

Structure and dynamics of 3'-aminoacetophenone and 4'-aminoacetophenone from rotational spectroscopy

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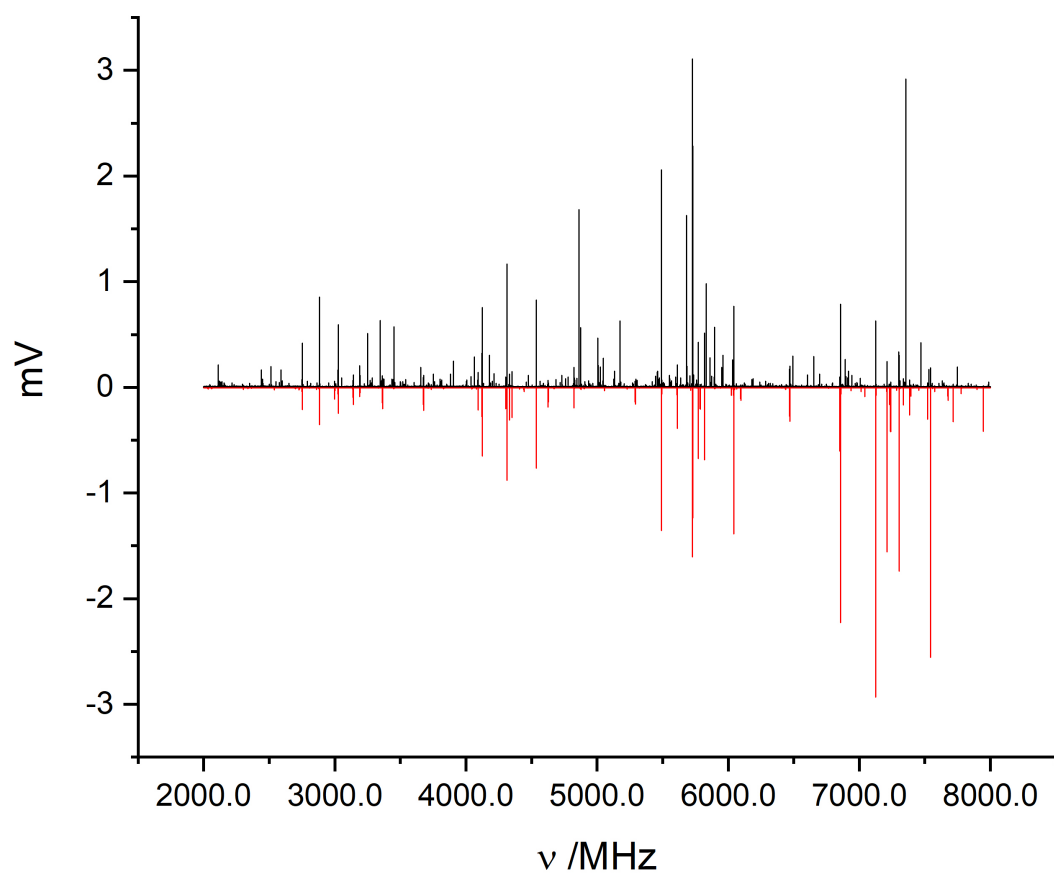


Figure S1: Measured (black) and simulated (red) CP-FTMW spectrum of 4'-aminoacetophenone.

