TH.GE.0.) GOTO 20
   16 T=-T
   20 C=1./SQRT(T*T+1.)
         S=T*C
         TH=S/(C+1.)
      F=T*F
         X(I)=X(I)-F
         X(K)=X(K)+F
         H(I,K)=0.
      NE=I-1
         IF (NE.LT.1) GOTO 23
   21 DO 22 J=1,NE
         E=H(J,I)
         G=H(J,K)
      H(J,I)=-(E*TH+G)*S+E
   22 H(J,K)=(-G*TH+E)*S+G
   23 NA=I+1
         NE=K-1
         IF (NE.LT.NA) GOTO 26
   24 DO 25 J=NA,NE
        E=H(I,J)
         G=H(J,K)
```

```
      H(I,J)=-(E*TH+G)*S+E
   25 H(J,K)=(-G*TH+E)*S+G
   26 NA=K+1
         IF (NA.GT.N) GOTO 29
   27 DO 28 J=NA,N
         E=H(I,J)
         G=H(K,J)
      H(I,J)=-(E*TH+G)*S+E
   28 H(K,J)=(-G*TH+E)*S+G
   29 IF (IV.NE.0) GOTO 32
   30 DO 31 J=1,N
         E=U(J,I)
         G=U(J,K)
      U(J,I)=-(E*TH+G)*S+E
   31 U(J,K)=(-G*TH+E)*S+G
   32 IR=IR+1
   33 CONTINUE
      DO 34 I=1,N
       H(I,I)=H(I,I)+X(I)
        X(I)=0.
   34 CONTINUE
   35 DO 39 I=1,N1
         J=I
         E=H(I,I)
         I1=I+1
      DO 37 K=I1,N
C-         IF (H(K,K).LE.E) GOTO 37
         IF (H(K,K).GE.E) GOTO 37
   36 J=K
         E=H(K,K)
   37 CONTINUE
      IF (J.EQ.I) GOTO 39
   38 H(J,J)=H(I,I)
         H(I,I)=E
        L=IQ(J)
      IQ(J)=IQ(I)
         IQ(I)=L
   39 CONTINUE
      IF (IV.NE.0) GOTO 49
   40 DO 48 I=1,N1
         IF (IQ(I).EQ.I) GOTO 48
   41 DO 42 J=1,N
   42 X(J)=U(J,I)
      L=I
   43 K=IQ(L)
         IF (K.EQ.I) GOTO 46
   44 IQ(L)=L
         DO 45 J=1,N
   45 U(J,L)=U(J,K)
      L=K
         GOTO 43
   46 IQ(L)=L
         DO 47 J=1,N
         U(J,L)=X(J)
   47 CONTINUE
   48 CONTINUE
   49 RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE FMZ1D(PARAM,VZ,NPER,NOPR)
C ................................................. called from MAIN
      IMPLICIT REAL*8 (A-H, O-Z)
      COMMON  NDX,NDY,NDZ,NX,NY,NZ,NDDX,NDDY,NDDZ,NCX,NCY,NCZ,NXY,NV,
     &        NA,JABC(25,3),RTP(25,3),AM(25),
     &        DX,DY,DZ, DRX,DRY,DRZ, DDX(2*91),DDY(2*91),DDZ(2*91),
     &        RGT(91*91,15),GDET(91*91)
      DIMENSION PARAM(20),C(3,25),R(91,3,25),G(91*4*4),
     &        VPS(91),VZ(91,2),EZ(91,2),
     &        U0(91*91),HP(91*91),UP(91*91),U(91*91,2)
C ......................................................................
```

```
C .... calculates energy levels and wavefunctions for dimer ............
C .... stretching mode (y2) for each of the potential surfaces .........
C .... associated with the tunnel doublet in the ground state ..........
C .... of the x and y1 modes ...........................................
C ......................................................................
C ............. conversion factors: ....................................
                CL=29979.25E0
                PI=3.14159265358979E0
      CALL DIFFCO(NDZ,DDZ)
        X = 0.
        Y = 0.
      DO 10 JZ = 1,NZ
        RZ = DRZ*DFLOAT(JZ-NDZ-1)
        Y2 = 1.+RZ
        PARAM(12) = Y2
      CALL MOVE(NA,X,Y,RTP(1,1),RTP(1,2),RTP(1,3),PARAM)
      CALL CARTO(NA,JABC(1,1),JABC(1,2),JABC(1,3),
     &                 RTP(1,1),RTP(1,2),RTP(1,3),C)
   10 CALL CONFIG(NA,NDZ,C,AM,R,JZ)
      DO 20 J=1,NZ
   20 CALL GTENJ(NA,NDZ,NPER,DDZ,DRZ,R,J,G,GDET(J))
      CALL VPSEU1(NDZ,NPER,DDZ,DRZ,G,GDET,VPS)
      DO 21 J=1,NZ
      VZ(J,1) = VZ(J,1)+VPS(J)
      VZ(J,2) = VZ(J,2)+VPS(J)
   21 CONTINUE
      IF (NOPR.EQ.0) THEN
      PRINT*
      PRINT*," FMZ1D: y2 motion"
      PRINT*," energy profiles for ground state doublet,"
      PRINT*," pseudopotential, and mobility coefficient"
      PRINT 911
      DO 22 J=1,NZ
      PRINT 912, J-NDZ-1,VZ(J,1),VZ(J,2),VPS(J),G(J+NZ*15)
   22 CONTINUE
  911 FORMAT(/,5H   JZ,8X,5HVZ(1),11X,5HVZ(2),10X,3HVPS,5X,9HG44 (MHZ))
  912 FORMAT(I5,2F16.2,2F12.2)
      ENDIF
      CALL SOLV1D(NDZ,DDZ,DRZ,G,VZ(1,1),U0,UP,HP,U(1,1),EZ(1,1))
      CALL SOLV1D(NDZ,DDZ,DRZ,G,VZ(1,2),U0,UP,HP,U(1,2),EZ(1,2))
      PRINT*
      PRINT*," potential profiles, energy levels 1 & 2 (cm^-1)"
      PRINT*," and wavefunctions"
      PRINT 915
      PRINT 916, (EZ(I,1)/CL,I=1,2), (EZ(I,2)/CL,I=1,2)
      PRINT 916, 0.,(EZ(2,1)-EZ(1,1))/CL,
     &           0.,(EZ(2,2)-EZ(1,2))/CL
      DO 42 J = 1,NZ
      RZ = DRZ*DFLOAT(J-NDZ-1)
      Y2 = 1.+RZ
      PRINT 917,Y2, VZ(J,1)/CL, (INT(1.E6*U(J+NZ*(I-1),1)),I=1,2),
     &    (VZ(J,2)-VZ(J,1))/CL, (INT(1.E6*U(J+NZ*(I-1),2)),I=1,2)
   42 CONTINUE
  915 FORMAT(8X,2HY2,13X,3HV0s,10X,3HEs1,9X,3HEs2,
     &           10X,7HV0a-V0s, 8X,3HEa1,9X,3HEa2)
  916 FORMAT(28X,2F12.2,16X,2F12.2)
  917 FORMAT(F12.3,F16.2,2I12,F16.2,2I12)
      PRINT 920, EZ(1,2)-EZ(1,1)
  920 FORMAT(//,32H ground state tunnel splitting =,F10.2,4H MHz,/)
      RETURN
      END
C ----------------------------------------------------------------------
C ------------- subroutines called by FMZ1D  --------------------------
C ----------------------------------------------------------------------
      SUBROUTINE SOLV1D(ND,D,DRV,G,V,U0,UP,HP,U,EP)
C ............................................. called from FMZ1D
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION D(4*ND+2),G(2*ND+1,4,4),V(2*ND+1),U0(2*ND+1,2*ND+1),
     &          U(2*ND+1,2*ND+1),HP((2*ND+1)**2),UP((2*ND+1)**2),
     &          EP(2*ND+1)
```

```
      CALL BASIS0(ND,U0)
      CALL EPSI0(ND,D,DRV,G(1,4,4),V,U0,UP,HP,U,EP,1)
      PM = 0.
      DO 10 J=1,2*ND+1
   10 PM = PM+U(J,1)
      IF(PM.LT.0.) THEN
      DO 12 J=1,2*ND+1
   12 U(J,1) = -U(J,1)
      ENDIF
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE EPSI0(ND,D,DRV,GXX,V,U0,UP,HP,U,EP,NOPR)
C .............................................. called from SOLV1D
C ..............................................................
C ...... solves ...... H psi = E psi ..................... for J = 0
C ...... in subspace spanned by first NV1 columns of U0
C ...... returns first NV eigenvalues in EP
C ...... and eigenfunctions in first NV columns of U0
C ..............................................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION D(4*ND+2),GXX(2*ND+1),V(2*ND+1),U0(2*ND+1,2*ND+1),
     &          U(2*ND+1,2*ND+1),HP(2*ND+1,2*ND+1),
     &          UP(2*ND+1,2*ND+1),EP(2*ND+1)
      NV1 = 2*ND+1
      C0 = 0.
      DO 10 L=1,NV1
   10 CALL HMEPSI(ND,D,DRV,GXX,V,C0,U0(1,L),U(1,L))
      DO 20 K=1,NV1
      DO 20 L=K,NV1
        HP(K,L)=0.
      DO 12 J=1,2*ND+1
   12 HP(K,L) = HP(K,L)+U0(J,K)*U(J,L)
   20 HP(L,K) = HP(K,L)
        CALL JACOB(NV1,0,HP,UP,NV1)
      DO 22 K=1,NV1
      EP(K)=HP(K,K)
      DO 22 J=1,2*ND+1
      U(J,K) = 0.
      DO 22 L=1,NV1
      U(J,K) = U(J,K)+U0(J,L)*UP(L,K)
   22 CONTINUE
      DO 24 K=1,NV1
      DO 24 J=1,2*ND+1
   24 U0(J,K) = U(J,K)
      IF(NOPR.EQ.0) PRINT 901, (EP(K),K=1,NV1)
  901 FORMAT(2X,6F13.2)
      RETURN
      END
C........|.........|.........|.........|.........|.........|.........|..
C ----------------------------------------------------------------------
      SUBROUTINE HMEPSI(ND,D,DRX,GXX,V,E,PSI,RESID)
C ................................................... called from EPSI0
C ..................................................
C ............  (H - E)psi = r ....................
C ..................................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION  D(4*ND+2),GXX(2*ND+1),V(2*ND+1),
     &           PSI(2*ND+1),RESID(2*ND+1),DF(101)
      DX = 2.*3.14159265358979/DFLOAT(2*ND+1)
      DO 10 JP=1,2*ND+1
   10 DF(JP)= -GXX(JP)*DFDX(ND,D,JP,PSI,0)*DX/DRX
      DO 20 JP=1,2*ND+1
      RESID(JP) = DFDX(ND,D,JP,DF,0)*DX/DRX
   20 RESID(JP) = RESID(JP)+(V(JP)-E)*PSI(JP)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE BASIS0(ND,U)
C ............................................... called from SOLV1D
```

```
C ..........................................
C ...... initial basis set .................
C ..........................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION U(2*ND+1,2*ND+1)
      DX=2.E0*3.14159265358979E0/DFLOAT(2*ND+1)
      C=1./SQRT(DFLOAT(2*ND+1))
      DO 10 J=1,2*ND+1
   10 U(J,1)=C
      C=C*SQRT(2.)
      DO 20 K=1,ND
      DO 20 J=1,2*ND+1
      U(J,2*K)   = C*SIN(DFLOAT(K*J)*DX)
   20 U(J,1+2*K) = C*COS(DFLOAT(K*J)*DX)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE PREPS0(E,PSI,ND,NV)
C ................................................ called from SOLV1D
C ....... printing E, psi .....................
C .............................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION E(NV),PSI(2*ND+1,NV)
      PRINT*
      PRINT*, '    E / cm^-1 , psi*1.E6 '
        CL=29979.25E0
        NREC=NV/12
        IF(NV.GT.12*NREC) NREC=NREC+1
      DO 30 N=0,NREC-1
      PRINT*
        L12=12
        IF((12*N+12).GT.NV) L12=NV-12*N
      PRINT 902, (E(12*N+I)/CL, I=1,L12)
      DO 20 J=1,2*ND+1
      PRINT 903, (INT(1.E6*PSI(J,12*N+I)),I=1,L12)
   20 CONTINUE
   30 CONTINUE
  902 FORMAT(2X,12F10.2)
  903 FORMAT(2X,12I10)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE CARTO(N,JA,JB,JC,VR,VT,VP,C)
C ......................................................................
C
C   INPUT
C        N   number of atoms (including dummies, if any)
C            for each atom (K=1,2 ... N):
C        JA(K), JB(K), JC(K)      numbers of reference atoms
C        VR(K), VT(K), VP(K)      polar coordinates (angles in degrees)
C
C
C          Y ^                   (X,Y) plane = (JA,JB,JC) plane
C     JC    |
C           |      K            VR(K) = distance JA <---> K
C           |                   VT(K) = angle JA -> K \/ JA -> JB
C           |                   VP(K) = angle of rotation of atom K,
C           |                          clockwise about x-axis,
C           |                          from (X,Y) plane
C           |
C             JA -------------JB ------> X
C
C     The common axis set (X,Y,Z) is the initial one, defined by
C     the first three (non-collinear) atoms, (JA,JB,JC) = (1,2,3).
C     No reference atom is needed for K = 1, one for K = 2 [JA(2)=1],
C     and two for K = 3 [JA(3)=1, JB(3)=2 or JA(3)=2, JB(3)=1]
C
C   OUTPUT   cartesian coordinates:   C(1,K) = X(K)
C                                C(2,K) = Y(K)
C                                C(3,K) = Z(K)
```

```
C
C       The original version of this subroutine was written
C       by R. Beaudet, Harvard University, ca. 1967
C .......................................................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION JA(N),JB(N),JC(N),VR(N),VT(N),VP(N),U(3,3),C(3,N),CI(3)
        PI1=3.14159265358979E0/180.E0
      DO 1 K=1,3
         DO 1 L=1,3
    1 C(L,K)=0.
      C(1,2)=VR(2)
         T=PI1*VT(3)
         IA=JA(3)
         IB=JB(3)
         IC=JC(3)
         X=VR(3)*(C(1,IB)-C(1,IA))*COS(T)
      C(1,3)=C(1,IA)+X/ABS(C(1,IB)-C(1,IA))
      C(2,3)=VR(3)*SIN(T)
      IF (N.GT.3) THEN
      DO 17 K=4,N
         IAP=IA
         IBP=IB
         ICP=IC
        IA=JA(K)
        IB=JB(K)
        IC=JC(K)
         R=VR(K)
         T=PI1*VT(K)
         P=PI1*VP(K)
      IF((IA.NE.IAP).OR.(IB.NE.IBP).OR.(IC.NE.ICP)) THEN
         S=0.
         SX=0.
         SY=0.
      DO 12 M=1,3
      X=C(M,IB)-C(M,IA)
         SX=SX+X*X
         U(M,1)=X
      Y=C(M,IC)-C(M,IA)
         SY=SY+Y*Y
         S=S+X*Y
   12 U(M,2)=Y
      X=SQRT(SX)
         S=S/X
         Y=SQRT(SY-S*S)
      DO 14 M=1,3
      U(M,1)=U(M,1)/X
   14 U(M,2)=(U(M,2)-S*U(M,1))/Y
        U(1,3)=U(2,1)*U(3,2)-U(3,1)*U(2,2)
        U(2,3)=U(3,1)*U(1,2)-U(1,1)*U(3,2)
        U(3,3)=U(1,1)*U(2,2)-U(2,1)*U(1,2)
      ENDIF
         Y=R*SIN(T)
         CI(1)=R*COS(T)
         CI(2)=Y*COS(P)
         CI(3)=Y*SIN(P)
      DO 17 L=1,3
      S=0.
      DO 16 M=1,3
   16 S=S+U(L,M)*CI(M)
   17 C(L,K)=C(L,IA)+S
      ENDIF
      RETURN
      END
C -----------------------------------------------------------------------
      SUBROUTINE CONFIG(NA,ND,C,VM,R,J)
C ............................................... called from FMZ1D
C .......... mass-weighted nuclear coordinates, ........
C .......... relative to center of mass, ..............
C .......... at configuration point J in array R .......
C ...............................................
```

```
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION C(3,NA),VM(NA),CM(3),R(2*ND+1,3,NA)
         CM(1)=0.
         CM(2)=0.
         CM(3)=0.
         SM=0.
      DO 10 K=1,NA
         SM=SM+VM(K)
         DO 10 I=1,3
   10 CM(I)=CM(I)+VM(K)*C(I,K)
      DO 20 I=1,3
         CM(I)=CM(I)/SM
      DO 20 K=1,NA
   20 R(J,I,K)=SQRT(VM(K))*(C(I,K)-CM(I))
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE GTENJ(NA,ND,NPER,D,DRV,R,J,G,DET)
C ................................................. called from FMZ1D
C ........ contravariant metric tensor,
C ........ its determinant DET,
C ........ and covariant metric tensor G
C ............................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION D(4*ND+2),R(2*ND+1,3,NA),G(2*ND+1,4,4),
     &          DR(4),GJ(4,4),UJ(4,4)
      DV = 2.*3.14159265358979/DFLOAT(2*ND+1)
      DO 10 I=1,4
      DO 10 K=1,4
   10 GJ(I,K)=0.
      DO 20 K=1,NA
        UJ(1,1)= 0.
        UJ(1,2)= R(J,3,K)
        UJ(1,3)=-R(J,2,K)
      UJ(2,1)=-UJ(1,2)
      UJ(2,2)= 0.
      UJ(2,3)= R(J,1,K)
        UJ(3,1)=-UJ(1,3)
        UJ(3,2)=-UJ(2,3)
        UJ(3,3)= 0.
      DO 12 I=1,3
   12 UJ(I,4) = DFDX(ND,D,J,R(1,I,K),NPER)*DV/DRV
        DO 16 I=1,4
        DO 16 L=I,4
        DO 16 M=1,3
   16 GJ(I,L)=GJ(I,L)+UJ(M,I)*UJ(M,L)
   20 CONTINUE
        DO 22 I=1,4
        DO 22 K=I,4
   22 GJ(K,I)=GJ(I,K)
        CALL JACOB(4,0,GJ,UJ,4)
        DET=1.
      DO 30 I=1,4
        DR(I) = 505379.05E0/GJ(I,I)
   30 DET=DET*GJ(I,I)
        DO 40 I=1,4
        DO 40 K=1,4
        G(J,I,K)=0.
      DO 40 M=1,4
   40 G(J,I,K)=G(J,I,K)+UJ(I,M)*DR(M)*UJ(K,M)
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE VPSEU1(ND,NPER,D,DRV,G,DET,VPS)
C ................................................. called from FMZ1D
C ............ pseudopotential function in Mz ..........
C ..... input: metric determinant contained in array DET
C ...................................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION D(4*ND+2),G(2*ND+1,4,4),DET(2*ND+1),VPS(2*ND+1)
```

```
      DV = 2.*3.14159265358979/DFLOAT(2*ND+1)
      DO 10 J=1,2*ND+1
   10 VPS(J)= -DFDX(ND,D,J,DET,NPER)*(DV/DRV)/(4.*DET(J))
      DO 20 J=1,2*ND+1
   20 DET(J)=VPS(J)*G(J,4,4)
      DO 30 J=1,2*ND+1
   30 VPS(J)=VPS(J)**2*G(J,4,4)-DFDX(ND,D,J,DET,NPER)*DV/DRV
      RETURN
      END
C ----------------------------------------------------------------------
      FUNCTION DFDX(ND,D,JP,F,NPER)
C ........................................... called from GTENJ, VPSEU1
C ......................................................................
C ...... Derivative of a function F(1, ... 2*ND+1) ....................
C ...... that represents F(x) in the range -pi<= x <= pi ..............
C ...... choose NPER = 0 for a cyclic function ........................
C ......        NPER = 1 for a noncyclic function .....................
C ...... the result DFDX is DF/DX at the point JP .....................
C ......................................................................
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION D(4*ND+2),F(2*ND+1)
        DX=2.E0*3.14159265358979E0/DFLOAT(2*ND+1)
        DF=0.
      IF(NPER.EQ.0) THEN
        K=2*ND+1-JP
        DO 10 J=1,2*ND+1
        K=K+1
   10   DF=DF+D(K)*F(J)
      ELSE
       IF((JP.GT.2).AND.(JP.LT.2*ND))
     &  DF=(4./3.*(F(JP+1)-F(JP-1))-1./6.*(F(JP+2)-F(JP-2)))/(2.*DX)
       IF(JP.EQ.1)
     &  DF=(-11.*F(JP)+18.*F(JP+1)-9.*F(JP+2)+2.*F(JP+3))/(6.*DX)
       IF(JP.EQ.2*ND+1)
     &  DF=(+11.*F(JP)-18.*F(JP-1)+9.*F(JP-2)-2.*F(JP-3))/(6.*DX)
       IF (JP.EQ.2)
     &  DF=(-2.*F(JP-1)-3.*F(JP)+6.*F(JP+1)-F(JP+2))/(6.*DX)
       IF (JP.EQ.2*ND)
     &  DF=(+2.*F(JP+1)+3.*F(JP)-6.*F(JP-1)+F(JP-2))/(6.*DX)
      ENDIF
             DFDX=DF
      RETURN
      END
C ----------------------------------------------------------------------
```

*c) Input File*