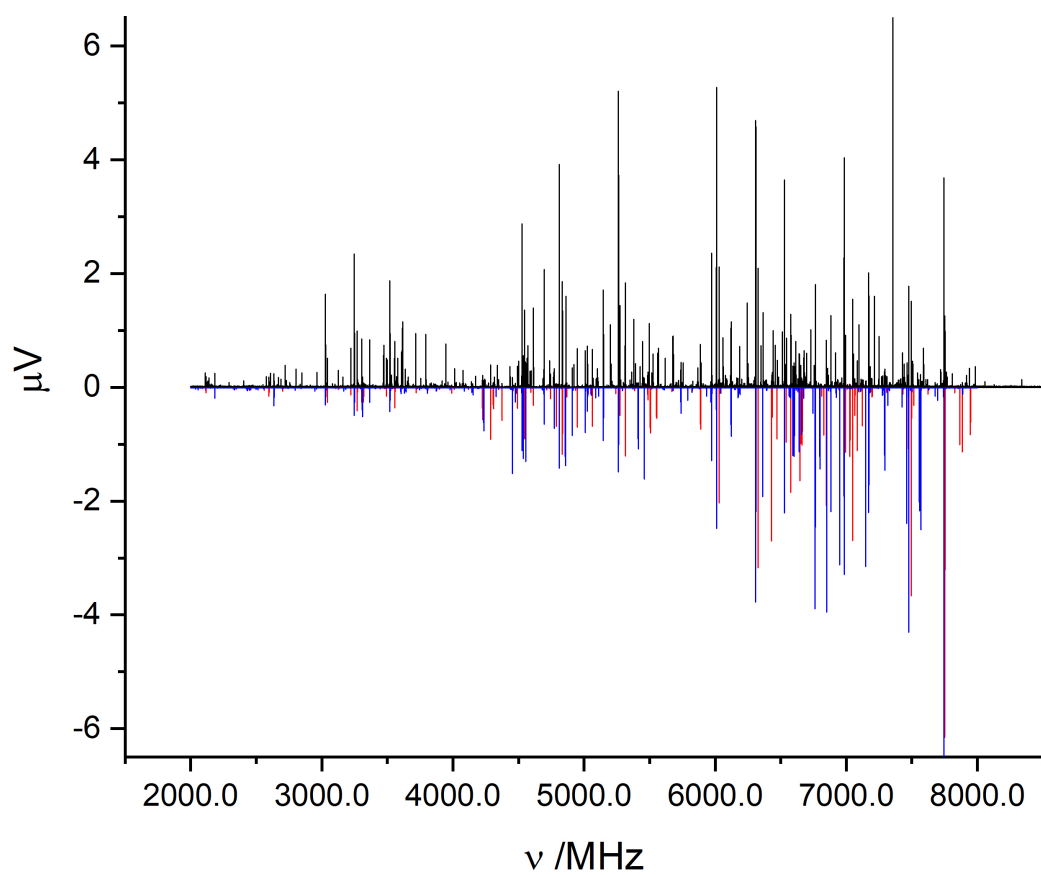


Figure S2: Measured (black) and simulated (3AA-Z blue, 3AA-E red) CP-FTMW spectrum of 3'-aminoacetophenone.

Table S1: Experimental rotational transition frequencies of 4'-aminoacetophenone (ν /MHz, $\Delta\nu = \nu_{obs} - \nu_{calc}$).

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
1	1	1	0	0	0	0	1	E	4303.724	0.009	
1	1	1	0	0	0	0	1	A	4303.724	-0.013	-0.008
1	1	1	0	0	0	2	1	E	4304.569	0.016	
1	1	1	0	0	0	2	1	A	4304.569	-0.007	-0.002
1	1	1	0	0	0	1	1	E	4305.121	0.009	
1	1	1	0	0	0	1	1	A	4305.121	-0.014	-0.009
1	1	0	1	0	1	1	1	E	2996.376	0.002	
1	1	0	1	0	1	1	1	A	2996.376	-0.011	-0.007
1	1	0	1	0	1	1	2	E	2997.109	0.007	
1	1	0	1	0	1	1	2	A	2997.109	-0.005	-0.001
1	1	0	1	0	1	2	1	E	2997.665	0.004	
1	1	0	1	0	1	2	1	A	2997.665	-0.008	-0.004
1	1	0	1	0	1	1	0	E	2998.211	0.018	
1	1	0	1	0	1	1	0	A	2998.211	0.006	0.011
1	1	0	1	0	1	2	2	E	2998.390	0.002	
1	1	0	1	0	1	2	2	A	2998.390	-0.011	-0.007
1	1	0	1	0	1	0	1	E	2999.610	0.020	
1	1	0	1	0	1	0	1	A	2999.610	0.007	0.010
2	0	2	1	0	1	1	1	E	2882.198	0.004	
2	0	2	1	0	1	1	1	A	2882.198	0.000	0.001
2	0	2	1	0	1	3	2	E	2883.381	0.001	
2	0	2	1	0	1	3	2	A	2883.381	-0.003	-0.002
2	0	2	1	0	1	2	1	E	2883.479	0.002	
2	0	2	1	0	1	2	1	A	2883.479	-0.003	-0.001
2	0	2	1	0	1	1	0	E	2884.014	0.002	
2	0	2	1	0	1	1	0	A	2884.014	-0.003	-0.001
2	0	2	1	0	1	2	2	E	2884.205	0.000	
2	0	2	1	0	1	2	2	A	2884.205	-0.004	-0.002
2	1	2	1	1	1	1	1	E	2749.212	0.001	
2	1	2	1	1	1	1	1	A	2749.212	0.002	0.003
2	1	2	1	1	1	3	2	E	2750.533	-0.003	
2	1	2	1	1	1	3	2	A	2750.533	-0.002	0.000
2	1	2	1	1	1	1	0	E	2750.608	-0.001	
2	1	2	1	1	1	1	0	A	2750.608	0.000	0.001
2	1	2	1	1	1	2	1	E	2751.358	0.003	
2	1	2	1	1	1	2	1	A	2751.358	0.004	0.005
2	1	2	1	1	1	2	2	E	2751.912	-0.002	
2	1	2	1	1	1	2	2	A	2751.912	-0.001	0.000
2	1	1	1	1	0	1	0	E	3024.149	0.010	
2	1	1	1	1	0	1	0	A	3024.149	0.000	0.001
2	1	1	1	1	0	2	2	E	3025.142	0.005	
2	1	1	1	1	0	2	2	A	3025.142	-0.005	-0.003
2	1	1	1	1	0	3	2	E	3025.741	0.005	
2	1	1	1	1	0	3	2	A	3025.741	-0.005	-0.004
2	1	1	1	1	0	2	1	E	3026.427	0.003	
2	1	1	1	1	0	2	1	A	3026.427	-0.007	-0.005
2	1	1	1	1	0	1	1	E	3027.363	0.008	
2	1	1	1	1	0	1	1	A	3027.363	-0.003	-0.002
2	1	2	1	0	1	1	1	E	5609.584	0.009	
2	1	2	1	0	1	1	1	A	5609.584	-0.011	-0.006
2	1	2	1	0	1	3	2	E	5611.080	0.011	
2	1	2	1	0	1	3	2	A	5611.080	-0.008	-0.003
2	1	2	1	0	1	1	0	E	5611.401	0.007	
2	1	2	1	0	1	1	0	A	5611.401	-0.012	-0.006
2	1	2	1	0	1	2	1	E	5611.730	0.010	
2	1	2	1	0	1	2	1	A	5611.730	-0.009	-0.004

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Table S1 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
2	1	2	1	0	1	2	2	E	5612.456	0.009	
2	1	2	1	0	1	2	2	A	5612.456	-0.011	-0.005
2	1	1	2	0	2	2	2	E	3139.336	0.016	
2	1	1	2	0	2	2	2	A	3139.336	-0.003	0.002
2	1	1	2	0	2	3	2	E	3139.941	0.022	
2	1	1	2	0	2	3	2	A	3139.941	0.003	0.007
2	1	1	2	0	2	2	3	E	3140.160	0.015	
2	1	1	2	0	2	2	3	A	3140.160	-0.004	0.001
2	1	1	2	0	2	1	2	E	3140.271	0.019	
2	1	1	2	0	2	1	2	A	3140.271	0.000	0.003
2	1	1	2	0	2	2	1	E	3140.615	0.011	
2	1	1	2	0	2	2	1	A	3140.615	-0.007	-0.002
2	1	1	2	0	2	3	3	E	3140.760	0.015	
2	1	1	2	0	2	3	3	A	3140.760	-0.003	0.001
2	1	1	2	0	2	1	1	E	3141.557	0.021	
2	1	1	2	0	2	1	1	A	3141.557	0.003	0.006
3	0	3	2	0	2	2	2	E	4311.904	0.003	
3	0	3	2	0	2	2	2	A	4311.904	-0.003	-0.002
3	0	3	2	0	2	4	3	E	4313.052	0.002	
3	0	3	2	0	2	4	3	A	4313.052	-0.005	-0.002
3	0	3	2	0	2	3	2	E	4313.152	0.000	
3	0	3	2	0	2	3	2	A	4313.152	-0.006	-0.004
3	0	3	2	0	2	2	1	E	4313.183	-0.002	
3	0	3	2	0	2	2	1	A	4313.183	-0.008	-0.005
3	0	3	2	0	2	3	3	E	4313.979	0.002	
3	0	3	2	0	2	3	3	A	4313.979	-0.004	-0.002
3	1	3	2	1	2	2	2	E	4121.076	-0.008	
3	1	3	2	1	2	2	2	A	4121.076	-0.011	-0.009
3	1	3	2	1	2	4	3	E	4123.037	-0.002	
3	1	3	2	1	2	4	3	A	4123.037	-0.005	-0.003
3	1	3	2	1	2	2	1	E	4123.226	-0.003	