```
 ----- formic acid dimer, March 2017 -------- (x, y1, y2) = (0,0,0)
  12
   1    0    0    0   0.00000     0.000     0.000          0.0000000
   2    1    0    0   1.00000     0.000     0.000          0.0000000
   3    1    2    0   1.77575    90.000     0.000         12.0000000
   4    1    2    3   1.77575    90.000   180.000         12.0000000
   5    3    1    2   1.26120    63.300     0.000         15.9949150
   6    3    1    2   1.26120    63.300   180.000         15.9949150
   7    4    1    2   1.26120    63.300     0.000         15.9949150
   8    4    1    2   1.26120    63.300   180.000         15.9949150
   9    3    5    1   1.09520   116.700   180.000          1.0078250
  10    4    7    1   1.09520   116.700   180.000          2.0141018
  11    1    4    2   1.11610    90.000     0.000          1.0078250
  12    1    4    2   1.11610    90.000   180.000          1.0078250
  1424000.    -13000.    597000.   <-  mobility constants HCOOH HOOCD
 ----- formic acid dimer, March 2017 -------- (x, y1, y2) = (0,0,0)
  12
   1    0    0    0   0.00000     0.000     0.000          0.0000000
   2    1    0    0   1.00000     0.000     0.000          0.0000000
   3    1    2    0   1.77575    90.000     0.000         12.0000000
   4    1    2    3   1.77575    90.000   180.000         12.0000000
   5    3    1    2   1.26120    63.300     0.000         15.9949150
   6    3    1    2   1.26120    63.300   180.000         15.9949150
   7    4    1    2   1.26120    63.300     0.000         15.9949150
   8    4    1    2   1.26120    63.300   180.000         15.9949150
   9    3    5    1   1.09520   116.700   180.000          1.0078250
  10    4    7    1   1.09520   116.700   180.000          2.0141018
  11    1    4    2   1.11610    90.000     0.000          2.0141018
  12    1    4    2   1.11610    90.000   180.000          2.0141018
   719000.    -13000.    597000.   <-  mobility constants HCOOD DOOCD
 ----- formic acid dimer, March 2017 -------- (x, y1, y2) = (0,0,0)
  12
   1    0    0    0   0.00000     0.000     0.000          0.0000000
   2    1    0    0   1.00000     0.000     0.000          0.0000000
   3    1    2    0   1.77575    90.000     0.000         12.0000000
   4    1    2    3   1.77575    90.000   180.000         12.0000000
   5    3    1    2   1.26120    63.300     0.000         15.9949150
   6    3    1    2   1.26120    63.300   180.000         15.9949150
   7    4    1    2   1.26120    63.300     0.000         15.9949150
   8    4    1    2   1.26120    63.300   180.000         15.9949150
   9    3    5    1   1.09520   116.700   180.000          1.0078250
  10    4    7    1   1.09520   116.700   180.000          1.0078250
  11    1    4    2   1.11610    90.000     0.000          1.0078250
  12    1    4    2   1.11610    90.000   180.000          1.0078250
  1424000.    -13000.    597000.   <-  mobility constants HCOOH HOOCH
 ----- formic acid dimer, March 2017 -------- (x, y1, y2) = (0,0,0)
  12
   1    0    0    0   0.00000     0.000     0.000          0.0000000
   2    1    0    0   1.00000     0.000     0.000          0.0000000
   3    1    2    0   1.77575    90.000     0.000         12.0000000
   4    1    2    3   1.77575    90.000   180.000         12.0000000
   5    3    1    2   1.26120    63.300     0.000         15.9949150
   6    3    1    2   1.26120    63.300   180.000         15.9949150
   7    4    1    2   1.26120    63.300     0.000         15.9949150
   8    4    1    2   1.26120    63.300   180.000         15.9949150
   9    3    5    1   1.09520   116.700   180.000          1.0078250
  10    4    7    1   1.09520   116.700   180.000          1.0078250
  11    1    4    2   1.11610    90.000     0.000          1.0078250
  12    1    4    2   1.11610    90.000   180.000          2.0141018
   958000.    -13000.    597000.   <-  mobility constants HCOOH DOOCH



  10    4    7    1   1.09520   116.700   180.000          2.0141018

---------------------------------------------------------------------------
```

## *d) Output file*

```
Standard configuration as read from input
 ******************************************************************************
   ----- formic acid dimer, March 2017 -------- (x, y1, y2) = (0,0,0)
 ******************************************************************************
 NA = 12
    1    0    0    0   0.00000     0.000     0.000           0.0000000
    2    1    0    0   1.00000     0.000     0.000           0.0000000
    3    1    2    0   1.77575    90.000     0.000          12.0000000
    4    1    2    3   1.77575    90.000   180.000          12.0000000
    5    3    1    2   1.26120    63.300     0.000          15.9949150
    6    3    1    2   1.26120    63.300   180.000          15.9949150
    7    4    1    2   1.26120    63.300     0.000          15.9949150
    8    4    1    2   1.26120    63.300   180.000          15.9949150
    9    3    5    1   1.09520   116.700   180.000           1.0078250
   10    4    7    1   1.09520   116.700   180.000           2.0141018
   11    1    4    2   1.11610    90.000     0.000           1.0078250
   12    1    4    2   1.11610    90.000   180.000           1.0078250

   ----------- grid properties -----------
   NDX   NDY   NDZ     DRX     DRY     DRZ    NV
    18    18    18   0.167   0.167   0.167    16

        mobility constants (MHz)
      GXXE        GXYE        GYYE
    1424000.     -13000.     597000.

 X=Y=0
          GXX    1424480.587  MHZ
          GXY     -13709.103
          GYY     599408.202
          G   0.18270934E+07  (AMU*A**2)**5



 TABLES: GXX, GXY, GYY (GHZ),  G/G(0,0), VG (GHZ)


  1423  1423  1423  1424  1424  1424  1424  1424  1424  1424  1424  1424  1424  1424  1424  1424  1423  1423  1423
  1423  1423  1423  1424  1424  1424  1424  1424  1424  1424  1424  1424  1424  1424  1424  1424  1423  1423  1423
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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
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| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
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| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -12 | -11 | -10 | -9 | -8 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
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| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
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| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10724 | 10617 | 10522 | 10439 | 10369 | 10313 | 10272 | 10247 | 10236 | 10242 | 10264 | 10302 | 10356 | 10425 | 10510 | 10609 | 10723 | 10850 | 10989 |
| 10704 | 10596 | 10500 | 10417 | 10346 | 10290 | 10248 | 10222 | 10211 | 10216 | 10237 | 10274 | 10327 | 10395 | 10479 | 10577 | 10690 | 10816 | 10954 |
| 10685 | 10577 | 10480 | 10396 | 10325 | 10268 | 10226 | 10198 | 10187 | 10191 | 10211 | 10247 | 10299 | 10367 | 10450 | 10547 | 10659 | 10783 | 10920 |
| 10668 | 10559 | 10462 | 10377 | 10305 | 10248 | 10205 | 10177 | 10164 | 10168 | 10187 | 10223 | 10274 | 10340 | 10422 | 10519 | 10629 | 10752 | 10888 |
| 10653 | 10543 | 10445 | 10360 | 10287 | 10229 | 10185 | 10156 | 10143 | 10146 | 10165 | 10199 | 10249 | 10315 | 10396 | 10492 | 10601 | 10723 | 10858 |
| 10639 | 10529 | 10430 | 10344 | 10271 | 10211 | 10167 | 10138 | 10124 | 10126 | 10144 | 10177 | 10227 | 10292 | 10372 | 10466 | 10574 | 10696 | 10829 |
| 10626 | 10516 | 10416 | 10329 | 10255 | 10196 | 10150 | 10120 | 10106 | 10107 | 10124 | 10157 | 10206 | 10270 | 10349 | 10442 | 10549 | 10670 | 10802 |
| 10616 | 10504 | 10404 | 10316 | 10242 | 10181 | 10135 | 10105 | 10089 | 10090 | 10106 | 10138 | 10186 | 10249 | 10327 | 10420 | 10526 | 10645 | 10776 |
| 10607 | 10494 | 10393 | 10305 | 10230 | 10169 | 10122 | 10090 | 10074 | 10074 | 10090 | 10121 | 10168 | 10230 | 10307 | 10399 | 10504 | 10622 | 10753 |
| 10599 | 10486 | 10384 | 10295 | 10219 | 10157 | 10110 | 10078 | 10061 | 10060 | 10075 | 10105 | 10151 | 10213 | 10289 | 10380 | 10484 | 10601 | 10730 |
| 10593 | 10479 | 10377 | 10287 | 10210 | 10148 | 10100 | 10067 | 10049 | 10047 | 10061 | 10091 | 10136 | 10197 | 10272 | 10362 | 10465 | 10582 | 10710 |
| 10588 | 10474 | 10371 | 10280 | 10203 | 10139 | 10091 | 10057 | 10039 | 10036 | 10049 | 10078 | 10123 | 10182 | 10257 | 10346 | 10448 | 10564 | 10691 |
| 10586 | 10470 | 10366 | 10275 | 10197 | 10133 | 10083 | 10049 | 10030 | 10026 | 10039 | 10067 | 10111 | 10169 | 10243 | 10331 | 10433 | 10547 | 10673 |
| 10584 | 10468 | 10363 | 10271 | 10192 | 10127 | 10077 | 10042 | 10022 | 10018 | 10030 | 10057 | 10100 | 10158 | 10231 | 10318 | 10419 | 10532 | 10657 |
| 10585 | 10468 | 10362 | 10269 | 10189 | 10124 | 10073 | 10037 | 10016 | 10011 | 10022 | 10049 | 10091 | 10148 | 10220 | 10307 | 10406 | 10519 | 10643 |
| 10586 | 10469 | 10362 | 10268 | 10188 | 10122 | 10070 | 10033 | 10012 | 10006 | 10016 | 10042 | 10083 | 10140 | 10211 | 10297 | 10395 | 10507 | 10630 |
| 10590 | 10471 | 10364 | 10269 | 10188 | 10121 | 10068 | 10031 | 10009 | 10002 | 10012 | 10037 | 10077 | 10133 | 10203 | 10288 | 10386 | 10497 | 10619 |
| 10595 | 10475 | 10367 | 10272 | 10190 | 10122 | 10068 | 10030 | 10007 | 10000 | 10009 | 10033 | 10073 | 10128 | 10197 | 10281 | 10378 | 10488 | 10609 |
| 10601 | 10481 | 10372 | 10276 | 10193 | 10124 | 10070 | 10031 | 10007 | 10000 | 10007 | 10031 | 10070 | 10124 | 10193 | 10276 | 10372 | 10481 | 10601 |
| 10609 | 10488 | 10378 | 10281 | 10197 | 10128 | 10073 | 10033 | 10009 | 10000 | 10007 | 10030 | 10068 | 10122 | 10190 | 10272 | 10367 | 10475 | 10595 |
| 10619 | 10497 | 10386 | 10288 | 10203 | 10133 | 10077 | 10037 | 10012 | 10002 | 10009 | 10031 | 10068 | 10121 | 10188 | 10269 | 10364 | 10471 | 10590 |
| 10630 | 10507 | 10395 | 10297 | 10211 | 10140 | 10083 | 10042 | 10016 | 10006 | 10012 | 10033 | 10070 | 10122 | 10188 | 10268 | 10362 | 10469 | 10586 |
| 10643 | 10519 | 10406 | 10307 | 10220 | 10148 | 10091 | 10049 | 10022 | 10011 | 10016 | 10037 | 10073 | 10124 | 10189 | 10269 | 10362 | 10468 | 10585 |
| 10657 | 10532 | 10419 | 10318 | 10231 | 10158 | 10100 | 10057 | 10030 | 10018 | 10022 | 10042 | 10077 | 10127 | 10192 | 10271 | 10363 | 10468 | 10584 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10673 | 10547 | 10433 | 10331 | 10243 | 10169 | 10111 | 10067 | 10039 | 10026 | 10030 | 10049 | 10083 | 10133 | 10197 | 10275 | 10366 | 10470 | 10586 |
| 10691 | 10564 | 10448 | 10346 | 10257 | 10182 | 10123 | 10078 | 10049 | 10036 | 10039 | 10057 | 10091 | 10139 | 10203 | 10280 | 10371 | 10474 | 10588 |
| 10710 | 10582 | 10465 | 10362 | 10272 | 10197 | 10136 | 10091 | 10061 | 10047 | 10049 | 10067 | 10100 | 10148 | 10210 | 10287 | 10377 | 10479 | 10593 |
| 10730 | 10601 | 10484 | 10380 | 10289 | 10213 | 10151 | 10105 | 10075 | 10060 | 10061 | 10078 | 10110 | 10157 | 10219 | 10295 | 10384 | 10486 | 10599 |
| 10753 | 10622 | 10504 | 10399 | 10307 | 10230 | 10168 | 10121 | 10090 | 10074 | 10074 | 10090 | 10122 | 10169 | 10230 | 10305 | 10393 | 10494 | 10607 |
| 10776 | 10645 | 10526 | 10420 | 10327 | 10249 | 10186 | 10138 | 10106 | 10090 | 10089 | 10105 | 10135 | 10181 | 10242 | 10316 | 10404 | 10504 | 10616 |
| 10802 | 10670 | 10549 | 10442 | 10349 | 10270 | 10206 | 10157 | 10124 | 10107 | 10106 | 10120 | 10150 | 10196 | 10255 | 10329 | 10416 | 10516 | 10626 |
| 10829 | 10696 | 10574 | 10466 | 10372 | 10292 | 10227 | 10177 | 10144 | 10126 | 10124 | 10138 | 10167 | 10211 | 10271 | 10344 | 10430 | 10529 | 10639 |
| 10858 | 10723 | 10601 | 10492 | 10396 | 10315 | 10249 | 10199 | 10165 | 10146 | 10143 | 10156 | 10185 | 10229 | 10287 | 10360 | 10445 | 10543 | 10653 |
| 10888 | 10752 | 10629 | 10519 | 10422 | 10340 | 10274 | 10223 | 10187 | 10168 | 10164 | 10177 | 10205 | 10248 | 10305 | 10377 | 10462 | 10559 | 10668 |
| 10920 | 10783 | 10659 | 10547 | 10450 | 10367 | 10299 | 10247 | 10211 | 10191 | 10187 | 10198 | 10226 | 10268 | 10325 | 10396 | 10480 | 10577 | 10685 |
| 10954 | 10816 | 10690 | 10577 | 10479 | 10395 | 10327 | 10274 | 10237 | 10216 | 10211 | 10222 | 10248 | 10290 | 10346 | 10417 | 10500 | 10596 | 10704 |
| 10989 | 10850 | 10723 | 10609 | 10510 | 10425 | 10356 | 10302 | 10264 | 10242 | 10236 | 10247 | 10272 | 10313 | 10369 | 10439 | 10522 | 10617 | 10724 |

pseudopotential function in GHz

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |

pseudopotential + potential energy (cm^-1)

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23835 | 23819 | 23819 | 23836 | 23865 | 23900 | 23932 | 23958 | 23977 | 23988 | 23994 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 | 23999 | 24000 |
| 23486 | 23431 | 23427 | 23477 | 23567 | 23674 | 23778 | 23863 | 23923 | 23961 | 23982 | 23992 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 | 23999 |

```
22710 22560 22538 22650 22868 23138 23405 23628 23789 23892 23949 23978 23991 23997 23999 23999 23999 23999 23999
21323 20987 20908 21105 21530 22084 22652 23142 23506 23743 23879 23948 23980 23993 23997 23999 23999 23999 23999
19288 18654 18446 18711 19389 20334 21354 22273 22983 23460 23741 23887 23955 23984 23994 23998 23999 23999 23999
16802 15764 15329 15579 16467 17824 19391 20891 22112 22969 23493 23775 23910 23967 23989 23996 23999 23999 23999
14236 12718 11949 12047 12997 14653 16738 18890 20767 22168 23069 23575 23825 23934 23978 23993 23998 23999 23999
12020  9968  8761  8545  9344 11065 13480 16214 18815 20915 22363 23222 23668 23872 23955 23986 23996 23998 23999
10548  7924  6180  5489  5906  7399  9829 12897 16134 19021 21199 22598 23373 23747 23908 23969 23991 23997 23999
10176  6953  4574  3258  3085  4063  6139  9145 12716 16300 19333 21496 22806 23491 23805 23932 23978 23993 23998
11251  7473  4380  2299  1357  1584  2975  5473  8884 12789 16568 19643 21743 22962 23573 23841 23947 23983 23995
13719  9620  5840  2890  1024   321   794  2434  5184  8833 12921 16790 19860 21902 23056 23619 23862 23954 23986
16978 13101  8954  5207  2344   588     0   588  2344  5207  8954 13101 16978 20011 22000 23109 23645 23872 23958
19937 16894 13035  8937  5259  2470   788   274   936  2761  5678  9439 13546 17328 20245 22134 23175 23673 23883
21834 19774 16719 12913  8936  5421  2808  1301   959  1789  3770  6796 10571 14558 18107 20754 22418 23313 23732
22764 21388 19104 15889 12091  8311  5130  2913  1817  1886  3117  5458  8733 12548 16307 19423 21593 22876 23531
23147 22115 20289 17532 14021 10260  6857  4272  2747  2368  3150  5060  7968 11559 15302 18594 21029 22552 23370
23277 22372 20732 18186 14843 11150  7703  4997  3312  2759  3363  5097  7843 11313 15003 18318 20824 22426 23304
23298 22417 20813 18311 15009 11340  7898  5180  3474  2897  3474  5180  7898 11340 15009 18311 20813 22417 23298
23304 22426 20824 18318 15003 11313  7843  5097  3363  2759  3312  4997  7703 11150 14843 18186 20732 22372 23277
23370 22552 21029 18594 15302 11559  7968  5060  3150  2368  2747  4272  6857 10260 14021 17532 20289 22115 23147
23531 22876 21593 19423 16307 12548  8733  5458  3117  1886  1817  2913  5130  8311 12091 15889 19104 21388 22764
23732 23313 22418 20754 18107 14558 10571  6796  3770  1789   959  1301  2808  5421  8936 12913 16719 19774 21834
23883 23673 23175 22134 20245 17328 13546  9439  5678  2761   936   274   788  2470  5259  8937 13035 16894 19937
23958 23872 23645 23109 22000 20011 16978 13101  8954  5207  2344   588     0   588  2344  5207  8954 13101 16978
23986 23954 23862 23619 23056 21902 19860 16790 12921  8833  5184  2434   794   321  1024  2890  5840  9620 13719
23995 23983 23947 23841 23573 22962 21743 19643 16568 12789  8884  5473  2975  1584  1357  2299  4380  7473 11251
23998 23993 23978 23932 23805 23491 22806 21496 19333 16300 12716  9145  6139  4063  3085  3258  4574  6953 10176
23999 23997 23991 23969 23908 23747 23373 22598 21199 19021 16134 12897  9829  7399  5906  5489  6180  7924 10548
23999 23998 23996 23986 23955 23872 23668 23222 22363 20915 18815 16214 13480 11065  9344  8545  8761  9968 12020
23999 23999 23998 23993 23978 23934 23825 23575 23069 22168 20767 18890 16738 14653 12997 12047 11949 12718 14236
23999 23999 23999 23996 23989 23967 23910 23775 23493 22969 22112 20891 19391 17824 16467 15579 15329 15764 16802
23999 23999 23999 23998 23994 23984 23955 23887 23741 23460 22983 22273 21354 20334 19389 18711 18446 18654 19288
23999 23999 23999 23999 23997 23993 23980 23948 23879 23743 23506 23142 22652 22084 21530 21105 20908 20987 21323
23999 23999 23999 23999 23999 23997 23991 23978 23949 23892 23789 23628 23405 23138 22868 22650 22538 22560 22710
23999 23999 23999 23999 23999 23999 23997 23992 23982 23961 23923 23863 23778 23674 23567 23477 23427 23431 23486
24000 23999 23999 23999 23999 23999 23999 23997 23994 23988 23977 23958 23932 23900 23865 23836 23819 23819 23835


Emax / cm^-1 =    45982.404211258210


                     energy levels (MHz)

  iteration cycle           11
 40646947.22  40647068.68  51355477.37  51358971.54  61962721.14  62004413.91
   72392805.39  72659131.48  82501955.30  83469753.01  92475259.90  94457470.54
102670330.03 104747183.19 106295543.34 106394742.95

Tunnel splitting, E0(2)-E0(1) =       121.47 MHz

  iteration cycle           12
 40646947.22  40647068.68  51355477.37  51358971.54  61962721.14  62004413.91
   72392805.39  72659131.48  82501955.30  83469753.01  92475259.90  94457470.54
102670329.92 104747183.19 106295543.31 106394742.95

Tunnel splitting, E0(2)-E0(1) =       121.47 MHz

  iteration cycle           13
 40646947.22  40647068.68  51355477.37  51358971.54  61962721.14  62004413.91
   72392805.39  72659131.48  82501955.30  83469753.01  92475259.90  94457470.54
102670329.92 104747183.19 106295543.31 106394742.95
```

Tunnel splitting, E0(2)-E0(1) =       121.47 MHz

energy levels (cm^-1) and wavefunctions:

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1355.836

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 2 | 20 | 34 | 14 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 16 | 153 | 334 | 181 | 25 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 55 | 683 | 1991 | 1444 | 276 | 15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 100 | 1677 | 6758 | 6848 | 1824 | 135 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 94 | 2174 | 12412 | 18097 | 7000 | 746 | 22 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 44 | 1441 | 11882 | 25423 | 14592 | 2316 | 104 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 10 | 490 | 5884 | 18688 | 16124 | 3867 | 261 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 92 | 1597 | 7543 | 9815 | 3564 | 363 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 11 | 274 | 1890 | 3681 | 2008 | 305 | 15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 35 | 350 | 1003 | 804 | 180 | 18 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 4 | 56 | 232 | 268 | 94 | 32 | 12 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 8 | 53 | 86 | 67 | 86 | 53 | 8 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 12 | 32 | 94 | 268 | 232 | 56 | 4 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 18 | 180 | 804 | 1003 | 350 | 35 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | 305 | 2008 | 3681 | 1890 | 274 | 11 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 | 363 | 3564 | 9815 | 7543 | 1597 | 92 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 261 | 3867 | 16124 | 18688 | 5884 | 490 | 10 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 104 | 2316 | 14592 | 25423 | 11882 | 1441 | 44 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 22 | 746 | 7000 | 18097 | 12412 | 2174 | 94 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 135 | 1824 | 6848 | 6758 | 1677 | 100 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | 276 | 1444 | 1991 | 683 | 55 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 25 | 181 | 334 | 153 | 16 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 14 | 34 | 20 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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1355.840

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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -2 | -20 | -34 | -14 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -16 | -153 | -334 | -181 | -25 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -55 | -683 | -1991 | -1444 | -276 | -15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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| 0 | 0 | -1 | -100 | -1678 | -6759 | -6848 | -1824 | -135 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -94 | -2174 | -12413 | -18097 | -7000 | -746 | -22 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -44 | -1441 | -11883 | -25424 | -14592 | -2316 | -104 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -10 | -490 | -5884 | -18688 | -16124 | -3866 | -260 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -1 | -92 | -1597 | -7543 | -9814 | -3562 | -360 | -9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -11 | -274 | -1890 | -3681 | -2006 | -299 | -9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | -35 | -350 | -1003 | -802 | -168 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -4 | -56 | -232 | -265 | -66 | 20 | 11 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -8 | -52 | -80 | 0 | 80 | 52 | 8 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -1 | -11 | -20 | 66 | 265 | 232 | 56 | 4 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | 0 | 168 | 802 | 1003 | 350 | 35 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | 299 | 2006 | 3681 | 1890 | 274 | 11 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | 360 | 3562 | 9814 | 7543 | 1597 | 92 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 260 | 3866 | 16124 | 18688 | 5884 | 490 | 10 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 104 | 2316 | 14592 | 25424 | 11883 | 1441 | 44 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 22 | 746 | 7000 | 18097 | 12413 | 2174 | 94 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 135 | 1824 | 6848 | 6759 | 1678 | 100 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | 276 | 1444 | 1991 | 683 | 55 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 25 | 181 | 334 | 153 | 16 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 14 | 34 | 20 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 1 | 5 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 11 | 63 | 68 | 11 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 2 | 69 | 472 | 638 | 118 | -17 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 228 | 2043 | 3604 | 786 | -225 | -34 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 7 | 405 | 4871 | 11577 | 2979 | -1710 | -325 | -11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 4 | 370 | 6127 | 20053 | 5880 | -7426 | -1900 | -94 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 170 | 3935 | 18020 | 5424 | -17307 | -6220 | -447 | -8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 40 | 1295 | 8321 | 1822 | -21232 | -10951 | -1163 | -31 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 5 | 235 | 2083 | -203 | -14309 | -10659 | -1681 | -69 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 27 | 324 | -314 | -5956 | -6371 | -1478 | -96 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 2 | 36 | -116 | -1812 | -2728 | -924 | -109 | -10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 4 | -29 | -475 | -987 | -516 | -158 | -33 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -7 | -123 | -355 | -382 | -355 | -123 | -7 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -1 | -33 | -158 | -516 | -987 | -475 | -29 | 4 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -10 | -109 | -924 | -2728 | -1812 | -116 | 36 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -96 | -1478 | -6371 | -5956 | -314 | 324 | 27 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -69 | -1681 | -10659 | -14309 | -203 | 2083 | 235 | 5 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -31 | -1163 | -10951 | -21232 | 1822 | 8321 | 1295 | 40 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -8 | -447 | -6220 | -17307 | 5424 | 18020 | 3935 | 170 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -94 | -1900 | -7426 | 5880 | 20053 | 6127 | 370 | 4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -11 | -325 | -1710 | 2979 | 11577 | 4871 | 405 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -34 | -225 | 786 | 3604 | 2043 | 228 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -17 | 118 | 638 | 472 | 69 | 2 | 0 | 0 |

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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 11 | 68 | 63 | 11 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | -1 | -5 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -11 | -63 | -68 | -11 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -2 | -69 | -472 | -638 | -118 | 17 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -229 | -2045 | -3606 | -786 | 225 | 34 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -7 | -405 | -4875 | -11584 | -2978 | 1711 | 325 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -4 | -370 | -6131 | -20063 | -5877 | 7430 | 1899 | 94 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -170 | -3938 | -18029 | -5418 | 17317 | 6215 | 444 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -40 | -1296 | -8325 | -1816 | 21242 | 10938 | 1151 | 28 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -5 | -235 | -2084 | 206 | 14314 | 10641 | 1652 | 57 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -27 | -324 | 315 | 5957 | 6350 | 1426 | 62 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -2 | -36 | 116 | 1812 | 2707 | 834 | 22 | -8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -4 | 29 | 474 | 958 | 341 | -73 | -31 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 7 | 122 | 306 | 0 | -306 | -122 | -7 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 31 | 73 | -341 | -958 | -474 | -29 | 4 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | -22 | -834 | -2707 | -1812 | -116 | 36 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -62 | -1426 | -6350 | -5957 | -315 | 324 | 27 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -57 | -1652 | -10641 | -14314 | -206 | 2084 | 235 | 5 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -28 | -1151 | -10938 | -21242 | 1816 | 8325 | 1296 | 40 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -7 | -444 | -6215 | -17317 | 5418 | 18029 | 3938 | 170 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -94 | -1899 | -7430 | 5877 | 20063 | 6131 | 370 | 4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -11 | -325 | -1711 | 2978 | 11584 | 4875 | 405 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -34 | -225 | 786 | 3606 | 2045 | 229 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -17 | 118 | 638 | 472 | 69 | 2 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 11 | 68 | 63 | 11 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 5 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 1 | 35 | 136 | 82 | -2 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 7 | 200 | 979 | 715 | -54 | -12 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 19 | 650 | 4107 | 3733 | -592 | -105 | 37 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 25 | 1128 | 9472 | 10969 | -3424 | -456 | 396 | 29 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 17 | 1010 | 11505 | 17173 | -10381 | -666 | 2526 | 241 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 456 | 7122 | 13711 | -16031 | 1235 | 8983 | 1189 | 32 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 106 | 2253 | 5481 | -12530 | 4789 | 17116 | 3238 | 127 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 14 | 391 | 1134 | -5216 | 5448 | 18037 | 4914 | 287 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 43 | 133 | -1298 | 3258 | 11721 | 4564 | 403 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 3 | 8 | -225 | 1331 | 5512 | 3048 | 439 | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -30 | 457 | 2237 | 1842 | 530 | 57 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -2 | 154 | 945 | 1433 | 945 | 154 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 57 | 530 | 1842 | 2237 | 457 | -30 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 25 | 439 | 3048 | 5512 | 1331 | -225 | 8 | 3 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 12 | 403 | 4564 | 11721 | 3258 | -1298 | 133 | 43 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 287 | 4914 | 18037 | 5448 | -5216 | 1134 | 391 | 14 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 127 | 3238 | 17116 | 4789 | -12530 | 5481 | 2253 | 106 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 32 | 1189 | 8983 | 1235 | -16031 | 13711 | 7122 | 456 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 241 | 2526 | -666 | -10381 | 17173 | 11505 | 1010 | 17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 29 | 396 | -456 | -3424 | 10969 | 9472 | 1128 | 25 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 37 | -105 | -592 | 3733 | 4107 | 650 | 19 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | -12 | -54 | 715 | 979 | 200 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -2 | 82 | 136 | 35 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 12 | 3 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -3 | -12 | -6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -35 | -137 | -82 | 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -7 | -202 | -985 | -718 | 55 | 12 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -19 | -655 | -4133 | -3745 | 599 | 104 | -37 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -25 | -1137 | -9531 | -11000 | 3456 | 447 | -398 | -28 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -17 | -1018 | -11576 | -17211 | 10461 | 620 | -2535 | -238 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -459 | -7165 | -13730 | 16136 | -1348 | -9003 | -1169 | -29 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -106 | -2266 | -5484 | 12599 | -4934 | -17124 | -3164 | -112 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -14 | -394 | -1133 | 5238 | -5547 | -17999 | -4742 | -233 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -1 | -44 | -133 | 1302 | -3297 | -11640 | -4281 | -268 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -3 | -8 | 226 | -1339 | -5402 | -2619 | -145 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 30 | -455 | -2086 | -1112 | 135 | 46 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 2 | -147 | -706 | 0 | 706 | 147 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -46 | -135 | 1112 | 2086 | 455 | -30 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -12 | 145 | 2619 | 5402 | 1339 | -226 | 8 | 3 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 268 | 4281 | 11640 | 3297 | -1302 | 133 | 44 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 233 | 4742 | 17999 | 5547 | -5238 | 1133 | 394 | 14 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 112 | 3164 | 17124 | 4934 | -12599 | 5484 | 2266 | 106 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 29 | 1169 | 9003 | 1348 | -16136 | 13730 | 7165 | 459 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 238 | 2535 | -620 | -10461 | 17211 | 11576 | 1018 | 17 | 0 | 0 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 28 | 398 | -447 | -3456 | 11000 | 9531 | 1137 | 25 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 37 | -104 | -599 | 3745 | 4133 | 655 | 19 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | -12 | -55 | 718 | 985 | 202 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -2 | 82 | 137 | 35 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 12 | 3 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

7
2414.764

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 8 | 20 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 82 | 224 | 59 | -10 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 22 | 460 | 1553 | 438 | -130 | 16 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 56 | 1462 | 6274 | 1876 | -973 | 204 | -8 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 73 | 2486 | 13907 | 4166 | -4153 | 1510 | -150 | -46 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 48 | 2180 | 16194 | 4109 | -9419 | 6248 | -1309 | -410 | -13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 16 | 962 | 9579 | 978 | -10625 | 13502 | -5860 | -2153 | -93 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 2 | 218 | 2882 | -778 | -5579 | 14799 | -13446 | -6236 | -380 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 28 | 473 | -506 | -1208 | 8373 | -16705 | -10099 | -886 | -17 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 2 | 49 | -128 | 0 | 2557 | -12714 | -10088 | -1275 | -36 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 4 | -20 | 65 | 365 | -7056 | -7344 | -1357 | -54 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -2 | 21 | -77 | -3480 | -4893 | -1407 | -75 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 5 | -99 | -1899 | -4019 | -1899 | -99 | 5 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -75 | -1407 | -4893 | -3480 | -77 | 21 | -2 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -54 | -1357 | -7344 | -7056 | 365 | 65 | -20 | 4 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -36 | -1275 | -10088 | -12714 | 2557 | 0 | -128 | 49 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -17 | -886 | -10099 | -16705 | 8373 | -1208 | -506 | 473 | 28 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | -380 | -6236 | -13446 | 14799 | -5579 | -778 | 2882 | 218 | 2 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -93 | -2153 | -5860 | 13502 | -10625 | 978 | 9579 | 962 | 16 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -13 | -410 | -1309 | 6248 | -9419 | 4109 | 16194 | 2180 | 48 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -46 | -150 | 1510 | -4153 | 4166 | 13907 | 2486 | 73 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -8 | 204 | -973 | 1876 | 6274 | 1462 | 56 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 16 | -130 | 438 | 1553 | 460 | 22 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -10 | 59 | 224 | 82 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 20 | 8 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

8
2423.647

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

```
     0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
     0      0      0      0     -1      0      0      0      0      0      0      0      0      0      0      0      0      0      0
     0      0      0     -9    -21     -5      0      0      0      0      0      0      0      0      0      0      0      0      0
     0      0     -5    -85   -231    -59     11     -1      0      0      0      0      0      0      0      0      0      0      0
     0      0    -23   -479  -1598   -435    133    -16      0      0      0      0      0      0      0      0      0      0      0
     0      0    -58  -1520  -6452  -1846    983   -211     10      3      0      0      0      0      0      0      0      0      0
     0      0    -76  -2583-14287  -4022   4163  -1548    171     46      1      0      0      0      0      0      0      0      0
     0      0    -50  -2263-16616  -3787   9344  -6347   1441    409     12      0      0      0      0      0      0      0      0
     0      0    -16   -998  -9816   -633  10385-13591   6301   2127     82      0      0      0      0      0      0      0      0
     0      0     -2   -226  -2949    959   5308-14736  14196   6068    322      3      0      0      0      0      0      0      0
     0      0      0    -29   -483    556   1063  -8216  17325   9594    697      8      0      0      0      0      0      0      0
     0      0      0     -2    -50    136    -44  -2449  12882   9141    856      9      0      0      0      0      0      0      0
     0      0      0      0     -4     21    -74   -330   6834   5893    585     -1      0      0      0      0      0      0      0
     0      0      0      0      0      2    -22     71   2965   2610    -27    -30      0      0      0      0      0      0      0
     0      0      0      0      0      0     -5     71   1032      0  -1032    -71      5      0      0      0      0      0      0
     0      0      0      0      0      0      0     30     27  -2610  -2965    -71     22     -2      0      0      0      0      0
     0      0      0      0      0      0      0      1   -585  -5893  -6834    330     74    -21      4      0      0      0      0
     0      0      0      0      0      0      0     -9   -856  -9141-12882   2449     44   -136     50      2      0      0      0
     0      0      0      0      0      0      0     -8   -697  -9594-17325   8216  -1063   -556    483     29      0      0      0
     0      0      0      0      0      0      0     -3   -322  -6068-14196  14736  -5308   -959   2949    226      2      0      0
     0      0      0      0      0      0      0      0    -82  -2127  -6301  13591-10385    633   9816    998     16      0      0
     0      0      0      0      0      0      0      0    -12   -409  -1441   6347  -9344   3787  16616   2263     50      0      0
     0      0      0      0      0      0      0      0     -1    -46   -171   1548  -4163   4022  14287   2583     76      0      0
     0      0      0      0      0      0      0      0      0     -3    -10    211   -983   1846   6452   1520     58      0      0
     0      0      0      0      0      0      0      0      0      0      0     16   -133    435   1598    479     23      0      0
     0      0      0      0      0      0      0      0      0      0      0      1    -11     59    231     85      5      0      0
     0      0      0      0      0      0      0      0      0      0      0      0      0      5     21      9      0      0      0
     0      0      0      0      0      0      0      0      0      0      0      0      0      0      1      0      0      0      0
     0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
     0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
     0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
     0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0
     0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0      0


 SELEST: lowest four energy levels in cm^-1
         at Y2 = 1 (JZ = NDZ+1)
      1355.84      1355.84      1713.03      1713.15
         0.00         0.00       357.20       357.31

reference at J = 19  VZ(J,1) =   1355.84 cm^-1

 effective potentials for A-type dimer stretching
   JZ   VZ1/cm^-1   VZ2/cm^-1  splitting / MHz
  -18    10010.86    10586.12    17245806.98
  -17     8128.87     8726.51    17916634.96
  -16     6559.46     7171.17    18338522.86
  -15     5281.35     5900.45    18559940.44
  -14     4257.27     4876.60    18566865.66
  -13     3445.78     4052.39    18185661.62
  -12     2806.99     3366.54    16774984.22
  -11     2304.53     2757.69    13585240.83
  -10     1905.36     2223.27     9530726.56
   -9     1578.04     1768.37     5705905.68
   -8     1291.28     1382.55     2736376.75
   -7     1020.46     1053.78      999062.80
   -6      764.24      774.01      292822.26
   -5      537.23      539.79       76806.16
   -4      349.45      350.10       19513.01
   -3      203.74      203.90        5037.28
```

| | | | |
|---|---|---|---|
| -2 | 99.03 | 99.07 | 1361.17 |
| -1 | 32.39 | 32.40 | 391.98 |
| 0 | 0.00 | 0.00 | 121.47 |
| 1 | -2.33 | -2.33 | 40.66 |
| 2 | 21.18 | 21.18 | 14.71 |
| 3 | 66.48 | 66.48 | 5.73 |
| 4 | 129.81 | 129.81 | 2.40 |
| 5 | 207.72 | 207.72 | 1.07 |
| 6 | 297.16 | 297.16 | 0.51 |
| 7 | 395.44 | 395.44 | 0.25 |
| 8 | 500.22 | 500.22 | 0.13 |
| 9 | 609.50 | 609.50 | 0.07 |
| 10 | 721.60 | 721.60 | 0.04 |
| 11 | 835.10 | 835.10 | 0.02 |
| 12 | 948.86 | 948.86 | 0.01 |
| 13 | 1061.95 | 1061.95 | 0.01 |
| 14 | 1173.62 | 1173.62 | 0.01 |
| 15 | 1283.30 | 1283.30 | 0.00 |
| 16 | 1390.56 | 1390.56 | 0.00 |
| 17 | 1495.07 | 1495.07 | 0.00 |
| 18 | 1596.59 | 1596.59 | 0.00 |

FMZ1D: y2 motion
energy profiles for ground state doublet,
pseudopotential, and mobility coefficient

| JZ | VZ(1) | VZ(2) | VPS | G44 (MHZ) |
|---|---|---|---|---|
| -18 | 300118713.22 | 317364520.20 | 569.84 | 312664.95 |
| -17 | 243698030.45 | 261614665.41 | 549.51 | 312677.84 |
| -16 | 196648240.17 | 214986763.02 | 527.86 | 312690.71 |
| -15 | 158331559.79 | 176891500.23 | 506.49 | 312703.58 |
| -14 | 127630315.14 | 146197180.80 | 486.57 | 312716.44 |
| -13 | 103302321.19 | 121487982.81 | 467.47 | 312729.30 |
| -12 | 84151766.16 | 100926750.38 | 449.28 | 312742.14 |
| -11 | 69088564.70 | 82673805.53 | 431.93 | 312754.97 |
| -10 | 57121687.99 | 66652414.55 | 415.37 | 312767.78 |
| -9 | 47308995.77 | 53014901.45 | 399.57 | 312780.59 |
| -8 | 38711936.79 | 41448313.54 | 384.49 | 312793.39 |
| -7 | 30592965.38 | 31592028.18 | 370.09 | 312806.17 |
| -6 | 22911788.07 | 23204610.34 | 356.34 | 312818.95 |
| -5 | 16105947.45 | 16182753.61 | 343.20 | 312831.71 |
| -4 | 10476505.21 | 10496018.22 | 330.64 | 312844.46 |
| -3 | 6108186.66 | 6113223.94 | 318.63 | 312857.20 |
| -2 | 2969109.99 | 2970471.16 | 307.16 | 312869.93 |
| -1 | 971374.30 | 971766.28 | 296.18 | 312882.65 |
| 0 | 285.68 | 407.15 | 285.68 | 312895.36 |
| 1 | -69602.52 | -69561.86 | 275.63 | 312908.05 |
| 2 | 635260.88 | 635275.59 | 266.02 | 312920.74 |
| 3 | 1993392.75 | 1993398.48 | 256.82 | 312933.41 |
| 4 | 3891745.01 | 3891747.41 | 248.00 | 312946.07 |
| 5 | 6227523.95 | 6227525.02 | 239.56 | 312958.72 |
| 6 | 8908938.62 | 8908939.12 | 231.47 | 312971.36 |
| 7 | 11855266.17 | 11855266.43 | 223.73 | 312983.99 |
| 8 | 14996490.55 | 14996490.68 | 216.30 | 312996.61 |
| 9 | 18272683.24 | 18272683.31 | 209.18 | 313009.21 |
| 10 | 21633234.46 | 21633234.51 | 202.35 | 313021.80 |
| 11 | 25036002.00 | 25036002.02 | 195.80 | 313034.39 |
| 12 | 28446418.98 | 28446419.00 | 189.52 | 313046.96 |
| 13 | 31836588.28 | 31836588.29 | 183.48 | 313059.52 |
| 14 | 35184386.37 | 35184386.38 | 177.71 | 313072.07 |

| | | | | |
|---|---|---|---|---|
| 15 | 38472599.05 | 38472599.05 | 172.07 | 313084.60 |
| 16 | 41688112.73 | 41688112.73 | 166.76 | 313097.13 |
| 17 | 44821180.17 | 44821180.17 | 161.73 | 313109.66 |
| 18 | 47864777.04 | 47864777.04 | 156.60 | 313122.17 |

potential profiles, energy levels 1 & 2 (cm^-1)
and wavefunctions

| Y2 | V0s | Es1 | Es2 | V0a-V0s | Ea1 | Ea2 |
|---|---|---|---|---|---|---|
| | | 66.70 | 207.40 | | 66.71 | 207.44 |
| | | 0.00 | 140.71 | | 0.00 | 140.74 |
| -2.000 | 10010.88 | 0 | 0 | 575.26 | 0 | 0 |
| -1.833 | 8128.89 | 0 | 0 | 597.63 | 0 | 0 |
| -1.667 | 6559.48 | 0 | 0 | 611.71 | 0 | 0 |
| -1.500 | 5281.37 | 0 | 0 | 619.09 | 0 | 0 |
| -1.333 | 4257.29 | 0 | 0 | 619.32 | 0 | 0 |
| -1.167 | 3445.79 | 0 | 0 | 606.61 | 0 | 0 |
| -1.000 | 2807.00 | 0 | 0 | 559.55 | 0 | 0 |
| -0.833 | 2304.55 | 0 | -1 | 453.15 | 0 | 0 |
| -0.667 | 1905.37 | 2 | -14 | 317.91 | 1 | -9 |
| -0.500 | 1578.06 | 23 | -115 | 190.33 | 19 | -93 |
| -0.333 | 1291.29 | 165 | -744 | 91.28 | 151 | -673 |
| -0.167 | 1020.47 | 962 | -3888 | 33.33 | 927 | -3729 |
| 0.000 | 764.25 | 4536 | -16257 | 9.77 | 4475 | -15998 |
| 0.167 | 537.24 | 17145 | -53428 | 2.56 | 17061 | -53096 |
| 0.333 | 349.46 | 51653 | -136083 | 0.65 | 51556 | -135744 |
| 0.500 | 203.75 | 124154 | -265125 | 0.17 | 124060 | -264869 |
| 0.667 | 99.04 | 239255 | -386571 | 0.05 | 239180 | -386482 |
| 0.833 | 32.40 | 372290 | -399321 | 0.01 | 372249 | -399423 |
| 1.000 | 0.01 | 471720 | -237473 | 0.00 | 471718 | -237690 |
| 1.167 | -2.32 | 491208 | 46406 | 0.00 | 491237 | 46210 |
| 1.333 | 21.19 | 424417 | 307170 | 0.00 | 424461 | 307093 |
| 1.500 | 66.49 | 307253 | 426198 | 0.00 | 307294 | 426246 |
| 1.667 | 129.81 | 188184 | 392819 | 0.00 | 188213 | 392932 |
| 1.833 | 207.73 | 98442 | 278352 | 0.00 | 98459 | 278464 |
| 2.000 | 297.17 | 44391 | 160284 | 0.00 | 44400 | 160362 |
| 2.167 | 395.45 | 17410 | 77302 | 0.00 | 17414 | 77345 |
| 2.333 | 500.23 | 5989 | 31858 | 0.00 | 5991 | 31878 |
| 2.500 | 609.51 | 1822 | 11391 | 0.00 | 1822 | 11399 |
| 2.667 | 721.61 | 494 | 3577 | 0.00 | 494 | 3579 |
| 2.833 | 835.11 | 120 | 996 | 0.00 | 120 | 997 |
| 3.000 | 948.87 | 26 | 248 | 0.00 | 26 | 249 |
| 3.167 | 1061.95 | 5 | 56 | 0.00 | 5 | 56 |
| 3.333 | 1173.62 | 0 | 11 | 0.00 | 0 | 11 |
| 3.500 | 1283.31 | 0 | 2 | 0.00 | 0 | 2 |
| 3.667 | 1390.57 | 0 | 0 | 0.00 | 0 | 0 |
| 3.833 | 1495.07 | 0 | 0 | 0.00 | 0 | 0 |
| 4.000 | 1596.60 | 0 | 0 | 0.00 | 0 | 0 |

ground state tunnel splitting = 331.27 MHz

Standard configuration as read from input

```
*******************************************************************************
  ----- formic acid dimer, March 2017 -------- (x, y1, y2) = (0,0,0)
*******************************************************************************
NA = 12
   1    0    0    0   0.00000     0.000     0.000           0.0000000
   2    1    0    0   1.00000     0.000     0.000           0.0000000
   3    1    2    0   1.77575    90.000     0.000          12.0000000
   4    1    2    3   1.77575    90.000   180.000          12.0000000
```

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 5 | 3 | 1 | 2 | 1.26120 | 63.300 | 0.000 | 15.9949150 |
| 6 | 3 | 1 | 2 | 1.26120 | 63.300 | 180.000 | 15.9949150 |
| 7 | 4 | 1 | 2 | 1.26120 | 63.300 | 0.000 | 15.9949150 |
| 8 | 4 | 1 | 2 | 1.26120 | 63.300 | 180.000 | 15.9949150 |
| 9 | 3 | 5 | 1 | 1.09520 | 116.700 | 180.000 | 1.0078250 |
| 10 | 4 | 7 | 1 | 1.09520 | 116.700 | 180.000 | 2.0141018 |
| 11 | 1 | 4 | 2 | 1.11610 | 90.000 | 0.000 | 2.0141018 |
| 12 | 1 | 4 | 2 | 1.11610 | 90.000 | 180.000 | 2.0141018 |

----------- grid properties -----------

| NDX | NDY | NDZ | DRX | DRY | DRZ | NV |
|---|---|---|---|---|---|---|
| 18 | 18 | 18 | 0.167 | 0.167 | 0.167 | 16 |

mobility constants (MHz)

| GXXE | GXYE | GYYE |
|---|---|---|
| 719000. | -13000. | 597000. |

X=Y=0

```
GXX     719391.798  MHZ
GXY     -13709.039
GYY     599408.156
G   0.37745265E+07  (AMU*A**2)**5
```

TABLES: GXX, GXY, GYY (GHZ),  G/G(0,0), VG (GHZ)