3	1	3	2	1	2	2	1	A	4123.226	-0.005	-0.003
3	1	3	2	1	2	3	2	E	4123.304	-0.003	
3	1	3	2	1	2	3	2	A	4123.304	-0.005	-0.003
3	1	3	2	1	2	3	3	E	4124.684	-0.001	
3	1	3	2	1	2	3	3	A	4124.684	-0.004	-0.002
3	1	2	2	1	1	3	3	E	4535.221	0.008	
3	1	2	2	1	1	3	3	A	4535.221	-0.003	0.000
3	1	2	2	1	1	2	1	E	4535.435	0.010	
3	1	2	2	1	1	2	1	A	4535.435	-0.001	0.002
3	1	2	2	1	1	4	3	E	4535.624	0.007	
3	1	2	2	1	1	4	3	A	4535.624	-0.004	-0.001
3	1	2	2	1	1	3	2	E	4535.819	0.007	
3	1	2	2	1	1	3	2	A	4535.819	-0.004	-0.001
3	1	2	2	1	1	2	2	E	4536.366	0.009	-0.001
3	2	2	2	2	1	2	1	A	4331.825	0.000	0.002
3	2	2	2	2	1	4	3	E	4332.649	-0.001	
3	2	2	2	2	1	4	3	A	4332.252	-0.006	-0.004
3	2	2	2	2	1	3	2	E	4333.427	-0.006	
3	2	2	2	2	1	3	2	A	4333.037	0.000	0.002
3	2	1	2	2	0	2	1	E	4350.777	-0.004	
3	2	1	2	2	0	2	1	A	4351.186	0.000	0.002
3	2	1	2	2	0	3	3	A	4351.478	-0.007	-0.005
3	2	1	2	2	0	4	3	E	4351.186	-0.011	
3	2	1	2	2	0	4	3	A	4351.600	-0.003	-0.001
3	2	1	2	2	0	3	2	E	4351.892	-0.008	
3	2	1	2	2	0	3	2	A	4352.306	-0.004	-0.002

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Table S1 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
3	2	1	2	2	0	2	2	A	4352.463	-0.007	-0.004
3	1	3	2	0	2	2	1	E	6850.613	0.003	
3	1	3	2	0	2	2	1	A	6850.613	-0.015	-0.009
3	1	3	2	0	2	4	3	E	6850.738	0.010	
3	1	3	2	0	2	4	3	A	6850.738	-0.007	-0.002
3	1	3	2	0	2	3	2	E	6851.555	0.006	
3	1	3	2	0	2	3	2	A	6851.555	-0.011	-0.006
3	1	3	2	0	2	3	3	E	6852.378	0.004	
3	1	3	2	0	2	3	3	A	6852.378	-0.013	-0.008
3	1	2	3	0	3	3	3	E	3362.002	0.021	
3	1	2	3	0	3	3	3	A	3362.002	-0.002	0.003
3	1	2	3	0	3	3	4	E	3362.922	0.015	
3	1	2	3	0	3	3	4	A	3362.922	-0.008	-0.003
3	1	2	3	0	3	4	4	E	3363.330	0.019	
3	1	2	3	0	3	4	4	A	3363.330	-0.004	0.001
3	1	2	3	0	3	2	2	E	3363.801	0.024	
3	1	2	3	0	3	2	2	A	3363.801	0.001	0.006
4	0	4	3	0	3	3	3	E	5727.270	0.002	
4	0	4	3	0	3	3	3	A	5727.270	-0.006	-0.003
4	0	4	3	0	3	5	4	E	5728.466	0.004	