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 718 | 718 | 718 | 718 | 718 | 718 | 719 | 719 | 719 | 719 | 719 | 719 | 719 | 718 | 718 | 718 | 718 | 718 | 718 |
| 718 | 718 | 718 | 718 | 718 | 718 | 719 | 719 | 719 | 719 | 719 | 719 | 719 | 718 | 718 | 718 | 718 | 718 | 718 |
| 718 | 718 | 718 | 718 | 718 | 719 | 719 | 719 | 719 | 719 | 719 | 719 | 719 | 719 | 718 | 718 | 718 | 718 | 718 |
| 718 | 718 | 718 | 718 | 718 | 719 | 719 | 719 | 719 | 719 | 719 | 719 | 719 | 719 | 718 | 718 | 718 | 718 | 718 |
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| 10917 | 10773 | 10643 | 10525 | 10423 | 10336 | 10264 | 10208 | 10169 | 10146 | 10140 | 10149 | 10175 | 10216 | 10272 | 10343 | 10428 | 10525 | 10634 |
| 10964 | 10818 | 10685 | 10566 | 10462 | 10373 | 10300 | 10242 | 10202 | 10177 | 10169 | 10177 | 10202 | 10241 | 10296 | 10366 | 10449 | 10545 | 10652 |
| 11014 | 10866 | 10731 | 10610 | 10504 | 10413 | 10338 | 10279 | 10237 | 10211 | 10201 | 10208 | 10231 | 10270 | 10323 | 10391 | 10473 | 10567 | 10674 |
| 11068 | 10917 | 10780 | 10657 | 10549 | 10457 | 10380 | 10319 | 10275 | 10248 | 10237 | 10242 | 10264 | 10301 | 10353 | 10420 | 10500 | 10593 | 10698 |
| 11124 | 10972 | 10833 | 10708 | 10598 | 10503 | 10425 | 10363 | 10317 | 10288 | 10275 | 10279 | 10299 | 10335 | 10386 | 10451 | 10530 | 10622 | 10725 |
| 11184 | 11029 | 10888 | 10761 | 10649 | 10553 | 10473 | 10409 | 10362 | 10331 | 10317 | 10319 | 10338 | 10372 | 10422 | 10486 | 10563 | 10654 | 10756 |
| 11247 | 11090 | 10947 | 10818 | 10704 | 10606 | 10524 | 10458 | 10409 | 10377 | 10362 | 10363 | 10380 | 10413 | 10461 | 10523 | 10600 | 10689 | 10790 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 11314 | 11154 | 11009 | 10878 | 10762 | 10662 | 10578 | 10510 | 10460 | 10426 | 10409 | 10409 | 10425 | 10456 | 10503 | 10564 | 10639 | 10727 | 10827 |
| 11384 | 11222 | 11074 | 10941 | 10823 | 10721 | 10635 | 10566 | 10514 | 10478 | 10460 | 10458 | 10472 | 10503 | 10548 | 10608 | 10682 | 10769 | 10867 |

pseudopotential function in GHz

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |

pseudopotential + potential energy (cm^-1)

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23835 | 23819 | 23819 | 23836 | 23865 | 23900 | 23932 | 23958 | 23977 | 23988 | 23994 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 | 23999 | 24000 |
| 23486 | 23431 | 23427 | 23477 | 23567 | 23674 | 23778 | 23863 | 23923 | 23961 | 23982 | 23992 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 | 23999 |
| 22710 | 22560 | 22538 | 22650 | 22868 | 23138 | 23405 | 23628 | 23789 | 23892 | 23949 | 23978 | 23991 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 |
| 21323 | 20987 | 20908 | 21105 | 21530 | 22084 | 22652 | 23142 | 23506 | 23743 | 23879 | 23948 | 23980 | 23993 | 23997 | 23999 | 23999 | 23999 | 23999 |
| 19288 | 18654 | 18446 | 18711 | 19389 | 20334 | 21354 | 22273 | 22983 | 23460 | 23741 | 23887 | 23955 | 23984 | 23994 | 23998 | 23999 | 23999 | 23999 |
| 16802 | 15764 | 15329 | 15579 | 16467 | 17824 | 19391 | 20891 | 22112 | 22969 | 23493 | 23775 | 23910 | 23967 | 23989 | 23996 | 23999 | 23999 | 23999 |
| 14236 | 12718 | 11949 | 12047 | 12997 | 14653 | 16738 | 18890 | 20767 | 22168 | 23069 | 23575 | 23825 | 23934 | 23978 | 23993 | 23998 | 23999 | 23999 |
| 12020 | 9968 | 8761 | 8545 | 9344 | 11065 | 13480 | 16214 | 18815 | 20915 | 22363 | 23222 | 23668 | 23872 | 23955 | 23986 | 23996 | 23998 | 23999 |
| 10548 | 7924 | 6180 | 5489 | 5906 | 7399 | 9829 | 12897 | 16134 | 19021 | 21199 | 22598 | 23373 | 23747 | 23908 | 23969 | 23991 | 23997 | 23999 |
| 10176 | 6953 | 4574 | 3258 | 3085 | 4063 | 6139 | 9145 | 12716 | 16300 | 19333 | 21496 | 22806 | 23491 | 23805 | 23932 | 23978 | 23993 | 23998 |
| 11251 | 7473 | 4380 | 2299 | 1357 | 1584 | 2975 | 5473 | 8884 | 12789 | 16568 | 19643 | 21743 | 22962 | 23573 | 23841 | 23947 | 23983 | 23995 |
| 13719 | 9620 | 5840 | 2890 | 1024 | 321 | 794 | 2434 | 5184 | 8833 | 12921 | 16790 | 19860 | 21902 | 23056 | 23619 | 23862 | 23954 | 23986 |
| 16978 | 13101 | 8954 | 5207 | 2344 | 588 | 0 | 588 | 2344 | 5207 | 8954 | 13101 | 16978 | 20011 | 22000 | 23109 | 23645 | 23872 | 23958 |

```
19937 16894 13035  8937  5259  2470   788   274   936  2761  5678  9439 13546 17328 20245 22134 23175 23673 23883
21834 19774 16719 12913  8936  5421  2808  1301   959  1789  3770  6796 10571 14558 18107 20754 22418 23313 23732
22764 21388 19104 15889 12091  8311  5130  2913  1817  1886  3117  5458  8733 12548 16307 19423 21593 22876 23531
23147 22115 20289 17532 14021 10260  6857  4272  2747  2368  3150  5060  7968 11559 15302 18594 21029 22552 23370
23277 22372 20732 18186 14843 11150  7703  4997  3312  2759  3363  5097  7843 11313 15003 18318 20824 22426 23304
23298 22417 20813 18311 15009 11340  7898  5180  3474  2897  3474  5180  7898 11340 15009 18311 20813 22417 23298
23304 22426 20824 18318 15003 11313  7843  5097  3363  2759  3312  4997  7703 11150 14843 18186 20732 22372 23277
23370 22552 21029 18594 15302 11559  7968  5060  3150  2368  2747  4272  6857 10260 14021 17532 20289 22115 23147
23531 22876 21593 19423 16307 12548  8733  5458  3117  1886  1817  2913  5130  8311 12091 15889 19104 21388 22764
23732 23313 22418 20754 18107 14558 10571  6796  3770  1789   959  1301  2808  5421  8936 12913 16719 19774 21834
23883 23673 23175 22134 20245 17328 13546  9439  5678  2761   936   274   788  2470  5259  8937 13035 16894 19937
23958 23872 23645 23109 22000 20011 16978 13101  8954  5207  2344   588     0   588  2344  5207  8954 13101 16978
23986 23954 23862 23619 23056 21902 19860 16790 12921  8833  5184  2434   794   321  1024  2890  5840  9620 13719
23995 23983 23947 23841 23573 22962 21743 19643 16568 12789  8884  5473  2975  1584  1357  2299  4380  7473 11251
23998 23993 23978 23932 23805 23491 22806 21496 19333 16300 12716  9145  6139  4063  3085  3258  4574  6953 10176
23999 23997 23991 23969 23908 23747 23373 22598 21199 19021 16134 12897  9829  7399  5906  5489  6180  7924 10548
23999 23998 23996 23986 23955 23872 23668 23222 22363 20915 18815 16214 13480 11065  9344  8545  8761  9968 12020
23999 23999 23998 23993 23978 23934 23825 23575 23069 22168 20767 18890 16738 14653 12997 12047 11949 12718 14236
23999 23999 23999 23996 23989 23967 23910 23775 23493 22969 22112 20891 19391 17824 16467 15579 15329 15764 16802
23999 23999 23999 23998 23994 23984 23955 23887 23741 23460 22983 22273 21354 20334 19389 18711 18446 18654 19288
23999 23999 23999 23999 23997 23993 23980 23948 23879 23743 23506 23142 22652 22084 21530 21105 20908 20987 21323
23999 23999 23999 23999 23999 23997 23991 23978 23949 23892 23789 23628 23405 23138 22868 22650 22538 22560 22710
23999 23999 23999 23999 23999 23999 23997 23992 23982 23961 23923 23863 23778 23674 23567 23477 23427 23431 23486
24000 23999 23999 23999 23999 23999 23999 23997 23994 23988 23977 23958 23932 23900 23865 23836 23819 23819 23835


Emax / cm^-1 =    38363.134216178216


                     energy levels (MHz)

  iteration cycle           11
 31384411.30  31384413.45  42048610.05  42048695.57  52630906.79  52632393.32
   63159733.28  63174993.86  73555294.06  73656762.50  81560899.87  81563469.88
 83676855.77  84147624.45  90433554.80  90497814.45

Tunnel splitting, E0(2)-E0(1) =         2.15 MHz

  iteration cycle           12
 31384411.30  31384413.45  42048610.05  42048695.57  52630906.79  52632393.32
   63159733.28  63174993.86  73555294.06  73656762.50  81560899.87  81563469.88
 83676855.77  84147624.45  90433554.80  90497814.45

Tunnel splitting, E0(2)-E0(1) =         2.15 MHz

  iteration cycle           13
 31384411.30  31384413.45  42048610.05  42048695.57  52630906.79  52632393.32
   63159733.28  63174993.86  73555294.06  73656762.50  81560899.87  81563469.88
 83676855.77  84147624.45  90433554.80  90497814.45

Tunnel splitting, E0(2)-E0(1) =         2.15 MHz



   energy levels (cm^-1) and wavefunctions:
          1
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    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
```

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 2 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 6 | 49 | 80 | 27 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 41 | 427 | 974 | 519 | 69 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 104 | 1598 | 5571 | 4534 | 889 | 45 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 104 | 2458 | 13447 | 17528 | 5594 | 448 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 40 | 1478 | 13095 | 28090 | 14870 | 1990 | 68 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 6 | 351 | 5071 | 18109 | 16242 | 3700 | 215 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 36 | 839 | 5049 | 7676 | 2966 | 291 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 2 | 76 | 720 | 1826 | 1185 | 191 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 2 | 66 | 282 | 291 | 74 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | 6 | 32 | 55 | 22 | 3 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 10 | 9 | 10 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 3 | 22 | 55 | 32 | 6 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 74 | 291 | 282 | 66 | 2 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 | 191 | 1185 | 1826 | 720 | 76 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 | 291 | 2966 | 7676 | 5049 | 839 | 36 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 215 | 3700 | 16242 | 18109 | 5071 | 351 | 6 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 68 | 1990 | 14870 | 28090 | 13095 | 1478 | 40 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | 448 | 5594 | 17528 | 13447 | 2458 | 104 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 45 | 889 | 4534 | 5571 | 1598 | 104 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 69 | 519 | 974 | 427 | 41 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 27 | 80 | 49 | 6 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 2 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 6 | 49 | 80 | 27 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 41 | 427 | 974 | 519 | 69 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 104 | 1598 | 5571 | 4534 | 889 | 45 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 104 | 2458 | 13447 | 17528 | 5594 | 448 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 40 | 1478 | 13095 | 28090 | 14870 | 1990 | 68 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 6 | 351 | 5071 | 18109 | 16242 | 3700 | 215 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 36 | 839 | 5049 | 7676 | 2966 | 291 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 2 | 76 | 720 | 1826 | 1185 | 191 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 2 | 66 | 282 | 291 | 74 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | 6 | 32 | 54 | 19 | 0 | 0 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 9 | 0 | -9 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | -19 | -54 | -32 | -6 | -1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -4 | -74 | -291 | -282 | -66 | -2 | 0 | 0 | 0 | 0 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -7 | -191 | -1185 | -1826 | -720 | -76 | -2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -7 | -291 | -2966 | -7676 | -5049 | -839 | -36 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -215 | -3700 | -16242 | -18109 | -5071 | -351 | -6 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -68 | -1990 | -14870 | -28090 | -13095 | -1478 | -40 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -9 | -448 | -5594 | -17528 | -13448 | -2458 | -104 | -1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -45 | -889 | -4534 | -5571 | -1598 | -104 | -1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -69 | -519 | -974 | -427 | -41 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -27 | -80 | -49 | -6 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -1 | -2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 2 | 9 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 30 | 165 | 176 | 30 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 4 | 177 | 1352 | 1962 | 405 | -36 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 7 | 428 | 4780 | 10138 | 2627 | -656 | -96 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 410 | 6925 | 21897 | 6410 | -5439 | -1071 | -36 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 151 | 3902 | 18739 | 4262 | -17931 | -5264 | -286 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 21 | 862 | 6240 | -1287 | -23597 | -10771 | -955 | -19 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 82 | 847 | -1582 | -13174 | -9487 | -1383 | -45 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 3 | 60 | -415 | -3687 | -4181 | -978 | -51 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -64 | -666 | -1140 | -411 | -34 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | -5 | -92 | -243 | -134 | -23 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -2 | -16 | -52 | -66 | -52 | -16 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -23 | -134 | -243 | -92 | -5 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -34 | -411 | -1140 | -666 | -64 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -51 | -978 | -4181 | -3687 | -415 | 60 | 3 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -45 | -1383 | -9487 | -13174 | -1582 | 847 | 82 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -19 | -955 | -10771 | -23597 | -1287 | 6240 | 862 | 21 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -286 | -5264 | -17931 | 4262 | 18739 | 3902 | 151 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -36 | -1071 | -5439 | 6410 | 21897 | 6925 | 410 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -96 | -656 | 2627 | 10138 | 4780 | 428 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -36 | 405 | 1962 | 1352 | 177 | 4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 30 | 176 | 165 | 30 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 9 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -2 | -9 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -30 | -165 | -176 | -30 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -4 | -177 | -1352 | -1962 | -405 | 36 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -7 | -428 | -4780 | -10139 | -2627 | 656 | 96 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -410 | -6926 | -21897 | -6410 | 5439 | 1071 | 36 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -151 | -3902 | -18739 | -4262 | 17932 | 5264 | 286 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -21 | -862 | -6240 | 1287 | 23598 | 10770 | 955 | 19 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -1 | -82 | -847 | 1582 | 13175 | 9486 | 1382 | 45 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -3 | -60 | 415 | 3687 | 4180 | 976 | 50 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 64 | 666 | 1139 | 406 | 29 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -1 | 5 | 92 | 240 | 116 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 2 | 16 | 42 | 0 | -42 | -16 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -116 | -240 | -92 | -5 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -29 | -406 | -1139 | -666 | -64 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -50 | -976 | -4180 | -3687 | -415 | 60 | 3 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -45 | -1382 | -9486 | -13175 | -1582 | 847 | 82 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -19 | -955 | -10770 | -23598 | -1287 | 6240 | 862 | 21 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -286 | -5264 | -17932 | 4262 | 18739 | 3902 | 151 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -36 | -1071 | -5439 | 6410 | 21897 | 6926 | 410 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -96 | -656 | 2627 | 10139 | 4780 | 428 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -36 | 405 | 1962 | 1352 | 177 | 4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 30 | 176 | 165 | 30 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 9 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 7 | 23 | 9 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 4 | 94 | 375 | 238 | 5 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 17 | 524 | 2888 | 2357 | -89 | -43 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 28 | 1215 | 9573 | 10452 | -1783 | -397 | 98 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 17 | 1118 | 12941 | 18712 | -9808 | -1096 | 1300 | 86 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 4 | 394 | 6751 | 12376 | -18619 | 2001 | 7520 | 736 | 13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 53 | 1364 | 2781 | -12629 | 9235 | 17689 | 2660 | 76 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 3 | 117 | 151 | -3311 | 8665 | 17755 | 4170 | 190 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 4 | -8 | -362 | 3472 | 8903 | 3206 | 227 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | -2 | -11 | 831 | 2774 | 1480 | 159 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 156 | 687 | 539 | 106 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 30 | 179 | 292 | 179 | 30 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 106 | 539 | 687 | 156 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 159 | 1480 | 2774 | 831 | -11 | -2 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 227 | 3206 | 8903 | 3472 | -362 | -8 | 4 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 190 | 4170 | 17755 | 8665 | -3311 | 151 | 117 | 3 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 76 | 2660 | 17689 | 9235 | -12629 | 2781 | 1364 | 53 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 13 | 736 | 7520 | 2001 | -18619 | 12376 | 6751 | 394 | 4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 86 | 1300 | -1096 | -9808 | 18712 | 12941 | 1118 | 17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 98 | -397 | -1783 | 10452 | 9573 | 1215 | 28 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -43 | -89 | 2357 | 2888 | 524 | 17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 5 | 238 | 375 | 94 | 4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 9 | 23 | 7 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 7 | 23 | 9 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 4 | 94 | 375 | 238 | 5 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 17 | 524 | 2889 | 2358 | -89 | -43 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 28 | 1216 | 9576 | 10454 | -1784 | -397 | 98 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 17 | 1119 | 12944 | 18714 | -9811 | -1095 | 1301 | 86 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 4 | 394 | 6753 | 12376 | -18623 | 2005 | 7521 | 736 | 13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 53 | 1364 | 2780 | -12631 | 9241 | 17689 | 2658 | 76 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 3 | 117 | 151 | -3311 | 8668 | 17752 | 4164 | 188 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 4 | -8 | -362 | 3472 | 8896 | 3190 | 220 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | -2 | -11 | 830 | 2764 | 1448 | 139 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 155 | 667 | 449 | 30 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 28 | 128 | 0 | -128 | -28 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | -30 | -449 | -667 | -155 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -139 | -1448 | -2764 | -830 | 11 | 2 | -1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -220 | -3190 | -8896 | -3472 | 362 | 8 | -4 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -188 | -4164 | -17752 | -8668 | 3311 | -151 | -117 | -3 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -76 | -2658 | -17689 | -9241 | 12631 | -2780 | -1364 | -53 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -13 | -736 | -7521 | -2005 | 18623 | -12376 | -6753 | -394 | -4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -86 | -1301 | 1095 | 9811 | -18714 | -12944 | -1119 | -17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | -98 | 397 | 1784 | -10454 | -9576 | -1216 | -28 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 43 | 89 | -2358 | -2889 | -524 | -17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 0 | -5 | -238 | -375 | -94 | -4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -9 | -23 | -7 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 1 | 20 | 43 | 11 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 13 | 230 | 656 | 204 | -22 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 52 | 1235 | 4731 | 1626 | -389 | 35 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 82 | 2747 | 14526 | 4939 | -3140 | 627 | -13 | -7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 50 | 2416 | 18027 | 3891 | -9499 | 4892 | -531 | -137 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 11 | 811 | 8521 | -2155 | -9421 | 13835 | -5038 | -1305 | -36 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 105 | 1524 | -2403 | -1494 | 13619 | -16040 | -5231 | -225 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 6 | 114 | -548 | 1012 | 3965 | -20363 | -9080 | -598 | -7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 2 | -54 | 337 | -385 | -12508 | -7744 | -769 | -15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 0 | 49 | -459 | -4728 | -4011 | -583 | -16 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | -1 | 0 | -163 | -1440 | -1677 | -389 | -22 | -1 | -1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | 1 | -45 | -498 | -1015 | -498 | -45 | 1 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -1 | -1 | -22 | -389 | -1677 | -1440 | -163 | 0 | -1 | -1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | -16 | -583 | -4011 | -4728 | -459 | 49 | 0 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -15 | -769 | -7744 | -12508 | -385 | 337 | -54 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -7 | -598 | -9080 | -20363 | 3965 | 1012 | -548 | 114 | 6 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -225 | -5231 | -16040 | 13619 | -1494 | -2403 | 1524 | 105 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -36 | -1305 | -5038 | 13835 | -9421 | -2155 | 8521 | 811 | 11 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -137 | -531 | 4892 | -9499 | 3891 | 18027 | 2416 | 50 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -7 | -13 | 627 | -3140 | 4939 | 14526 | 2747 | 82 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 35 | -389 | 1626 | 4731 | 1235 | 52 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -22 | 204 | 656 | 230 | 13 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 11 | 43 | 20 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