4	0	4	3	0	3	5	4	A	5728.466	-0.004	-0.002
4	0	4	3	0	3	3	2	E	5728.520	0.002	
4	0	4	3	0	3	3	2	A	5728.520	-0.006	-0.004
4	0	4	3	0	3	4	3	E	5728.578	0.000	
4	0	4	3	0	3	4	3	A	5728.578	-0.008	-0.006
4	0	4	3	0	3	4	4	E	5729.506	0.001	
4	0	4	3	0	3	4	4	A	5729.506	-0.007	-0.004
4	1	4	3	1	3	3	3	E	5489.946	-0.002	
4	1	4	3	1	3	3	3	A	5489.946	-0.006	-0.003
4	1	4	3	1	3	5	4	E	5492.051	-0.002	
4	1	4	3	1	3	5	4	A	5492.051	-0.006	-0.004
4	1	4	3	1	3	3	2	E	5492.148	-0.022	
4	1	4	3	1	3	3	2	A	5492.148	-0.026	-0.023
4	1	4	3	1	3	4	3	E	5492.204	0.009	
4	1	4	3	1	3	4	3	A	5492.204	0.005	0.007
4	1	4	3	1	3	4	4	E	5493.838	-0.003	
4	1	4	3	1	3	4	4	A	5493.838	-0.007	-0.005
4	1	3	3	1	2	4	4	E	6041.315	0.011	
4	1	3	3	1	2	4	4	A	6041.315	-0.003	0.001
4	1	3	3	1	2	3	2	E	6041.552	0.005	
4	1	3	3	1	2	3	2	A	6041.552	-0.009	-0.006
4	1	3	3	1	2	5	4	E	6041.623	0.013	
4	1	3	3	1	2	5	4	A	6041.623	-0.001	0.003
4	1	3	3	1	2	4	3	E	6041.716	0.008	
4	1	3	3	1	2	4	3	A	6041.716	-0.006	-0.002
4	1	3	3	1	2	3	3	E	6042.101	0.008	
4	1	3	3	1	2	3	3	A	6042.101	-0.006	-0.003
4	2	3	3	2	2	3	2	A	5772.628	0.001	0.003
4	2	3	3	2	2	5	4	E	5772.771	-0.010	
4	2	3	3	2	2	5	4	A	5772.720	0.005	0.007
4	2	3	3	2	2	4	3	E	5773.113	-0.011	
4	2	3	3	2	2	4	3	A	5773.057	0.000	0.003
4	2	2	3	2	1	3	2	E	5820.633	-0.006	
4	2	2	3	2	1	3	2	A	5820.722	-0.002	0.001
4	2	2	3	2	1	5	4	A	5820.798	0.000	0.003
4	2	2	3	2	1	4	3	E	5820.954	-0.003	
4	2	2	3	2	1	4	3	A	5821.041	-0.001	0.002

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Table S1 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
4	3	2	3	3	1	3	2	A	5785.494	-0.006	-0.003
4	3	2	3	3	1	5	4	A	5785.826	0.051	0.054
4	3	2	3	3	1	4	3	A	5786.472	-0.002	0.001
4	3	1	3	3	0	3	2	A	5786.140	0.000	0.002
4	3	1	3	3	0	5	4	A	5786.421	0.006	0.009
4	3	1	3	3	0	4	3	A	5787.095	-0.016	-0.013
4	0	4	3	1	3	4	3	E	3190.181	0.000	
4	0	4	3	1	3	4	3	A	3190.181	0.003	0.003