8
2107.291

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 20 | 43 | 11 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 13 | 231 | 658 | 204 | -22 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 52 | 1239 | 4741 | 1627 | -389 | 35 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 83 | 2754 | 14555 | 4935 | -3144 | 628 | -14 | -7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 50 | 2423 | 18060 | 3871 | -9500 | 4900 | -536 | -137 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 11 | 813 | 8535 | -2180 | -9403 | 13842 | -5063 | -1305 | -37 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 105 | 1526 | -2413 | -1472 | 13607 | -16089 | -5224 | -222 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 6 | 114 | -549 | 1020 | 3947 | -20392 | -9045 | -588 | -7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 2 | -54 | 338 | -391 | -12492 | -7659 | -735 | -12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 0 | 50 | -458 | -4679 | -3850 | -502 | -11 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | -1 | 0 | -159 | -1342 | -1310 | -152 | 4 | 1 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | 1 | -36 | -271 | 0 | 271 | 36 | -1 | -1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -1 | -1 | -4 | 152 | 1310 | 1342 | 159 | 0 | 1 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 11 | 502 | 3850 | 4679 | 458 | -50 | 0 | -1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 12 | 735 | 7659 | 12492 | 391 | -338 | 54 | -2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 | 588 | 9045 | 20392 | -3947 | -1020 | 549 | -114 | -6 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 222 | 5224 | 16089 | -13607 | 1472 | 2413 | -1526 | -105 | -1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 37 | 1305 | 5063 | -13842 | 9403 | 2180 | -8535 | -813 | -11 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 137 | 536 | -4900 | 9500 | -3871 | -18060 | -2423 | -50 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 | 14 | -628 | 3144 | -4935 | -14555 | -2754 | -83 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -35 | 389 | -1627 | -4741 | -1239 | -52 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 22 | -204 | -658 | -231 | -13 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 0 | -11 | -43 | -20 | -1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

```
 SELEST: lowest four energy levels in cm^-1
         at Y2 = 1 (JZ = NDZ+1)
      1046.87     1046.87     1402.59     1402.59
         0.00        0.00      355.72      355.72

reference at J = 19  VZ(J,1) =   1046.87 cm^-1
```

effective potentials for A-type dimer stretching

| JZ | VZ1/cm^-1 | VZ2/cm^-1 | splitting / MHz |
|---|---|---|---|
| -18 | 10038.54 | 10616.01 | 17311989.43 |
| -17 | 8185.02 | 8784.34 | 17967326.63 |
| -16 | 6646.72 | 7259.69 | 18376215.69 |
| -15 | 5400.12 | 6019.40 | 18565663.47 |
| -14 | 4406.49 | 5018.77 | 18355559.44 |
| -13 | 3623.28 | 4171.45 | 16433773.98 |
| -12 | 3009.08 | 3427.41 | 12541304.84 |
| -11 | 2524.38 | 2805.73 | 8434512.69 |
| -10 | 2128.70 | 2285.17 | 4690605.93 |
| -9 | 1776.51 | 1839.69 | 1893963.17 |
| -8 | 1432.52 | 1449.76 | 516862.14 |
| -7 | 1102.49 | 1106.09 | 107724.95 |
| -6 | 807.27 | 807.94 | 19958.19 |
| -5 | 557.75 | 557.87 | 3624.36 |
| -4 | 357.12 | 357.14 | 684.90 |
| -3 | 204.46 | 204.46 | 139.29 |
| -2 | 96.79 | 96.79 | 31.13 |
| -1 | 30.14 | 30.14 | 7.74 |
| 0 | 0.00 | 0.00 | 2.15 |
| 1 | 1.63 | 1.63 | 0.67 |
| 2 | 30.38 | 30.38 | 0.23 |
| 3 | 81.87 | 81.87 | 0.09 |
| 4 | 152.12 | 152.12 | 0.04 |
| 5 | 237.51 | 237.51 | 0.02 |
| 6 | 334.87 | 334.87 | 0.01 |
| 7 | 441.39 | 441.39 | 0.00 |
| 8 | 554.64 | 554.64 | 0.00 |

| | | | |
|---|---|---|---|
| 9 | 672.56 | 672.56 | 0.00 |
| 10 | 793.38 | 793.38 | 0.00 |
| 11 | 915.65 | 915.65 | 0.00 |
| 12 | 1038.15 | 1038.15 | 0.00 |
| 13 | 1159.91 | 1159.91 | 0.00 |
| 14 | 1280.15 | 1280.15 | 0.00 |
| 15 | 1398.25 | 1398.25 | 0.00 |
| 16 | 1513.75 | 1513.75 | 0.00 |
| 17 | 1626.30 | 1626.30 | 0.00 |
| 18 | 1735.66 | 1735.66 | 0.00 |

FMZ1D: y2 motion
energy profiles for ground state doublet,
pseudopotential, and mobility coefficient

| JZ | VZ(1) | VZ(2) | VPS | G44 (MHZ) |
|---|---|---|---|---|
| -18 | 300948469.36 | 318260458.79 | 564.76 | 312664.09 |
| -17 | 245381199.67 | 263348526.30 | 544.91 | 312676.99 |
| -16 | 199264256.51 | 217640472.20 | 523.74 | 312689.85 |
| -15 | 161891996.99 | 180457660.45 | 502.82 | 312702.73 |
| -14 | 132103852.29 | 150459411.73 | 483.31 | 312715.59 |
| -13 | 108623778.75 | 125057552.73 | 464.59 | 312728.44 |
| -12 | 90210472.21 | 102751777.04 | 446.73 | 312741.28 |
| -11 | 75679550.77 | 84114063.46 | 429.69 | 312754.11 |
| -10 | 63817376.83 | 68507982.76 | 413.42 | 312766.93 |
| -9 | 53258980.54 | 55152943.71 | 397.88 | 312779.73 |
| -8 | 42946290.51 | 43463152.65 | 383.03 | 312792.53 |
| -7 | 33052303.39 | 33160028.34 | 368.84 | 312805.32 |
| -6 | 24201850.66 | 24221808.85 | 355.27 | 312818.09 |
| -5 | 16721227.32 | 16724851.69 | 342.30 | 312830.85 |
| -4 | 10706554.24 | 10707239.14 | 329.90 | 312843.60 |
| -3 | 6129868.90 | 6130008.19 | 318.03 | 312856.34 |
| -2 | 2901955.43 | 2901986.55 | 306.68 | 312869.07 |
| -1 | 903909.24 | 903916.98 | 295.82 | 312881.79 |
| 0 | 285.42 | 287.57 | 285.42 | 312894.50 |
| 1 | 49092.37 | 49093.04 | 275.46 | 312907.19 |
| 2 | 910887.21 | 910887.44 | 265.93 | 312919.88 |
| 3 | 2454666.26 | 2454666.35 | 256.79 | 312932.55 |
| 4 | 4560558.16 | 4560558.20 | 248.04 | 312945.21 |
| 5 | 7120712.56 | 7120712.58 | 239.66 | 312957.86 |
| 6 | 10039399.11 | 10039399.11 | 231.62 | 312970.50 |
| 7 | 13232708.16 | 13232708.16 | 223.91 | 312983.13 |
| 8 | 16627975.86 | 16627975.86 | 216.52 | 312995.75 |
| 9 | 20163014.10 | 20163014.11 | 209.43 | 313008.35 |
| 10 | 23785228.28 | 23785228.28 | 202.63 | 313020.95 |
| 11 | 27450691.24 | 27450691.24 | 196.11 | 313033.53 |
| 12 | 31123216.62 | 31123216.62 | 189.84 | 313046.10 |
| 13 | 34773452.23 | 34773452.23 | 183.82 | 313058.66 |
| 14 | 38378001.89 | 38378001.89 | 178.07 | 313071.21 |
| 15 | 41918581.67 | 41918581.67 | 172.44 | 313083.75 |
| 16 | 45381221.38 | 45381221.38 | 167.13 | 313096.27 |
| 17 | 48755523.95 | 48755523.95 | 162.11 | 313108.80 |
| 18 | 52033999.83 | 52033999.83 | 156.99 | 313121.31 |

potential profiles, energy levels 1 & 2 (cm^-1)
and wavefunctions

| Y2 | V0s | Es1 | Es2 | V0a-V0s | Ea1 | Ea2 |
|---|---|---|---|---|---|---|
| | | 71.22 | 217.34 | | 71.22 | 217.34 |
| | | 0.00 | 146.12 | | 0.00 | 146.12 |
| -2.000 | 10038.56 | 0 | 0 | 577.47 | 0 | 0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| -1.833 | 8185.03 | 0 | 0 | 599.33 | 0 | 0 |
| -1.667 | 6646.74 | 0 | 0 | 612.96 | 0 | 0 |
| -1.500 | 5400.13 | 0 | 0 | 619.28 | 0 | 0 |
| -1.333 | 4406.51 | 0 | 0 | 612.28 | 0 | 0 |
| -1.167 | 3623.30 | 0 | 0 | 548.17 | 0 | 0 |
| -1.000 | 3009.10 | 0 | 0 | 418.33 | 0 | 0 |
| -0.833 | 2524.40 | 0 | 0 | 281.35 | 0 | 0 |
| -0.667 | 2128.72 | 1 | -9 | 156.46 | 1 | -8 |
| -0.500 | 1776.53 | 18 | -89 | 63.18 | 17 | -85 |
| -0.333 | 1432.53 | 144 | -646 | 17.24 | 143 | -637 |
| -0.167 | 1102.51 | 918 | -3686 | 3.59 | 915 | -3672 |
| 0.000 | 807.29 | 4578 | -16299 | 0.67 | 4575 | -16283 |
| 0.167 | 557.76 | 17882 | -55265 | 0.12 | 17878 | -55248 |
| 0.333 | 357.13 | 54776 | -142622 | 0.02 | 54772 | -142608 |
| 0.500 | 204.47 | 132281 | -277351 | 0.00 | 132278 | -277341 |
| 0.667 | 96.80 | 253674 | -397460 | 0.00 | 253671 | -397458 |
| 0.833 | 30.15 | 389631 | -394146 | 0.00 | 389630 | -394151 |
| 1.000 | 0.01 | 483895 | -207309 | 0.00 | 483895 | -207317 |
| 1.167 | 1.64 | 490828 | 90951 | 0.00 | 490829 | 90945 |
| 1.333 | 30.38 | 410820 | 341896 | 0.00 | 410822 | 341894 |
| 1.500 | 81.88 | 286669 | 434326 | 0.00 | 286671 | 434329 |
| 1.667 | 152.12 | 168463 | 376795 | 0.00 | 168464 | 376800 |
| 1.833 | 237.52 | 84196 | 252583 | 0.00 | 84196 | 252587 |
| 2.000 | 334.88 | 36130 | 137582 | 0.00 | 36130 | 137584 |
| 2.167 | 441.40 | 13433 | 62654 | 0.00 | 13433 | 62655 |
| 2.333 | 554.65 | 4365 | 24323 | 0.00 | 4365 | 24323 |
| 2.500 | 672.57 | 1250 | 8169 | 0.00 | 1250 | 8169 |
| 2.667 | 793.39 | 318 | 2403 | 0.00 | 318 | 2403 |
| 2.833 | 915.66 | 72 | 625 | 0.00 | 72 | 625 |
| 3.000 | 1038.16 | 14 | 145 | 0.00 | 14 | 145 |
| 3.167 | 1159.92 | 2 | 30 | 0.00 | 2 | 30 |
| 3.333 | 1280.15 | 0 | 5 | 0.00 | 0 | 5 |
| 3.500 | 1398.25 | 0 | 1 | 0.00 | 0 | 1 |
| 3.667 | 1513.75 | 0 | 0 | 0.00 | 0 | 0 |
| 3.833 | 1626.31 | 0 | 0 | 0.00 | 0 | 0 |
| 4.000 | 1735.67 | 0 | 0 | 0.00 | 0 | 0 |

```
ground state tunnel splitting =     10.06 MHz

Standard configuration as read from input
******************************************************************************
  ----- formic acid dimer, March 2017 -------- (x, y1, y2) = (0,0,0)
******************************************************************************
NA = 12
   1    0    0    0   0.00000     0.000     0.000           0.0000000
   2    1    0    0   1.00000     0.000     0.000           0.0000000
   3    1    2    0   1.77575    90.000     0.000          12.0000000
   4    1    2    3   1.77575    90.000   180.000          12.0000000
   5    3    1    2   1.26120    63.300     0.000          15.9949150
   6    3    1    2   1.26120    63.300   180.000          15.9949150
   7    4    1    2   1.26120    63.300     0.000          15.9949150
   8    4    1    2   1.26120    63.300   180.000          15.9949150
   9    3    5    1   1.09520   116.700   180.000           1.0078250
  10    4    7    1   1.09520   116.700   180.000           1.0078250
  11    1    4    2   1.11610    90.000     0.000           1.0078250
  12    1    4    2   1.11610    90.000   180.000           1.0078250

  ----------- grid properties -----------
  NDX   NDY   NDZ     DRX     DRY     DRZ    NV
```

18 18 18 0.167 0.167 0.167 16

mobility constants (MHz)

| GXXE | GXYE | GYYE |
|---|---|---|
| 1424000. | -13000. | 597000. |

X=Y=0

| | | |
|---|---|---|
| GXX | 1424878.111 | MHZ |
| GXY | -13994.187 | |
| GYY | 599612.648 | |
| G | 0.17041314E+07 | (AMU*A**2)**5 |

TABLES: GXX, GXY, GYY (GHZ), G/G(0,0), VG (GHZ)

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1423 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1423 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 |
| 1423 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1424 | 1423 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
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| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
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| 10735 | 10628 | 10531 | 10448 | 10378 | 10322 | 10280 | 10255 | 10245 | 10251 | 10273 | 10312 | 10367 | 10438 | 10524 | 10625 | 10740 | 10869 | 11010 |
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| 10661 | 10551 | 10452 | 10366 | 10293 | 10234 | 10190 | 10161 | 10148 | 10151 | 10170 | 10206 | 10257 | 10324 | 10406 | 10503 | 10614 | 10738 | 10874 |
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| 10634 | 10522 | 10422 | 10334 | 10260 | 10200 | 10154 | 10124 | 10109 | 10111 | 10128 | 10162 | 10211 | 10277 | 10357 | 10452 | 10560 | 10682 | 10817 |
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| 10599 | 10484 | 10381 | 10290 | 10213 | 10150 | 10101 | 10068 | 10051 | 10049 | 10063 | 10093 | 10139 | 10201 | 10278 | 10369 | 10473 | 10591 | 10721 |
| 10595 | 10479 | 10375 | 10283 | 10205 | 10141 | 10092 | 10058 | 10040 | 10037 | 10051 | 10080 | 10125 | 10186 | 10262 | 10352 | 10456 | 10572 | 10701 |
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| 10590 | 10473 | 10367 | 10274 | 10195 | 10129 | 10078 | 10043 | 10023 | 10019 | 10031 | 10058 | 10102 | 10161 | 10235 | 10323 | 10425 | 10540 | 10666 |
| 10591 | 10473 | 10366 | 10272 | 10191 | 10125 | 10074 | 10037 | 10017 | 10012 | 10023 | 10050 | 10093 | 10151 | 10224 | 10311 | 10412 | 10526 | 10651 |
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| 10608 | 10486 | 10376 | 10279 | 10195 | 10125 | 10071 | 10031 | 10007 | 10000 | 10007 | 10031 | 10071 | 10125 | 10195 | 10279 | 10376 | 10486 | 10608 |
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| 10638 | 10513 | 10401 | 10301 | 10214 | 10142 | 10085 | 10043 | 10017 | 10006 | 10012 | 10033 | 10071 | 10123 | 10190 | 10271 | 10366 | 10474 | 10592 |
| 10651 | 10526 | 10412 | 10311 | 10224 | 10151 | 10093 | 10050 | 10023 | 10012 | 10017 | 10037 | 10074 | 10125 | 10191 | 10272 | 10366 | 10473 | 10591 |
| 10666 | 10540 | 10425 | 10323 | 10235 | 10161 | 10102 | 10058 | 10031 | 10019 | 10023 | 10043 | 10078 | 10129 | 10195 | 10274 | 10367 | 10473 | 10590 |
| 10683 | 10555 | 10439 | 10337 | 10247 | 10173 | 10113 | 10069 | 10040 | 10027 | 10031 | 10050 | 10084 | 10134 | 10199 | 10278 | 10370 | 10475 | 10592 |
| 10701 | 10572 | 10456 | 10352 | 10262 | 10186 | 10125 | 10080 | 10051 | 10037 | 10040 | 10058 | 10092 | 10141 | 10205 | 10283 | 10375 | 10479 | 10595 |
| 10721 | 10591 | 10473 | 10369 | 10278 | 10201 | 10139 | 10093 | 10063 | 10049 | 10051 | 10068 | 10101 | 10150 | 10213 | 10290 | 10381 | 10484 | 10599 |
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| 10790 | 10657 | 10536 | 10428 | 10335 | 10255 | 10191 | 10143 | 10110 | 10093 | 10092 | 10108 | 10139 | 10185 | 10246 | 10321 | 10409 | 10510 | 10623 |
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| 10845 | 10709 | 10586 | 10476 | 10381 | 10299 | 10233 | 10183 | 10149 | 10130 | 10128 | 10142 | 10171 | 10216 | 10275 | 10349 | 10436 | 10536 | 10647 |
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| 10906 | 10768 | 10643 | 10531 | 10433 | 10350 | 10282 | 10230 | 10194 | 10174 | 10170 | 10182 | 10210 | 10253 | 10312 | 10384 | 10469 | 10568 | 10677 |
| 10939 | 10800 | 10674 | 10561 | 10462 | 10378 | 10309 | 10256 | 10219 | 10198 | 10193 | 10205 | 10232 | 10275 | 10332 | 10404 | 10488 | 10586 | 10695 |
| 10974 | 10834 | 10706 | 10592 | 10492 | 10407 | 10337 | 10283 | 10245 | 10224 | 10218 | 10229 | 10255 | 10297 | 10354 | 10425 | 10509 | 10606 | 10714 |
| 11010 | 10869 | 10740 | 10625 | 10524 | 10438 | 10367 | 10312 | 10273 | 10251 | 10245 | 10255 | 10280 | 10322 | 10378 | 10448 | 10531 | 10628 | 10735 |

pseudopotential function in GHz

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |

pseudopotential + potential energy (cm^-1)

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23835 | 23819 | 23819 | 23836 | 23865 | 23900 | 23932 | 23958 | 23977 | 23988 | 23994 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 | 23999 | 24000 |
| 23486 | 23431 | 23427 | 23477 | 23567 | 23674 | 23778 | 23863 | 23923 | 23961 | 23982 | 23992 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 | 23999 |
| 22710 | 22560 | 22538 | 22650 | 22868 | 23138 | 23405 | 23628 | 23789 | 23892 | 23949 | 23978 | 23991 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 |
| 21323 | 20987 | 20908 | 21105 | 21530 | 22084 | 22652 | 23142 | 23506 | 23743 | 23879 | 23948 | 23980 | 23993 | 23997 | 23999 | 23999 | 23999 | 23999 |
| 19288 | 18654 | 18446 | 18711 | 19389 | 20334 | 21354 | 22273 | 22983 | 23460 | 23741 | 23887 | 23955 | 23984 | 23994 | 23998 | 23999 | 23999 | 23999 |
| 16802 | 15764 | 15329 | 15579 | 16467 | 17824 | 19391 | 20891 | 22112 | 22969 | 23493 | 23775 | 23910 | 23967 | 23989 | 23996 | 23999 | 23999 | 23999 |
| 14236 | 12718 | 11949 | 12047 | 12997 | 14653 | 16738 | 18890 | 20767 | 22168 | 23069 | 23575 | 23825 | 23934 | 23978 | 23993 | 23998 | 23999 | 23999 |
| 12020 | 9968 | 8761 | 8545 | 9344 | 11065 | 13480 | 16214 | 18815 | 20915 | 22363 | 23222 | 23668 | 23872 | 23955 | 23986 | 23996 | 23998 | 23999 |
| 10548 | 7924 | 6180 | 5489 | 5906 | 7399 | 9829 | 12897 | 16134 | 19021 | 21199 | 22598 | 23373 | 23747 | 23908 | 23969 | 23991 | 23997 | 23999 |
| 10176 | 6953 | 4574 | 3258 | 3085 | 4063 | 6139 | 9145 | 12716 | 16300 | 19333 | 21496 | 22806 | 23491 | 23805 | 23932 | 23978 | 23993 | 23998 |
| 11251 | 7473 | 4380 | 2299 | 1357 | 1584 | 2975 | 5473 | 8884 | 12789 | 16568 | 19643 | 21743 | 22962 | 23573 | 23841 | 23947 | 23983 | 23995 |
| 13719 | 9620 | 5840 | 2890 | 1024 | 321 | 794 | 2434 | 5184 | 8833 | 12921 | 16790 | 19860 | 21902 | 23056 | 23619 | 23862 | 23954 | 23986 |
| 16978 | 13101 | 8954 | 5207 | 2344 | 588 | 0 | 588 | 2344 | 5208 | 8954 | 13101 | 16978 | 20011 | 22000 | 23109 | 23645 | 23872 | 23958 |
| 19937 | 16894 | 13035 | 8937 | 5259 | 2470 | 788 | 274 | 936 | 2761 | 5678 | 9439 | 13546 | 17328 | 20245 | 22134 | 23175 | 23673 | 23883 |
| 21834 | 19774 | 16719 | 12913 | 8936 | 5421 | 2808 | 1301 | 959 | 1789 | 3770 | 6796 | 10571 | 14558 | 18107 | 20754 | 22418 | 23313 | 23732 |
| 22764 | 21388 | 19104 | 15889 | 12091 | 8311 | 5130 | 2913 | 1817 | 1886 | 3117 | 5458 | 8733 | 12548 | 16307 | 19423 | 21593 | 22876 | 23531 |
| 23147 | 22115 | 20289 | 17532 | 14021 | 10260 | 6857 | 4272 | 2747 | 2368 | 3150 | 5060 | 7968 | 11559 | 15302 | 18594 | 21029 | 22552 | 23370 |
| 23277 | 22372 | 20732 | 18186 | 14843 | 11150 | 7703 | 4997 | 3312 | 2759 | 3363 | 5097 | 7843 | 11313 | 15003 | 18318 | 20824 | 22426 | 23304 |
| 23298 | 22417 | 20813 | 18311 | 15009 | 11340 | 7898 | 5180 | 3474 | 2897 | 3474 | 5180 | 7898 | 11340 | 15009 | 18311 | 20813 | 22417 | 23298 |
| 23304 | 22426 | 20824 | 18318 | 15003 | 11313 | 7843 | 5097 | 3363 | 2759 | 3312 | 4997 | 7703 | 11150 | 14843 | 18186 | 20732 | 22372 | 23277 |
| 23370 | 22552 | 21029 | 18594 | 15302 | 11559 | 7968 | 5060 | 3150 | 2368 | 2747 | 4272 | 6857 | 10260 | 14021 | 17532 | 20289 | 22115 | 23147 |
| 23531 | 22876 | 21593 | 19423 | 16307 | 12548 | 8733 | 5458 | 3117 | 1886 | 1817 | 2913 | 5130 | 8311 | 12091 | 15889 | 19104 | 21388 | 22764 |
| 23732 | 23313 | 22418 | 20754 | 18107 | 14558 | 10571 | 6796 | 3770 | 1789 | 959 | 1301 | 2808 | 5421 | 8936 | 12913 | 16719 | 19774 | 21834 |
| 23883 | 23673 | 23175 | 22134 | 20245 | 17328 | 13546 | 9439 | 5678 | 2761 | 936 | 274 | 788 | 2470 | 5259 | 8937 | 13035 | 16894 | 19937 |

```
23958 23872 23645 23109 22000 20011 16978 13101  8954  5208  2344   588     0   588  2344  5207  8954 13101 16978
23986 23954 23862 23619 23056 21902 19860 16790 12921  8833  5184  2434   794   321  1024  2890  5840  9620 13719
23995 23983 23947 23841 23573 22962 21743 19643 16568 12789  8884  5473  2975  1584  1357  2299  4380  7473 11251
23998 23993 23978 23932 23805 23491 22806 21496 19333 16300 12716  9145  6139  4063  3085  3258  4574  6953 10176
23999 23997 23991 23969 23908 23747 23373 22598 21199 19021 16134 12897  9829  7399  5906  5489  6180  7924 10548
23999 23998 23996 23986 23955 23872 23668 23222 22363 20915 18815 16214 13480 11065  9344  8545  8761  9968 12020
23999 23999 23998 23993 23978 23934 23825 23575 23069 22168 20767 18890 16738 14653 12997 12047 11949 12718 14236
23999 23999 23999 23996 23989 23967 23910 23775 23493 22969 22112 20891 19391 17824 16467 15579 15329 15764 16802
23999 23999 23999 23998 23994 23984 23955 23887 23741 23460 22983 22273 21354 20334 19389 18711 18446 18654 19288
23999 23999 23999 23999 23997 23993 23980 23948 23879 23743 23506 23142 22652 22084 21530 21105 20908 20987 21323
23999 23999 23999 23999 23999 23997 23991 23978 23949 23892 23789 23628 23405 23138 22868 22650 22538 22560 22710
23999 23999 23999 23999 23999 23999 23997 23992 23982 23961 23923 23863 23778 23674 23567 23477 23427 23431 23486
24000 23999 23999 23999 23999 23999 23999 23997 23994 23988 23977 23958 23932 23900 23865 23836 23819 23819 23835


Emax / cm^-1 =    45982.404211258232


                     energy levels (MHz)

  iteration cycle           11
 40647039.67  40647161.14  51355569.72  51359063.89  61962813.36  62004506.10
   72392897.49  72659223.44  82502047.27  83469844.67  92475351.56  94457561.92
102670421.54 104747275.10 106295636.09 106394835.47

Tunnel splitting, E0(2)-E0(1) =       121.47 MHz

  iteration cycle           12
 40647039.67  40647161.14  51355569.72  51359063.89  61962813.36  62004506.10
   72392897.49  72659223.44  82502047.27  83469844.67  92475351.56  94457561.92
102670421.44 104747275.09 106295636.05 106394835.47

Tunnel splitting, E0(2)-E0(1) =       121.47 MHz

  iteration cycle           13
 40647039.67  40647161.14  51355569.72  51359063.89  61962813.36  62004506.10
   72392897.49  72659223.44  82502047.27  83469844.67  92475351.56  94457561.92
102670421.43 104747275.09 106295636.05 106394835.47

Tunnel splitting, E0(2)-E0(1) =       121.47 MHz



   energy levels (cm^-1) and wavefunctions:
          1
 1355.839

    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     1     2     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     2    20    34    14     1     0     0     0     0     0     0     0     0     0     0     0
    0     0     0    16   153   334   181    25     1     0     0     0     0     0     0     0     0     0     0
    0     0     1    55   683  1991  1444   276    15     0     0     0     0     0     0     0     0     0     0
    0     0     1   100  1677  6758  6848  1824   135     3     0     0     0     0     0     0     0     0     0
    0     0     0    94  2174 12412 18097  7000   746    22     0     0     0     0     0     0     0     0     0
    0     0     0    44  1441 11882 25423 14592  2316   104     1     0     0     0     0     0     0     0     0
```