4	0	4	3	1	3	5	4	E	3190.785	0.000	
4	0	4	3	1	3	5	4	A	3190.785	0.003	0.003
4	0	4	3	1	3	3	2	E	3191.096	0.003	
4	0	4	3	1	3	3	2	A	3191.096	0.006	0.006
4	0	4	3	1	3	4	4	E	3191.823	-0.004	
4	0	4	3	1	3	4	4	A	3191.823	-0.001	-0.002
4	1	3	4	0	4	4	4	E	3675.136	0.026	
4	1	3	4	0	4	4	4	A	3675.136	-0.003	0.003
4	1	3	4	0	4	5	5	E	3676.484	0.025	
4	1	3	4	0	4	5	5	A	3676.484	-0.004	0.002
4	1	3	4	0	4	3	3	E	3676.835	0.030	
4	1	3	4	0	4	3	3	A	3676.835	0.001	0.006
5	0	5	4	0	4	4	4	E	7124.315	0.004	
5	0	5	4	0	4	4	4	A	7124.315	-0.005	-0.003
5	0	5	4	0	4	6	5	E	7125.587	-0.006	
5	0	5	4	0	4	6	5	A	7125.587	-0.015	-0.012
5	0	5	4	0	4	4	3	E	7125.641	0.019	
5	0	5	4	0	4	4	3	A	7125.641	0.010	0.013
5	0	5	4	0	4	5	4	E	7125.729	0.003	
5	0	5	4	0	4	5	4	A	7125.729	-0.006	-0.003
5	0	5	4	0	4	5	5	E	7126.771	0.002	
5	0	5	4	0	4	5	5	A	7126.771	-0.007	-0.004
5	1	5	4	1	4	4	4	E	6854.548	-0.003	
5	1	5	4	1	4	4	4	A	6854.548	-0.008	-0.005
5	1	5	4	1	4	6	5	E	6856.719	-0.004	
5	1	5	4	1	4	6	5	A	6856.719	-0.009	-0.006
5	1	5	4	1	4	4	3	E	6856.782	-0.016	
5	1	5	4	1	4	4	3	A	6856.782	-0.021	-0.019
5	1	5	4	1	4	5	4	E	6856.829	0.010	
5	1	5	4	1	4	5	4	A	6856.829	0.005	0.007
5	1	5	4	1	4	5	5	E	6858.605	-0.002	
5	1	5	4	1	4	5	5	A	6858.605	-0.007	-0.005
5	1	4	4	1	3	4	3	E	7542.169	-0.008	
5	1	4	4	1	3	4	3	A	7542.169	-0.025	-0.021
5	1	4	4	1	3	6	5	E	7542.229	0.021	
5	1	4	4	1	3	6	5	A	7542.229	0.004	0.008
5	1	4	4	1	3	5	4	E	7542.289	0.011	
5	1	4	4	1	3	5	4	A	7542.289	-0.006	-0.002
5	2	4	4	2	3	6	5	E	7209.908	-0.002	
5	2	4	4	2	3	6	5	A	7209.908	0.008	0.011
5	2	4	4	2	3	5	4	E	7210.094	-0.008	
5	2	4	4	2	3	5	4	A	7210.094	0.003	0.006
5	2	3	4	2	2	4	3	A	7304.938	-0.038	-0.035
5	2	3	4	2	2	6	5	A	7304.995	0.011	0.015
5	2	3	4	2	2	5	4	A	7305.062	0.007	0.011
5	3	3	4	3	2	4	3	A	7236.077	-0.002	0.001
5	3	3	4	3	2	6	5	A	7236.164	-0.005	-0.001
5	3	3	4	3	2	5	4	A	7236.515	-0.008	-0.005
5	3	2	4	3	1	4	3	A	7238.309	-0.006	-0.002