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 10 | 490 | 5884 | 18688 | 16124 | 3867 | 261 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 92 | 1597 | 7543 | 9815 | 3564 | 363 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 11 | 274 | 1890 | 3681 | 2008 | 305 | 15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 35 | 350 | 1003 | 804 | 180 | 18 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 4 | 56 | 232 | 268 | 94 | 32 | 12 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 8 | 53 | 86 | 67 | 86 | 53 | 8 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 12 | 32 | 94 | 268 | 232 | 56 | 4 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 18 | 180 | 804 | 1003 | 350 | 35 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | 305 | 2008 | 3681 | 1890 | 274 | 11 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 | 363 | 3564 | 9815 | 7543 | 1597 | 92 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 261 | 3867 | 16124 | 18688 | 5884 | 490 | 10 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 104 | 2316 | 14592 | 25423 | 11882 | 1441 | 44 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 22 | 746 | 7000 | 18097 | 12412 | 2174 | 94 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 135 | 1824 | 6848 | 6758 | 1677 | 100 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | 276 | 1444 | 1991 | 683 | 55 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 25 | 181 | 334 | 153 | 16 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 14 | 34 | 20 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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1355.843

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -2 | -20 | -34 | -14 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -16 | -153 | -334 | -181 | -25 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -55 | -683 | -1991 | -1444 | -276 | -15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -100 | -1678 | -6759 | -6848 | -1824 | -135 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -94 | -2174 | -12413 | -18097 | -7000 | -746 | -22 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -44 | -1441 | -11883 | -25424 | -14592 | -2316 | -104 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -10 | -490 | -5884 | -18688 | -16124 | -3866 | -260 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -1 | -92 | -1597 | -7543 | -9814 | -3562 | -360 | -9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -11 | -274 | -1890 | -3681 | -2006 | -299 | -9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | -35 | -350 | -1003 | -802 | -168 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -4 | -56 | -232 | -265 | -66 | 20 | 11 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -8 | -52 | -80 | 0 | 80 | 52 | 8 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -1 | -11 | -20 | 66 | 265 | 232 | 56 | 4 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | 0 | 168 | 802 | 1003 | 350 | 35 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | 299 | 2006 | 3681 | 1890 | 274 | 11 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | 360 | 3562 | 9814 | 7543 | 1597 | 92 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 260 | 3866 | 16124 | 18688 | 5884 | 490 | 10 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 104 | 2316 | 14592 | 25424 | 11883 | 1441 | 44 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 22 | 746 | 7000 | 18097 | 12413 | 2174 | 94 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 135 | 1824 | 6848 | 6759 | 1678 | 100 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | 276 | 1444 | 1991 | 683 | 55 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 25 | 181 | 334 | 153 | 16 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 14 | 34 | 20 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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1713.037

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 5 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 11 | 63 | 68 | 11 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 2 | 69 | 472 | 638 | 118 | -17 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 228 | 2043 | 3604 | 786 | -225 | -34 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 7 | 405 | 4871 | 11577 | 2979 | -1710 | -325 | -11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 4 | 370 | 6127 | 20053 | 5880 | -7426 | -1900 | -94 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 170 | 3935 | 18020 | 5424 | -17307 | -6220 | -447 | -8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 40 | 1295 | 8321 | 1822 | -21232 | -10951 | -1163 | -31 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 5 | 235 | 2083 | -203 | -14309 | -10659 | -1681 | -69 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 27 | 324 | -314 | -5956 | -6371 | -1478 | -96 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 2 | 36 | -116 | -1812 | -2728 | -924 | -109 | -10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 4 | -29 | -475 | -987 | -516 | -158 | -33 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -7 | -123 | -355 | -382 | -355 | -123 | -7 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -1 | -33 | -158 | -516 | -987 | -475 | -29 | 4 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -10 | -109 | -924 | -2728 | -1812 | -116 | 36 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -96 | -1478 | -6371 | -5956 | -314 | 324 | 27 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -69 | -1681 | -10659 | -14309 | -203 | 2083 | 235 | 5 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -31 | -1163 | -10951 | -21232 | 1822 | 8321 | 1295 | 40 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -8 | -447 | -6220 | -17307 | 5424 | 18020 | 3935 | 170 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -94 | -1900 | -7426 | 5880 | 20053 | 6127 | 370 | 4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -11 | -325 | -1710 | 2979 | 11577 | 4871 | 405 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -34 | -225 | 786 | 3604 | 2043 | 228 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -17 | 118 | 638 | 472 | 69 | 2 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 11 | 68 | 63 | 11 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 5 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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1713.154

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -1 | -5 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -11 | -63 | -68 | -11 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -2 | -69 | -472 | -638 | -118 | 17 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -229 | -2045 | -3606 | -786 | 225 | 34 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | -7 | -405 | -4875 | -11584 | -2978 | 1711 | 325 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -4 | -370 | -6131 | -20063 | -5877 | 7430 | 1899 | 94 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -170 | -3938 | -18029 | -5418 | 17317 | 6215 | 444 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -40 | -1296 | -8325 | -1816 | 21242 | 10938 | 1151 | 28 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -5 | -235 | -2084 | 206 | 14314 | 10641 | 1652 | 57 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -27 | -324 | 315 | 5957 | 6350 | 1426 | 62 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -2 | -36 | 116 | 1812 | 2707 | 834 | 22 | -8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -4 | 29 | 474 | 958 | 341 | -73 | -31 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 7 | 122 | 306 | 0 | -306 | -122 | -7 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 31 | 73 | -341 | -958 | -474 | -29 | 4 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | -22 | -834 | -2707 | -1812 | -116 | 36 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -62 | -1426 | -6350 | -5957 | -315 | 324 | 27 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -57 | -1652 | -10641 | -14314 | -206 | 2084 | 235 | 5 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -28 | -1151 | -10938 | -21242 | 1816 | 8325 | 1296 | 40 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -7 | -444 | -6215 | -17317 | 5418 | 18029 | 3938 | 170 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -94 | -1899 | -7430 | 5877 | 20063 | 6131 | 370 | 4 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -11 | -325 | -1711 | 2978 | 11584 | 4875 | 405 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -34 | -225 | 786 | 3606 | 2045 | 229 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -17 | 118 | 638 | 472 | 69 | 2 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 11 | 68 | 63 | 11 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 5 | 1 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 3 | 12 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 35 | 136 | 82 | -2 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 7 | 200 | 979 | 715 | -54 | -12 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 19 | 650 | 4107 | 3733 | -592 | -105 | 37 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 25 | 1128 | 9472 | 10969 | -3424 | -456 | 396 | 29 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 17 | 1010 | 11505 | 17173 | -10381 | -666 | 2526 | 241 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 456 | 7122 | 13711 | -16031 | 1235 | 8983 | 1189 | 32 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 106 | 2253 | 5481 | -12530 | 4789 | 17116 | 3238 | 127 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 14 | 391 | 1134 | -5216 | 5448 | 18037 | 4914 | 287 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 43 | 133 | -1298 | 3258 | 11721 | 4564 | 403 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 3 | 8 | -225 | 1331 | 5512 | 3048 | 439 | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -30 | 457 | 2237 | 1842 | 530 | 57 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -2 | 154 | 945 | 1433 | 945 | 154 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 57 | 530 | 1842 | 2237 | 457 | -30 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 25 | 439 | 3048 | 5512 | 1331 | -225 | 8 | 3 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 12 | 403 | 4564 | 11721 | 3258 | -1298 | 133 | 43 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 287 | 4914 | 18037 | 5448 | -5216 | 1134 | 391 | 14 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 127 | 3238 | 17116 | 4789 | -12530 | 5481 | 2253 | 106 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 32 | 1189 | 8983 | 1235 | -16031 | 13711 | 7122 | 456 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 241 | 2526 | -666 | -10381 | 17173 | 11505 | 1010 | 17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 29 | 396 | -456 | -3424 | 10969 | 9472 | 1128 | 25 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 37 | -105 | -592 | 3733 | 4107 | 650 | 19 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -2 | 82 | 136 | 35 | 1 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -3 | -12 | -6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -35 | -137 | -82 | 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -7 | -202 | -985 | -718 | 55 | 12 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -19 | -655 | -4133 | -3745 | 599 | 104 | -37 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -25 | -1137 | -9531 | -11000 | 3456 | 447 | -398 | -28 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -17 | -1018 | -11576 | -17211 | 10461 | 620 | -2535 | -238 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -459 | -7165 | -13730 | 16136 | -1348 | -9003 | -1169 | -29 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -106 | -2266 | -5484 | 12599 | -4934 | -17124 | -3164 | -112 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -14 | -394 | -1133 | 5238 | -5547 | -17999 | -4742 | -233 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -1 | -44 | -133 | 1302 | -3297 | -11640 | -4281 | -268 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -3 | -8 | 226 | -1339 | -5402 | -2619 | -145 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 30 | -455 | -2086 | -1112 | 135 | 46 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 2 | -147 | -706 | 0 | 706 | 147 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -46 | -135 | 1112 | 2086 | 455 | -30 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -12 | 145 | 2619 | 5402 | 1339 | -226 | 8 | 3 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 268 | 4281 | 11640 | 3297 | -1302 | 133 | 44 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 233 | 4742 | 17999 | 5547 | -5238 | 1133 | 394 | 14 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 112 | 3164 | 17124 | 4934 | -12599 | 5484 | 2266 | 106 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 29 | 1169 | 9003 | 1348 | -16136 | 13730 | 7165 | 459 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 238 | 2535 | -620 | -10461 | 17211 | 11576 | 1018 | 17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 28 | 398 | -447 | -3456 | 11000 | 9531 | 1137 | 25 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 37 | -104 | -599 | 3745 | 4133 | 655 | 19 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | -12 | -55 | 718 | 985 | 202 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -2 | 82 | 137 | 35 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 12 | 3 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 5 | 82 | 224 | 59 | -10 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 22 | 460 | 1553 | 438 | -130 | 16 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 56 | 1462 | 6274 | 1876 | -973 | 204 | -8 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 73 | 2486 | 13907 | 4166 | -4153 | 1510 | -150 | -46 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 48 | 2180 | 16194 | 4109 | -9419 | 6248 | -1309 | -410 | -13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 16 | 962 | 9579 | 978 | -10625 | 13502 | -5860 | -2153 | -93 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 2 | 218 | 2882 | -778 | -5579 | 14799 | -13446 | -6236 | -380 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 28 | 473 | -506 | -1208 | 8373 | -16705 | -10099 | -886 | -17 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 2 | 49 | -128 | 0 | 2557 | -12714 | -10088 | -1275 | -36 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 4 | -20 | 65 | 365 | -7056 | -7344 | -1357 | -54 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -2 | 21 | -77 | -3480 | -4893 | -1407 | -75 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 5 | -99 | -1899 | -4019 | -1899 | -99 | 5 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -75 | -1407 | -4893 | -3480 | -77 | 21 | -2 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -54 | -1357 | -7344 | -7056 | 365 | 65 | -20 | 4 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -36 | -1275 | -10088 | -12714 | 2557 | 0 | -128 | 49 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -17 | -886 | -10099 | -16705 | 8373 | -1208 | -506 | 473 | 28 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | -380 | -6236 | -13446 | 14799 | -5579 | -778 | 2882 | 218 | 2 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -93 | -2153 | -5860 | 13502 | -10625 | 978 | 9579 | 962 | 16 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -13 | -410 | -1309 | 6248 | -9419 | 4109 | 16194 | 2180 | 48 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -46 | -150 | 1510 | -4153 | 4166 | 13907 | 2486 | 73 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -8 | 204 | -973 | 1876 | 6274 | 1462 | 56 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 16 | -130 | 438 | 1553 | 460 | 22 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -10 | 59 | 224 | 82 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 20 | 8 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -9 | -21 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -85 | -231 | -59 | 11 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -23 | -479 | -1598 | -435 | 133 | -16 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -58 | -1520 | -6452 | -1846 | 983 | -211 | 10 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -76 | -2583 | -14287 | -4022 | 4163 | -1548 | 171 | 46 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -50 | -2263 | -16616 | -3787 | 9344 | -6347 | 1441 | 409 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -16 | -998 | -9816 | -633 | 10385 | -13591 | 6301 | 2127 | 82 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -2 | -226 | -2949 | 959 | 5308 | -14736 | 14196 | 6068 | 322 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -29 | -483 | 556 | 1063 | -8216 | 17325 | 9594 | 697 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -2 | -50 | 136 | -44 | -2449 | 12882 | 9141 | 856 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -4 | 21 | -74 | -330 | 6834 | 5893 | 585 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 2 | -22 | 71 | 2965 | 2610 | -27 | -30 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -5 | 71 | 1032 | 0 | -1032 | -71 | 5 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 30 | 27 | -2610 | -2965 | -71 | 22 | -2 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -585 | -5893 | -6834 | 330 | 74 | -21 | 4 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -9 | -856 | -9141 | -12882 | 2449 | 44 | -136 | 50 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -8 | -697 | -9594 | -17325 | 8216 | -1063 | -556 | 483 | 29 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -322 | -6068 | -14196 | 14736 | -5308 | -959 | 2949 | 226 | 2 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -82 | -2127 | -6301 | 13591 | -10385 | 633 | 9816 | 998 | 16 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -12 | -409 | -1441 | 6347 | -9344 | 3787 | 16616 | 2263 | 50 | 0 | 0 |

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    0     0     0     0     0     0     0     0    -1   -46  -171  1548 -4163  4022 14287  2583    76     0     0
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    0     0     0     0     0     0     0     0     0     0     0     0     0     5    21     9     0     0     0
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    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
    0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0


 SELEST: lowest four energy levels in cm^-1
         at Y2 = 1 (JZ = NDZ+1)
      1355.84     1355.84     1713.04     1713.15
         0.00        0.00      357.20      357.31

reference at J = 19  VZ(J,1) =   1355.84 cm^-1

 effective potentials for A-type dimer stretching
   JZ   VZ1/cm^-1   VZ2/cm^-1  splitting / MHz
  -18    10010.86    10586.12    17245805.02
  -17     8128.87     8726.51    17916633.30
  -16     6559.46     7171.17    18338521.46
  -15     5281.36     5900.45    18559939.26
  -14     4257.27     4876.60    18566864.65
  -13     3445.78     4052.39    18185660.77
  -12     2806.99     3366.54    16774983.58
  -11     2304.53     2757.69    13585240.44
  -10     1905.36     2223.27     9530726.34
   -9     1578.05     1768.37     5705905.54
   -8     1291.28     1382.55     2736376.64
   -7     1020.46     1053.78      999062.71
   -6      764.24      774.01      292822.21
   -5      537.23      539.79       76806.14
   -4      349.45      350.10       19513.00
   -3      203.74      203.90        5037.27
   -2       99.03       99.07        1361.17
   -1       32.39       32.40         391.98
    0        0.00        0.00         121.47
    1       -2.33       -2.33          40.66
    2       21.18       21.18          14.71
    3       66.48       66.48           5.73
    4      129.81      129.81           2.40
    5      207.72      207.72           1.07
    6      297.16      297.16           0.51
    7      395.44      395.44           0.25
    8      500.22      500.22           0.13
    9      609.50      609.50           0.07
   10      721.60      721.60           0.04
   11      835.10      835.10           0.02
   12      948.86      948.86           0.01
   13     1061.95     1061.95           0.01
   14     1173.62     1173.62           0.01
   15     1283.30     1283.30           0.00
   16     1390.56     1390.56           0.00
   17     1495.07     1495.07           0.00
   18     1596.59     1596.59           0.00
```

FMZ1D: y2 motion
energy profiles for ground state doublet,
pseudopotential, and mobility coefficient

| JZ | VZ(1) | VZ(2) | VPS | G44 (MHZ) |
|---|---|---|---|---|
| -18 | 300118739.99 | 317364545.01 | 560.07 | 316405.30 |
| -17 | 243698063.55 | 261614696.84 | 541.14 | 316418.50 |
| -16 | 196648275.94 | 214986797.39 | 520.58 | 316431.68 |
| -15 | 158331595.88 | 176891535.14 | 500.10 | 316444.86 |
| -14 | 127630350.17 | 146197214.82 | 481.01 | 316458.04 |
| -13 | 103302354.31 | 121488015.08 | 462.65 | 316471.20 |
| -12 | 84151796.92 | 100926780.49 | 445.11 | 316484.35 |
| -11 | 69088592.87 | 82673833.31 | 428.34 | 316497.48 |
| -10 | 57121713.49 | 66652439.83 | 412.30 | 316510.61 |
| -9 | 47309018.60 | 53014924.14 | 396.97 | 316523.73 |
| -8 | 38711956.97 | 41448333.61 | 382.29 | 316536.83 |
| -7 | 30592982.89 | 31592045.60 | 368.25 | 316549.92 |
| -6 | 22911802.90 | 23204625.11 | 354.82 | 316563.00 |
| -5 | 16105959.60 | 16182765.75 | 341.96 | 316576.08 |
| -4 | 10476514.75 | 10496027.76 | 329.66 | 316589.13 |
| -3 | 6108193.65 | 6113230.92 | 317.88 | 316602.18 |
| -2 | 2969114.49 | 2970475.66 | 306.60 | 316615.22 |
| -1 | 971376.40 | 971768.37 | 295.79 | 316628.24 |
| 0 | 285.45 | 406.91 | 285.45 | 316641.25 |
| 1 | -69605.01 | -69564.35 | 275.53 | 316654.26 |
| 2 | 635256.22 | 635270.92 | 266.04 | 316667.25 |
| 3 | 1993385.98 | 1993391.71 | 256.94 | 316680.22 |
| 4 | 3891736.20 | 3891738.60 | 248.21 | 316693.19 |
| 5 | 6227513.16 | 6227514.23 | 239.85 | 316706.15 |
| 6 | 8908925.91 | 8908926.42 | 231.83 | 316719.09 |
| 7 | 11855251.60 | 11855251.85 | 224.14 | 316732.02 |
| 8 | 14996474.16 | 14996474.29 | 216.76 | 316744.94 |
| 9 | 18272665.08 | 18272665.16 | 209.69 | 316757.85 |
| 10 | 21633214.58 | 21633214.62 | 202.89 | 316770.75 |
| 11 | 25035980.44 | 25035980.46 | 196.37 | 316783.64 |
| 12 | 28446395.78 | 28446395.80 | 190.12 | 316796.51 |
| 13 | 31836563.49 | 31836563.50 | 184.10 | 316809.37 |
| 14 | 35184360.03 | 35184360.04 | 178.35 | 316822.22 |
| 15 | 38472571.20 | 38472571.20 | 172.72 | 316835.06 |
| 16 | 41688083.42 | 41688083.42 | 167.42 | 316847.89 |
| 17 | 44821149.43 | 44821149.43 | 162.40 | 316860.72 |
| 18 | 47864744.90 | 47864744.90 | 157.25 | 316873.53 |

potential profiles, energy levels 1 & 2 (cm^-1)
and wavefunctions

| Y2 | V0s | Es1 | Es2 | V0a-V0s | Ea1 | Ea2 |
|---|---|---|---|---|---|---|
| | | 67.12 | 208.64 | | 67.13 | 208.69 |
| | | 0.00 | 141.53 | | 0.00 | 141.56 |
| -2.000 | 10010.88 | 0 | 0 | 575.26 | 0 | 0 |
| -1.833 | 8128.89 | 0 | 0 | 597.63 | 0 | 0 |
| -1.667 | 6559.48 | 0 | 0 | 611.71 | 0 | 0 |
| -1.500 | 5281.37 | 0 | 0 | 619.09 | 0 | 0 |
| -1.333 | 4257.29 | 0 | 0 | 619.32 | 0 | 0 |
| -1.167 | 3445.80 | 0 | 0 | 606.61 | 0 | 0 |
| -1.000 | 2807.00 | 0 | 0 | 559.55 | 0 | 0 |
| -0.833 | 2304.55 | 0 | -1 | 453.15 | 0 | 0 |
| -0.667 | 1905.38 | 2 | -15 | 317.91 | 2 | -10 |
| -0.500 | 1578.06 | 24 | -122 | 190.33 | 20 | -99 |
| -0.333 | 1291.29 | 173 | -776 | 91.28 | 158 | -702 |
| -0.167 | 1020.47 | 995 | -4014 | 33.33 | 960 | -3850 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.000 | 764.26 | 4653 | -16630 | 9.77 | 4591 | -16365 |
| 0.167 | 537.24 | 17452 | -54230 | 2.56 | 17366 | -53893 |
| 0.333 | 349.46 | 52239 | -137245 | 0.65 | 52141 | -136903 |
| 0.500 | 203.75 | 124925 | -266053 | 0.17 | 124830 | -265796 |
| 0.667 | 99.04 | 239836 | -386522 | 0.05 | 239761 | -386433 |
| 0.833 | 32.40 | 372266 | -398398 | 0.01 | 372225 | -398501 |
| 1.000 | 0.01 | 471094 | -236867 | 0.00 | 471092 | -237086 |
| 1.167 | -2.32 | 490510 | 45717 | 0.00 | 490540 | 45519 |
| 1.333 | 21.19 | 424248 | 305664 | 0.00 | 424291 | 305585 |
| 1.500 | 66.49 | 307768 | 425262 | 0.00 | 307809 | 425309 |
| 1.667 | 129.81 | 189079 | 393254 | 0.00 | 189108 | 393367 |
| 1.833 | 207.73 | 99307 | 279813 | 0.00 | 99325 | 279926 |
| 2.000 | 297.17 | 45001 | 161927 | 0.00 | 45010 | 162007 |
| 2.167 | 395.45 | 17751 | 78546 | 0.00 | 17755 | 78590 |
| 2.333 | 500.23 | 6147 | 32584 | 0.00 | 6148 | 32604 |
| 2.500 | 609.51 | 1883 | 11735 | 0.00 | 1884 | 11743 |
| 2.667 | 721.61 | 514 | 3714 | 0.00 | 514 | 3717 |
| 2.833 | 835.11 | 126 | 1044 | 0.00 | 126 | 1045 |
| 3.000 | 948.87 | 28 | 263 | 0.00 | 28 | 263 |
| 3.167 | 1061.95 | 5 | 59 | 0.00 | 5 | 59 |
| 3.333 | 1173.62 | 1 | 12 | 0.00 | 1 | 12 |
| 3.500 | 1283.31 | 0 | 2 | 0.00 | 0 | 2 |
| 3.667 | 1390.56 | 0 | 0 | 0.00 | 0 | 0 |
| 3.833 | 1495.07 | 0 | 0 | 0.00 | 0 | 0 |
| 4.000 | 1596.60 | 0 | 0 | 0.00 | 0 | 0 |

```
ground state tunnel splitting =    334.89 MHz

Standard configuration as read from input
******************************************************************************
  ----- formic acid dimer, March 2017 -------- (x, y1, y2) = (0,0,0)
******************************************************************************
NA = 12
   1    0    0    0   0.00000     0.000     0.000           0.0000000
   2    1    0    0   1.00000     0.000     0.000           0.0000000
   3    1    2    0   1.77575    90.000     0.000          12.0000000
   4    1    2    3   1.77575    90.000   180.000          12.0000000
   5    3    1    2   1.26120    63.300     0.000          15.9949150
   6    3    1    2   1.26120    63.300   180.000          15.9949150
   7    4    1    2   1.26120    63.300     0.000          15.9949150
   8    4    1    2   1.26120    63.300   180.000          15.9949150
   9    3    5    1   1.09520   116.700   180.000           1.0078250
  10    4    7    1   1.09520   116.700   180.000           1.0078250
  11    1    4    2   1.11610    90.000     0.000           1.0078250
  12    1    4    2   1.11610    90.000   180.000           2.0141018

  ----------- grid properties -----------
  NDX   NDY   NDZ     DRX     DRY     DRZ    NV
   18    18    18   0.167   0.167   0.167    16

       mobility constants (MHz)
     GXXE        GXYE        GYYE
    958000.     -13000.     597000.

X=Y=0
         GXX     958342.639  MHZ
         GXY     -13994.186
         GYY     599612.648
         G   0.25881273E+07  (AMU*A**2)**5
```

TABLES: GXX, GXY, GYY (GHZ), G/G(0,0), VG (GHZ)

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 957 | 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 | 957 |
| 957 | 957 | 957 | 957 | 957 | 957 | 958 | 958 | 958 | 958 | 958 | 958 | 958 | 957 | 957 | 957 | 957 | 957 | 957 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -9 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -9 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |
| -8 | -9 | -10 | -11 | -12 | -12 | -13 | -13 | -13 | -13 | -13 | -13 | -13 | -12 | -12 | -11 | -10 | -9 | -8 |

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| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 588 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 588 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 585 | 587 | 590 | 592 | 594 | 596 | 597 | 598 | 599 | 599 | 599 | 598 | 597 | 596 | 594 | 592 | 590 | 587 | 585 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10808 | 10705 | 10614 | 10535 | 10470 | 10419 | 10384 | 10364 | 10360 | 10373 | 10402 | 10449 | 10511 | 10591 | 10686 | 10797 | 10922 | 11062 | 11215 |
| 10777 | 10673 | 10581 | 10501 | 10435 | 10383 | 10346 | 10325 | 10321 | 10332 | 10360 | 10405 | 10467 | 10545 | 10638 | 10747 | 10871 | 11009 | 11161 |
| 10748 | 10643 | 10550 | 10469 | 10402 | 10349 | 10311 | 10289 | 10283 | 10294 | 10321 | 10365 | 10425 | 10501 | 10593 | 10701 | 10823 | 10959 | 11109 |
| 10722 | 10616 | 10522 | 10440 | 10371 | 10318 | 10279 | 10256 | 10249 | 10258 | 10284 | 10326 | 10385 | 10460 | 10551 | 10657 | 10777 | 10912 | 11060 |
| 10698 | 10591 | 10496 | 10413 | 10344 | 10289 | 10249 | 10225 | 10216 | 10225 | 10249 | 10290 | 10348 | 10421 | 10510 | 10615 | 10734 | 10867 | 11013 |
| 10677 | 10569 | 10472 | 10388 | 10318 | 10262 | 10221 | 10196 | 10186 | 10193 | 10217 | 10257 | 10313 | 10385 | 10473 | 10576 | 10693 | 10825 | 10969 |
| 10658 | 10549 | 10451 | 10366 | 10295 | 10238 | 10196 | 10169 | 10159 | 10165 | 10187 | 10225 | 10280 | 10351 | 10437 | 10539 | 10655 | 10785 | 10927 |
| 10641 | 10531 | 10432 | 10346 | 10274 | 10216 | 10173 | 10145 | 10134 | 10138 | 10159 | 10196 | 10250 | 10319 | 10404 | 10505 | 10619 | 10747 | 10888 |
| 10627 | 10516 | 10416 | 10329 | 10255 | 10196 | 10152 | 10123 | 10111 | 10114 | 10134 | 10170 | 10222 | 10290 | 10374 | 10473 | 10586 | 10712 | 10851 |
| 10616 | 10503 | 10402 | 10314 | 10239 | 10179 | 10133 | 10104 | 10090 | 10092 | 10111 | 10146 | 10197 | 10263 | 10346 | 10443 | 10554 | 10679 | 10817 |
| 10606 | 10493 | 10390 | 10301 | 10225 | 10164 | 10117 | 10087 | 10072 | 10073 | 10090 | 10124 | 10173 | 10239 | 10320 | 10416 | 10526 | 10649 | 10785 |
| 10600 | 10484 | 10381 | 10291 | 10214 | 10151 | 10104 | 10072 | 10056 | 10056 | 10072 | 10104 | 10153 | 10217 | 10297 | 10391 | 10500 | 10621 | 10756 |
| 10595 | 10479 | 10374 | 10283 | 10204 | 10141 | 10092 | 10059 | 10042 | 10041 | 10056 | 10087 | 10134 | 10197 | 10275 | 10369 | 10476 | 10596 | 10729 |
| 10593 | 10475 | 10370 | 10277 | 10198 | 10133 | 10083 | 10049 | 10030 | 10028 | 10042 | 10072 | 10118 | 10180 | 10257 | 10348 | 10454 | 10573 | 10704 |
| 10593 | 10475 | 10368 | 10273 | 10193 | 10127 | 10076 | 10041 | 10021 | 10018 | 10030 | 10059 | 10104 | 10165 | 10240 | 10331 | 10435 | 10553 | 10682 |
| 10596 | 10476 | 10368 | 10272 | 10191 | 10124 | 10072 | 10035 | 10014 | 10010 | 10021 | 10049 | 10093 | 10152 | 10226 | 10315 | 10418 | 10535 | 10663 |
| 10601 | 10480 | 10370 | 10274 | 10191 | 10123 | 10069 | 10032 | 10010 | 10004 | 10014 | 10041 | 10083 | 10141 | 10215 | 10302 | 10404 | 10519 | 10646 |
| 10609 | 10486 | 10375 | 10277 | 10193 | 10124 | 10069 | 10031 | 10008 | 10001 | 10010 | 10035 | 10076 | 10133 | 10205 | 10292 | 10392 | 10505 | 10631 |
| 10619 | 10495 | 10382 | 10283 | 10198 | 10127 | 10072 | 10032 | 10008 | 10000 | 10008 | 10032 | 10072 | 10127 | 10198 | 10283 | 10382 | 10495 | 10619 |
| 10631 | 10505 | 10392 | 10292 | 10205 | 10133 | 10076 | 10035 | 10010 | 10001 | 10008 | 10031 | 10069 | 10124 | 10193 | 10277 | 10375 | 10486 | 10609 |
| 10646 | 10519 | 10404 | 10302 | 10215 | 10141 | 10083 | 10041 | 10014 | 10004 | 10010 | 10032 | 10069 | 10123 | 10191 | 10274 | 10370 | 10480 | 10601 |
| 10663 | 10535 | 10418 | 10315 | 10226 | 10152 | 10093 | 10049 | 10021 | 10010 | 10014 | 10035 | 10072 | 10124 | 10191 | 10272 | 10368 | 10476 | 10596 |
| 10682 | 10553 | 10435 | 10331 | 10240 | 10165 | 10104 | 10059 | 10030 | 10018 | 10021 | 10041 | 10076 | 10127 | 10193 | 10273 | 10368 | 10475 | 10593 |
| 10704 | 10573 | 10454 | 10348 | 10257 | 10180 | 10118 | 10072 | 10042 | 10028 | 10030 | 10049 | 10083 | 10133 | 10198 | 10277 | 10370 | 10475 | 10593 |
| 10729 | 10596 | 10476 | 10369 | 10275 | 10197 | 10134 | 10087 | 10056 | 10041 | 10042 | 10059 | 10092 | 10141 | 10204 | 10283 | 10374 | 10479 | 10595 |
| 10756 | 10621 | 10500 | 10391 | 10297 | 10217 | 10153 | 10104 | 10072 | 10056 | 10056 | 10072 | 10104 | 10151 | 10214 | 10291 | 10381 | 10484 | 10600 |
| 10785 | 10649 | 10526 | 10416 | 10320 | 10239 | 10173 | 10124 | 10090 | 10073 | 10072 | 10087 | 10117 | 10164 | 10225 | 10301 | 10390 | 10493 | 10606 |
| 10817 | 10679 | 10554 | 10443 | 10346 | 10263 | 10197 | 10146 | 10111 | 10092 | 10090 | 10104 | 10133 | 10179 | 10239 | 10314 | 10402 | 10503 | 10616 |
| 10851 | 10712 | 10586 | 10473 | 10374 | 10290 | 10222 | 10170 | 10134 | 10114 | 10111 | 10123 | 10152 | 10196 | 10255 | 10329 | 10416 | 10516 | 10627 |
| 10888 | 10747 | 10619 | 10505 | 10404 | 10319 | 10250 | 10196 | 10159 | 10138 | 10134 | 10145 | 10173 | 10216 | 10274 | 10346 | 10432 | 10531 | 10641 |
| 10927 | 10785 | 10655 | 10539 | 10437 | 10351 | 10280 | 10225 | 10187 | 10165 | 10159 | 10169 | 10196 | 10238 | 10295 | 10366 | 10451 | 10549 | 10658 |
| 10969 | 10825 | 10693 | 10576 | 10473 | 10385 | 10313 | 10257 | 10217 | 10193 | 10186 | 10196 | 10221 | 10262 | 10318 | 10388 | 10472 | 10569 | 10677 |
| 11013 | 10867 | 10734 | 10615 | 10510 | 10421 | 10348 | 10290 | 10249 | 10225 | 10216 | 10225 | 10249 | 10289 | 10344 | 10413 | 10496 | 10591 | 10698 |
| 11060 | 10912 | 10777 | 10657 | 10551 | 10460 | 10385 | 10326 | 10284 | 10258 | 10249 | 10256 | 10279 | 10318 | 10371 | 10440 | 10522 | 10616 | 10722 |
| 11109 | 10959 | 10823 | 10701 | 10593 | 10501 | 10425 | 10365 | 10321 | 10294 | 10283 | 10289 | 10311 | 10349 | 10402 | 10469 | 10550 | 10643 | 10748 |
| 11161 | 11009 | 10871 | 10747 | 10638 | 10545 | 10467 | 10405 | 10360 | 10332 | 10321 | 10325 | 10346 | 10383 | 10435 | 10501 | 10581 | 10673 | 10777 |
| 11215 | 11062 | 10922 | 10797 | 10686 | 10591 | 10511 | 10449 | 10402 | 10373 | 10360 | 10364 | 10384 | 10419 | 10470 | 10535 | 10614 | 10705 | 10808 |

pseudopotential function in GHz

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |

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| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 2 | 3 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 2 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |
| 1 | 2 | 2 | 2 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 1 |

pseudopotential + potential energy (cm^-1)

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23835 | 23819 | 23819 | 23836 | 23865 | 23900 | 23932 | 23958 | 23977 | 23988 | 23994 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 | 23999 | 24000 |
| 23486 | 23431 | 23427 | 23477 | 23567 | 23674 | 23778 | 23863 | 23923 | 23961 | 23982 | 23992 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 | 23999 |
| 22710 | 22560 | 22538 | 22650 | 22868 | 23138 | 23405 | 23628 | 23789 | 23892 | 23949 | 23978 | 23991 | 23997 | 23999 | 23999 | 23999 | 23999 | 23999 |
| 21323 | 20987 | 20908 | 21105 | 21530 | 22084 | 22652 | 23142 | 23506 | 23743 | 23879 | 23948 | 23980 | 23993 | 23997 | 23999 | 23999 | 23999 | 23999 |
| 19288 | 18654 | 18446 | 18711 | 19389 | 20334 | 21354 | 22273 | 22983 | 23460 | 23741 | 23887 | 23955 | 23984 | 23994 | 23998 | 23999 | 23999 | 23999 |
| 16802 | 15764 | 15329 | 15579 | 16467 | 17824 | 19391 | 20891 | 22112 | 22969 | 23493 | 23775 | 23910 | 23967 | 23989 | 23996 | 23999 | 23999 | 23999 |
| 14236 | 12718 | 11949 | 12047 | 12997 | 14653 | 16738 | 18890 | 20767 | 22168 | 23069 | 23575 | 23825 | 23934 | 23978 | 23993 | 23998 | 23999 | 23999 |
| 12020 | 9968 | 8761 | 8545 | 9344 | 11065 | 13480 | 16214 | 18815 | 20915 | 22363 | 23222 | 23668 | 23872 | 23955 | 23986 | 23996 | 23998 | 23999 |
| 10548 | 7924 | 6180 | 5489 | 5906 | 7399 | 9829 | 12897 | 16134 | 19021 | 21199 | 22598 | 23373 | 23747 | 23908 | 23969 | 23991 | 23997 | 23999 |
| 10176 | 6953 | 4574 | 3258 | 3085 | 4063 | 6139 | 9145 | 12716 | 16300 | 19333 | 21496 | 22806 | 23491 | 23805 | 23932 | 23978 | 23993 | 23998 |
| 11251 | 7473 | 4380 | 2299 | 1357 | 1584 | 2975 | 5473 | 8884 | 12789 | 16568 | 19643 | 21743 | 22962 | 23573 | 23841 | 23947 | 23983 | 23995 |
| 13719 | 9620 | 5840 | 2890 | 1024 | 321 | 794 | 2434 | 5184 | 8833 | 12921 | 16790 | 19860 | 21902 | 23056 | 23619 | 23862 | 23954 | 23986 |
| 16978 | 13101 | 8954 | 5207 | 2344 | 588 | 0 | 588 | 2344 | 5208 | 8954 | 13101 | 16978 | 20011 | 22000 | 23109 | 23645 | 23872 | 23958 |
| 19937 | 16894 | 13035 | 8937 | 5259 | 2470 | 788 | 274 | 936 | 2761 | 5678 | 9439 | 13546 | 17328 | 20245 | 22134 | 23175 | 23673 | 23883 |
| 21834 | 19774 | 16719 | 12913 | 8936 | 5421 | 2808 | 1301 | 959 | 1789 | 3770 | 6796 | 10571 | 14558 | 18107 | 20754 | 22418 | 23313 | 23732 |
| 22764 | 21388 | 19104 | 15889 | 12091 | 8311 | 5130 | 2913 | 1817 | 1886 | 3117 | 5458 | 8733 | 12548 | 16307 | 19423 | 21593 | 22876 | 23531 |
| 23147 | 22115 | 20289 | 17532 | 14021 | 10260 | 6857 | 4272 | 2747 | 2368 | 3150 | 5060 | 7968 | 11559 | 15302 | 18594 | 21029 | 22552 | 23370 |
| 23277 | 22372 | 20732 | 18186 | 14843 | 11150 | 7703 | 4997 | 3312 | 2759 | 3363 | 5097 | 7843 | 11313 | 15003 | 18318 | 20824 | 22426 | 23304 |
| 23298 | 22417 | 20813 | 18311 | 15009 | 11340 | 7898 | 5180 | 3474 | 2897 | 3474 | 5180 | 7898 | 11340 | 15009 | 18311 | 20813 | 22417 | 23298 |
| 23304 | 22426 | 20824 | 18318 | 15003 | 11313 | 7843 | 5097 | 3363 | 2759 | 3312 | 4997 | 7703 | 11150 | 14843 | 18186 | 20732 | 22372 | 23277 |
| 23370 | 22552 | 21029 | 18594 | 15302 | 11559 | 7968 | 5060 | 3150 | 2368 | 2747 | 4272 | 6857 | 10260 | 14021 | 17532 | 20289 | 22115 | 23147 |
| 23531 | 22876 | 21593 | 19423 | 16307 | 12548 | 8733 | 5458 | 3117 | 1886 | 1817 | 2913 | 5130 | 8311 | 12091 | 15889 | 19104 | 21388 | 22764 |
| 23732 | 23313 | 22418 | 20754 | 18107 | 14558 | 10571 | 6796 | 3770 | 1789 | 959 | 1301 | 2808 | 5421 | 8936 | 12913 | 16719 | 19774 | 21834 |
| 23883 | 23673 | 23175 | 22134 | 20245 | 17328 | 13546 | 9439 | 5678 | 2761 | 936 | 274 | 788 | 2470 | 5259 | 8937 | 13035 | 16894 | 19937 |
| 23958 | 23872 | 23645 | 23109 | 22000 | 20011 | 16978 | 13101 | 8954 | 5208 | 2344 | 588 | 0 | 588 | 2344 | 5207 | 8954 | 13101 | 16978 |
| 23986 | 23954 | 23862 | 23619 | 23056 | 21902 | 19860 | 16790 | 12921 | 8833 | 5184 | 2434 | 794 | 321 | 1024 | 2890 | 5840 | 9620 | 13719 |
| 23995 | 23983 | 23947 | 23841 | 23573 | 22962 | 21743 | 19643 | 16568 | 12789 | 8884 | 5473 | 2975 | 1584 | 1357 | 2299 | 4380 | 7473 | 11251 |
| 23998 | 23993 | 23978 | 23932 | 23805 | 23491 | 22806 | 21496 | 19333 | 16300 | 12716 | 9145 | 6139 | 4063 | 3085 | 3258 | 4574 | 6953 | 10176 |
| 23999 | 23997 | 23991 | 23969 | 23908 | 23747 | 23373 | 22598 | 21199 | 19021 | 16134 | 12897 | 9829 | 7399 | 5906 | 5489 | 6180 | 7924 | 10548 |
| 23999 | 23998 | 23996 | 23986 | 23955 | 23872 | 23668 | 23222 | 22363 | 20915 | 18815 | 16214 | 13480 | 11065 | 9344 | 8545 | 8761 | 9968 | 12020 |
| 23999 | 23999 | 23998 | 23993 | 23978 | 23934 | 23825 | 23575 | 23069 | 22168 | 20767 | 18890 | 16738 | 14653 | 12997 | 12047 | 11949 | 12718 | 14236 |
| 23999 | 23999 | 23999 | 23996 | 23989 | 23967 | 23910 | 23775 | 23493 | 22969 | 22112 | 20891 | 19391 | 17824 | 16467 | 15579 | 15329 | 15764 | 16802 |
| 23999 | 23999 | 23999 | 23998 | 23994 | 23984 | 23955 | 23887 | 23741 | 23460 | 22983 | 22273 | 21354 | 20334 | 19389 | 18711 | 18446 | 18654 | 19288 |
| 23999 | 23999 | 23999 | 23999 | 23997 | 23993 | 23980 | 23948 | 23879 | 23743 | 23506 | 23142 | 22652 | 22084 | 21530 | 21105 | 20908 | 20987 | 21323 |
| 23999 | 23999 | 23999 | 23999 | 23999 | 23997 | 23991 | 23978 | 23949 | 23892 | 23789 | 23628 | 23405 | 23138 | 22868 | 22650 | 22538 | 22560 | 22710 |

```
23999 23999 23999 23999 23999 23999 23997 23992 23982 23961 23923 23863 23778 23674 23567 23477 23427 23431 23486
24000 23999 23999 23999 23999 23999 23999 23997 23994 23988 23977 23958 23932 23900 23865 23836 23819 23819 23835


Emax / cm^-1 =    40946.120781886209


                     energy levels (MHz)

  iteration cycle          11
 34905992.75  34906006.51  45627993.58  45628463.42  56273981.36  56280879.71
   66832587.20  66889988.31  77210062.76  77507108.37  87230546.22  88229962.82
 91219151.74  91223954.40  96639506.32  99001116.40

Tunnel splitting, E0(2)-E0(1) =        13.76 MHz

  iteration cycle          12
 34905992.75  34906006.51  45627993.58  45628463.42  56273981.36  56280879.71
   66832587.20  66889988.31  77210062.76  77507108.37  87230546.22  88229962.82
 91219151.74  91223954.40  96639506.30  99001116.39

Tunnel splitting, E0(2)-E0(1) =        13.76 MHz

  iteration cycle          13
 34905992.75  34906006.51  45627993.58  45628463.42  56273981.36  56280879.71
   66832587.20  66889988.31  77210062.76  77507108.37  87230546.22  88229962.82
 91219151.74  91223954.40  96639506.30  99001116.39

Tunnel splitting, E0(2)-E0(1) =        13.76 MHz



   energy levels (cm^-1) and wavefunctions:
          1
 1164.338

     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0     0
     0     0     0     1     7     8     3     0     0     0     0     0     0     0     0     0     0     0     0
     0     0     0    10    85   155    66     6     0     0     0     0     0     0     0     0     0     0     0
     0     0     0    48   540  1371   833   128     5     0     0     0     0     0     0     0     0     0     0
     0     0     1   104  1659  6154  5503  1231    73     1     0     0     0     0     0     0     0     0     0
     0     0     1   100  2350 13085 17874  6180   558    13     0     0     0     0     0     0     0     0     0
     0     0     0    42  1472 12616 26958 14731  2112    81     0     0     0     0     0     0     0     0     0
     0     0     0     7   410  5454 18457 16205  3751   231     3     0     0     0     0     0     0     0     0
     0     0     0     0    55  1131  6092  8610  3217   317     8     0     0     0     0     0     0     0     0
     0     0     0     0     4   135  1123  2528  1509   235     9     0     0     0     0     0     0     0     0
     0     0     0     0     0    10   143   504   465   110     7     0     0     0     0     0     0     0     0
     0     0     0     0     0     1    16    81   114    42     8     1     0     0     0     0     0     0     0
     0     0     0     0     0     0     1    14    27    24    27    14     1     0     0     0     0     0     0
     0     0     0     0     0     0     0     1     8    42   114    81    16     1     0     0     0     0     0
     0     0     0     0     0     0     0     0     7   110   465   504   143    10     0     0     0     0     0
     0     0     0     0     0     0     0     0     9   235  1509  2528  1123   135     4     0     0     0     0
     0     0     0     0     0     0     0     0     8   317  3217  8610  6092  1131    55     0     0     0     0
     0     0     0     0     0     0     0     0     3   231  3751 16205 18457  5454   410     7     0     0     0
```

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 81 | 2112 | 14731 | 26957 | 12616 | 1472 | 42 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 13 | 558 | 6180 | 17874 | 13085 | 2350 | 100 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 73 | 1231 | 5502 | 6154 | 1659 | 104 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 128 | 833 | 1371 | 540 | 48 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 66 | 155 | 85 | 10 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 8 | 7 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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1164.339

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -1 | -7 | -8 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -10 | -85 | -155 | -66 | -6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -48 | -540 | -1371 | -833 | -128 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -104 | -1659 | -6154 | -5502 | -1231 | -73 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -100 | -2350 | -13085 | -17874 | -6180 | -558 | -13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -42 | -1472 | -12616 | -26957 | -14731 | -2112 | -81 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -7 | -410 | -5454 | -18457 | -16205 | -3751 | -230 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -55 | -1131 | -6092 | -8610 | -3216 | -317 | -8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -4 | -135 | -1123 | -2528 | -1509 | -234 | -8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -10 | -143 | -504 | -464 | -108 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -1 | -16 | -81 | -113 | -35 | 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -1 | -13 | -24 | 0 | 24 | 13 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -2 | 35 | 113 | 81 | 16 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 108 | 464 | 504 | 143 | 10 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | 234 | 1509 | 2528 | 1123 | 135 | 4 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | 317 | 3216 | 8610 | 6092 | 1131 | 55 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 230 | 3751 | 16205 | 18457 | 5454 | 410 | 7 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 81 | 2112 | 14731 | 26958 | 12616 | 1472 | 42 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 13 | 558 | 6180 | 17874 | 13085 | 2350 | 100 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 73 | 1231 | 5503 | 6154 | 1659 | 104 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 128 | 833 | 1371 | 540 | 48 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | 66 | 155 | 85 | 10 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 8 | 7 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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1521.986

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 5 | 23 | 19 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 45 | 273 | 319 | 55 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 204 | 1662 | 2614 | 546 | -86 | -10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 7 | 425 | 4891 | 10844 | 2743 | -1045 | -167 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 397 | 6623 | 21162 | 6016 | -6351 | -1383 | -55 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 161 | 3955 | 18537 | 4672 | -17793 | -5652 | -343 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 29 | 1046 | 7186 | 65 | -22634 | -10812 | -1027 | -23 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 2 | 133 | 1304 | -1094 | -13772 | -9992 | -1490 | -52 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 9 | 132 | -430 | -4627 | -5072 | -1167 | -63 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 7 | -91 | -1059 | -1704 | -588 | -52 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | -13 | -199 | -463 | -245 | -52 | -6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -2 | -39 | -125 | -148 | -125 | -39 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -6 | -52 | -245 | -463 | -199 | -13 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -52 | -588 | -1704 | -1059 | -91 | 7 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -63 | -1167 | -5072 | -4627 | -430 | 132 | 9 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -52 | -1490 | -9992 | -13772 | -1094 | 1304 | 133 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -23 | -1027 | -10812 | -22634 | 65 | 7186 | 1046 | 29 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | -343 | -5652 | -17793 | 4672 | 18537 | 3955 | 161 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -55 | -1383 | -6351 | 6016 | 21162 | 6623 | 397 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -4 | -167 | -1045 | 2743 | 10844 | 4891 | 425 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -10 | -86 | 546 | 2614 | 1662 | 204 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | 55 | 319 | 273 | 45 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 19 | 23 | 5 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -5 | -23 | -19 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -45 | -273 | -319 | -55 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -204 | -1662 | -2615 | -546 | 87 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -7 | -425 | -4891 | -10844 | -2743 | 1045 | 167 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -397 | -6623 | -21164 | -6016 | 6352 | 1383 | 55 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -161 | -3955 | -18538 | -4671 | 17795 | 5651 | 343 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -29 | -1046 | -7187 | -65 | 22636 | 10810 | 1025 | 22 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -2 | -133 | -1304 | 1094 | 13773 | 9989 | 1486 | 50 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -9 | -132 | 430 | 4627 | 5069 | 1158 | 58 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -7 | 91 | 1059 | 1699 | 569 | 34 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -1 | 13 | 199 | 454 | 194 | -7 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 2 | 38 | 106 | 0 | -106 | -38 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | 7 | -194 | -454 | -199 | -13 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -34 | -569 | -1699 | -1059 | -91 | 7 | 0 | 0 | 0 | 0 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | -58 | -1158 | -5069 | -4627 | -430 | 132 | 9 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -50 | -1486 | -9989 | -13773 | -1094 | 1304 | 133 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -22 | -1025 | -10810 | -22636 | 65 | 7187 | 1046 | 29 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | -343 | -5651 | -17795 | 4671 | 18538 | 3955 | 161 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -55 | -1383 | -6352 | 6016 | 21164 | 6623 | 397 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -4 | -167 | -1045 | 2743 | 10844 | 4891 | 425 | 7 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -10 | -87 | 546 | 2615 | 1662 | 204 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | 55 | 319 | 273 | 45 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 19 | 23 | 5 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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1877.098

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 16 | 53 | 27 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 137 | 593 | 393 | -7 | -4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 18 | 592 | 3445 | 2910 | -259 | -64 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 27 | 1198 | 9655 | 10659 | -2531 | -418 | 188 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 17 | 1085 | 12407 | 17950 | -10271 | -791 | 1781 | 136 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 5 | 426 | 7001 | 13045 | -17601 | 1955 | 8201 | 902 | 19 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 74 | 1739 | 3927 | -12784 | 7397 | 17492 | 2868 | 92 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 6 | 207 | 472 | -4197 | 7427 | 17960 | 4436 | 218 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 13 | 19 | -701 | 3541 | 10145 | 3720 | 277 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | -2 | -67 | 1075 | 3820 | 2030 | 235 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -2 | 265 | 1185 | 933 | 213 | 18 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | 65 | 387 | 606 | 387 | 65 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 18 | 213 | 933 | 1185 | 265 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | 235 | 2030 | 3820 | 1075 | -67 | -2 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 277 | 3720 | 10145 | 3541 | -701 | 19 | 13 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 218 | 4436 | 17960 | 7427 | -4197 | 472 | 207 | 6 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 92 | 2868 | 17492 | 7397 | -12784 | 3927 | 1739 | 74 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 19 | 902 | 8201 | 1955 | -17601 | 13045 | 7001 | 426 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 136 | 1781 | -791 | -10271 | 17950 | 12407 | 1085 | 17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 | 188 | -418 | -2531 | 10659 | 9655 | 1198 | 27 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | -64 | -259 | 2910 | 3445 | 592 | 18 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -4 | -7 | 393 | 593 | 137 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 27 | 53 | 16 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -2 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -16 | -53 | -27 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -137 | -593 | -394 | 7 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -18 | -593 | -3449 | -2912 | 259 | 64 | -9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -27 | -1200 | -9666 | -10665 | 2536 | 418 | -189 | -11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -17 | -1086 | -12421 | -17958 | 10285 | 784 | -1782 | -135 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -5 | -427 | -7008 | -13048 | 17620 | -1975 | -8205 | -899 | -19 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -74 | -1741 | -3926 | 12795 | -7424 | -17493 | -2857 | -90 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -6 | -207 | -472 | 4199 | -7443 | -17949 | -4406 | -209 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -13 | -18 | 701 | -3545 | -10124 | -3662 | -251 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | 2 | 67 | -1075 | -3790 | -1924 | -165 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 2 | -264 | -1135 | -698 | -7 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -1 | -62 | -283 | 0 | 283 | 62 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -12 | 7 | 698 | 1135 | 264 | -2 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 165 | 1924 | 3790 | 1075 | -67 | -2 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | 251 | 3662 | 10124 | 3545 | -701 | 18 | 13 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 209 | 4406 | 17949 | 7443 | -4199 | 472 | 207 | 6 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 90 | 2857 | 17493 | 7424 | -12795 | 3926 | 1741 | 74 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 19 | 899 | 8205 | 1975 | -17620 | 13048 | 7008 | 427 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 135 | 1782 | -784 | -10285 | 17958 | 12421 | 1086 | 17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 | 189 | -418 | -2536 | 10665 | 9666 | 1200 | 27 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | -64 | -259 | 2912 | 3449 | 593 | 18 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -4 | -7 | 394 | 593 | 137 | 5 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 27 | 53 | 16 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 2 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 2 | 4 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 2 | 39 | 93 | 24 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 17 | 327 | 991 | 289 | -51 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 56 | 1372 | 5462 | 1709 | -604 | 82 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 80 | 2690 | 14435 | 4405 | -3559 | 967 | -54 | -16 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 50 | 2356 | 17395 | 3688 | -9328 | 5508 | -879 | -225 | -5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 13 | 895 | 9136 | -875 | -9811 | 13676 | -5634 | -1629 | -54 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 150 | 2089 | -1854 | -3252 | 14222 | -15241 | -5623 | -274 | -3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 13 | 226 | -608 | 230 | 5995 | -19057 | -9443 | -684 | -9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 12 | -89 | 301 | 746 | -12871 | -8642 | -922 | -21 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | -6 | 73 | -250 | -5784 | -5216 | -817 | -27 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | -1 | 8 | -177 | -2188 | -2708 | -686 | -40 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 1 | -75 | -934 | -1912 | -934 | -75 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -40 | -686 | -2708 | -2188 | -177 | 8 | -1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -27 | -817 | -5216 | -5784 | -250 | 73 | -6 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -21 | -922 | -8642 | -12871 | 746 | 301 | -89 | 12 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -9 | -684 | -9443 | -19057 | 5995 | 230 | -608 | 226 | 13 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -3 | -274 | -5623 | -15241 | 14222 | -3252 | -1854 | 2089 | 150 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -54 | -1629 | -5634 | 13676 | -9811 | -875 | 9136 | 895 | 13 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | -225 | -879 | 5508 | -9328 | 3688 | 17395 | 2356 | 50 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -16 | -54 | 967 | -3559 | 4405 | 14435 | 2690 | 80 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 82 | -604 | 1709 | 5462 | 1372 | 56 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | -51 | 289 | 991 | 327 | 17 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | 24 | 93 | 39 | 2 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 4 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -2 | -4 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -2 | -39 | -94 | -24 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -18 | -330 | -999 | -289 | 52 | -2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -56 | -1384 | -5501 | -1708 | 607 | -83 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -81 | -2714 | -14531 | -4381 | 3567 | -974 | 57 | 16 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -51 | -2377 | -17504 | -3615 | 9320 | -5532 | 900 | 226 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -13 | -902 | -9190 | 960 | 9750 | -13697 | 5727 | 1628 | 53 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | -1 | -151 | -2100 | 1893 | 3180 | -14190 | 15413 | 5591 | 263 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | -13 | -227 | 616 | -262 | -5942 | 19176 | 9318 | 644 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -12 | 89 | -308 | -720 | 12857 | 8379 | 815 | 13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | -1 | 6 | -74 | 253 | 5668 | 4765 | 584 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | -8 | 169 | 1970 | 1853 | 139 | -12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | -1 | 59 | 512 | 0 | -512 | -59 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 12 | -139 | -1853 | -1970 | -169 | 8 | -1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -9 | -584 | -4765 | -5668 | -253 | 74 | -6 | 1 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -13 | -815 | -8379 | -12857 | 720 | 308 | -89 | 12 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -8 | -644 | -9318 | -19176 | 5942 | 262 | -616 | 227 | 13 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | -263 | -5591 | -15413 | 14190 | -3180 | -1893 | 2100 | 151 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -53 | -1628 | -5727 | 13697 | -9750 | -960 | 9190 | 902 | 13 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -5 | -226 | -900 | 5532 | -9320 | 3615 | 17504 | 2377 | 51 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -16 | -57 | 974 | -3567 | 4381 | 14531 | 2714 | 81 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 83 | -607 | 1708 | 5501 | 1384 | 56 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | -52 | 289 | 999 | 330 | 18 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -2 | 24 | 94 | 39 | 2 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 4 | 2 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

SELEST: lowest four energy levels in cm^-1
at Y2 = 1 (JZ = NDZ+1)

| | | | |
|---|---|---|---|
| 1164.34 | 1164.34 | 1521.99 | 1522.00 |
| 0.00 | 0.00 | 357.65 | 357.66 |

reference at J = 19  VZ(J,1) =   1164.34 cm^-1

effective potentials for A-type dimer stretching

| JZ | VZ1/cm^-1 | VZ2/cm^-1 | splitting / MHz |
|---|---|---|---|
| -18 | 10027.32 | 10603.99 | 17288124.52 |
| -17 | 8162.76 | 8761.50 | 17949854.75 |
| -16 | 6612.45 | 7225.06 | 18365420.00 |
| -15 | 5353.68 | 5973.30 | 18575487.56 |
| -14 | 4348.26 | 4965.96 | 18518284.60 |
| -13 | 3554.02 | 4143.83 | 17682087.58 |
| -12 | 2930.18 | 3421.69 | 14735042.65 |
| -11 | 2438.70 | 2791.79 | 10585454.80 |
| -10 | 2042.85 | 2261.00 | 6539804.37 |
| -9 | 1704.11 | 1811.15 | 3208984.23 |
| -8 | 1385.77 | 1423.80 | 1140161.55 |
| -7 | 1076.90 | 1086.98 | 302149.96 |
| -6 | 794.08 | 796.36 | 68226.60 |
| -5 | 551.78 | 552.26 | 14597.44 |
| -4 | 355.31 | 355.42 | 3156.13 |
| -3 | 204.85 | 204.87 | 717.09 |
| -2 | 98.01 | 98.02 | 175.41 |
| -1 | 31.16 | 31.17 | 46.85 |
| 0 | 0.00 | 0.00 | 13.76 |
| 1 | -0.02 | -0.02 | 4.44 |
| 2 | 26.63 | 26.63 | 1.58 |
| 3 | 75.69 | 75.69 | 0.61 |
| 4 | 143.24 | 143.24 | 0.26 |
| 5 | 225.75 | 225.75 | 0.12 |
| 6 | 320.07 | 320.07 | 0.06 |
| 7 | 423.44 | 423.44 | 0.03 |
| 8 | 533.46 | 533.46 | 0.02 |
| 9 | 648.09 | 648.09 | 0.01 |
| 10 | 765.60 | 765.60 | 0.01 |
| 11 | 884.54 | 884.54 | 0.00 |
| 12 | 1003.73 | 1003.73 | 0.00 |
| 13 | 1122.20 | 1122.20 | 0.00 |
| 14 | 1239.19 | 1239.19 | 0.00 |
| 15 | 1354.11 | 1354.11 | 0.00 |
| 16 | 1466.49 | 1466.49 | 0.00 |
| 17 | 1576.00 | 1576.00 | 0.00 |
| 18 | 1682.39 | 1682.39 | 0.00 |

FMZ1D: y2 motion
energy profiles for ground state doublet,
pseudopotential, and mobility coefficient

| JZ | VZ(1) | VZ(2) | VPS | G44 (MHZ) |
|---|---|---|---|---|
| -18 | 300612081.93 | 317900206.45 | 557.24 | 316405.30 |
| -17 | 244714019.84 | 262663874.59 | 538.57 | 316418.50 |
| -16 | 198236953.94 | 216602373.94 | 518.28 | 316431.68 |
| -15 | 160499943.96 | 179075431.52 | 498.06 | 316444.86 |
| -14 | 130357906.82 | 148876191.42 | 479.19 | 316458.04 |
| -13 | 106547193.99 | 124229281.57 | 461.03 | 316471.20 |

| | | | | |
|---|---|---|---|---|
| -12 | 87845058.78 | 102580101.43 | 443.69 | 316484.35 |
| -11 | 73110821.48 | 83696276.28 | 427.09 | 316497.48 |
| -10 | 61243617.97 | 67783422.34 | 411.21 | 316510.61 |
| -9 | 51088343.05 | 54297327.29 | 396.01 | 316523.73 |
| -8 | 41544700.58 | 42684862.12 | 381.47 | 316536.83 |
| -7 | 32285086.54 | 32587236.50 | 367.54 | 316549.92 |
| -6 | 23806362.11 | 23874588.71 | 354.22 | 316563.00 |
| -5 | 16542230.10 | 16556827.55 | 341.45 | 316576.08 |
| -4 | 10652376.61 | 10655532.74 | 329.23 | 316589.13 |
| -3 | 6141485.06 | 6142202.15 | 317.53 | 316602.18 |
| -2 | 2938670.94 | 2938846.34 | 306.32 | 316615.22 |
| -1 | 934567.31 | 934614.17 | 295.58 | 316628.24 |
| 0 | 285.29 | 299.04 | 285.29 | 316641.25 |
| 1 | -205.19 | -200.75 | 275.42 | 316654.26 |
| 2 | 798633.06 | 798634.63 | 265.97 | 316667.25 |
| 3 | 2269374.39 | 2269375.00 | 256.91 | 316680.22 |
| 4 | 4294584.47 | 4294584.73 | 248.22 | 316693.19 |
| 5 | 6768167.82 | 6768167.93 | 239.89 | 316706.15 |
| 6 | 9595770.62 | 9595770.68 | 231.90 | 316719.09 |
| 7 | 12694616.95 | 12694616.98 | 224.23 | 316732.02 |
| 8 | 15992993.41 | 15992993.43 | 216.87 | 316744.94 |
| 9 | 19429521.72 | 19429521.73 | 209.81 | 316757.85 |
| 10 | 22952315.61 | 22952315.62 | 203.04 | 316770.75 |
| 11 | 26518085.26 | 26518085.26 | 196.53 | 316783.64 |
| 12 | 30091226.65 | 30091226.66 | 190.28 | 316796.51 |
| 13 | 33642916.44 | 33642916.44 | 184.28 | 316809.37 |
| 14 | 37150225.50 | 37150225.50 | 178.54 | 316822.22 |
| 15 | 40595264.42 | 40595264.42 | 172.91 | 316835.06 |
| 16 | 43964377.89 | 43964377.89 | 167.62 | 316847.89 |
| 17 | 47247404.15 | 47247404.15 | 162.59 | 316860.72 |
| 18 | 50437016.82 | 50437016.82 | 157.45 | 316873.53 |

potential profiles, energy levels 1 & 2 (cm^-1)
and wavefunctions

| Y2 | V0s | Es1 | Es2 | V0a-V0s | Ea1 | Ea2 |
|---|---|---|---|---|---|---|
| | | 69.94 | 214.89 | | 69.94 | 214.90 |
| | | 0.00 | 144.95 | | 0.00 | 144.95 |
| -2.000 | 10027.34 | 0 | 0 | 576.67 | 0 | 0 |
| -1.833 | 8162.78 | 0 | 0 | 598.74 | 0 | 0 |
| -1.667 | 6612.47 | 0 | 0 | 612.60 | 0 | 0 |
| -1.500 | 5353.70 | 0 | 0 | 619.61 | 0 | 0 |
| -1.333 | 4348.27 | 0 | 0 | 617.70 | 0 | 0 |
| -1.167 | 3554.03 | 0 | 0 | 589.81 | 0 | 0 |
| -1.000 | 2930.20 | 0 | 0 | 491.51 | 0 | 0 |
| -0.833 | 2438.71 | 0 | -1 | 353.09 | 0 | 0 |
| -0.667 | 2042.87 | 2 | -12 | 218.14 | 1 | -9 |
| -0.500 | 1704.12 | 20 | -101 | 107.04 | 19 | -92 |
| -0.333 | 1385.78 | 156 | -697 | 38.03 | 151 | -674 |
| -0.167 | 1076.91 | 954 | -3830 | 10.08 | 945 | -3787 |
| 0.000 | 794.09 | 4636 | -16501 | 2.28 | 4623 | -16443 |
| 0.167 | 551.79 | 17794 | -55028 | 0.49 | 17778 | -54963 |
| 0.333 | 355.32 | 53922 | -140718 | 0.11 | 53905 | -140657 |
| 0.500 | 204.86 | 129519 | -272972 | 0.02 | 129504 | -272929 |
| 0.667 | 98.02 | 248205 | -393018 | 0.01 | 248194 | -393006 |
| 0.833 | 31.17 | 382567 | -395830 | 0.00 | 382561 | -395849 |
| 1.000 | 0.01 | 478603 | -219529 | 0.00 | 478603 | -219565 |
| 1.167 | -0.01 | 490707 | 72176 | 0.00 | 490712 | 72145 |
| 1.333 | 26.64 | 416465 | 327044 | 0.00 | 416472 | 327035 |
| 1.500 | 75.70 | 295524 | 431058 | 0.00 | 295530 | 431068 |
| 1.667 | 143.25 | 177075 | 384237 | 0.00 | 177080 | 384257 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 1.833 | 225.76 | 90463 | 264339 | 0.00 | 90466 | 264358 |
| 2.000 | 320.08 | 39773 | 147885 | 0.00 | 39774 | 147897 |
| 2.167 | 423.45 | 15185 | 69268 | 0.00 | 15186 | 69274 |
| 2.333 | 533.47 | 5078 | 27703 | 0.00 | 5078 | 27706 |
| 2.500 | 648.10 | 1499 | 9602 | 0.00 | 1499 | 9603 |
| 2.667 | 765.61 | 394 | 2920 | 0.00 | 394 | 2920 |
| 2.833 | 884.55 | 92 | 787 | 0.00 | 92 | 787 |
| 3.000 | 1003.74 | 19 | 189 | 0.00 | 19 | 189 |
| 3.167 | 1122.21 | 3 | 41 | 0.00 | 3 | 41 |
| 3.333 | 1239.20 | 0 | 8 | 0.00 | 0 | 8 |
| 3.500 | 1354.11 | 0 | 1 | 0.00 | 0 | 1 |
| 3.667 | 1466.49 | 0 | 0 | 0.00 | 0 | 0 |
| 3.833 | 1576.00 | 0 | 0 | 0.00 | 0 | 0 |
| 4.000 | 1682.40 | 0 | 0 | 0.00 | 0 | 0 |

ground state tunnel splitting =     49.80 MHz