Continued on next page

Table S1 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
5	3	2	4	3	1	6	5	A	7238.399	-0.004	-0.001
5	3	2	4	3	1	5	4	A	7238.742	-0.010	-0.007
5	0	5	4	1	4	5	4	E	4823.715	0.003	
5	0	5	4	1	4	5	4	A	4823.715	0.001	0.001
5	0	5	4	1	4	6	5	E	4824.328	0.003	
5	0	5	4	1	4	6	5	A	4824.328	0.001	0.001
5	0	5	4	1	4	4	3	E	4824.549	0.004	
5	0	5	4	1	4	4	3	A	4824.549	0.002	0.002
5	1	4	5	0	5	5	5	A	4091.689	-0.010	-0.003
5	1	4	5	0	5	6	6	A	4093.100	-0.010	-0.004
5	1	4	5	0	5	4	4	A	4093.397	-0.001	0.005
5	2	3	5	1	4	4	4	E	7944.323	0.061	
5	2	3	5	1	4	4	4	A	7944.323	0.039	0.050
5	2	3	5	1	4	6	6	E	7944.403	0.053	
5	2	3	5	1	4	6	6	A	7944.403	0.031	0.042
5	2	3	5	1	4	5	5	E	7944.765	-0.018	
5	2	3	5	1	4	5	5	A	7944.765	-0.040	-0.030
6	1	6	5	1	5	7	6	A	8216.353	-0.003	-0.001
6	1	6	5	1	5	6	5	A	8216.429	-0.004	-0.002
6	0	6	5	1	5	6	5	E	6468.642	0.005	
6	0	6	5	1	5	6	5	A	6468.642	-0.002	-0.001
6	0	6	5	1	5	7	6	E	6469.203	0.004	
6	0	6	5	1	5	7	6	A	6469.203	-0.003	-0.002
6	0	6	5	1	5	5	4	E	6469.365	0.005	
6	0	6	5	1	5	5	4	A	6469.365	-0.001	-0.001
6	1	5	6	0	6	6	6	A	4625.677	-0.012	-0.004
6	1	5	6	0	6	7	7	A	4627.172	-0.011	-0.004
6	1	5	6	0	6	5	5	A	4627.431	-0.004	0.003
6	2	4	6	1	5	5	5	E	7714.828	0.010	
6	2	4	6	1	5	5	5	A	7714.828	-0.018	-0.008
6	2	4	6	1	5	7	7	E	7714.896	0.017	
6	2	4	6	1	5	7	7	A	7714.896	-0.011	-0.001
6	2	4	6	1	5	6	6	E	7715.246	0.010	
6	2	4	6	1	5	6	6	A	7715.246	-0.018	-0.008
7	1	6	7	0	7	7	7	A	5290.035	-0.014	-0.005
7	1	6	7	0	7	8	8	A	5291.626	-0.007	0.001
7	1	6	7	0	7	6	6	A	5291.851	-0.011	-0.002
7	2	5	7	1	6	6	6	E	7519.477	-0.026	
7	2	5	7	1	6	6	6	A	7519.534	0.000	0.010
7	2	5	7	1	6	8	8	E	7519.534	-0.003	
7	2	5	7	1	6	8	8	A	7519.579	0.011	0.021
7	2	5	7	1	6	7	7	E	7519.771	-0.004	
7	2	5	7	1	6	7	7	A	7519.810	0.004	0.014
8	1	7	7	2	6	8	7	E	5056.196	0.035	
8	1	7	7	2	6	8	7	A	5056.196	0.035	0.030
8	1	7	7	2	6	9	8	E	5056.985	0.037	
8	1	7	7	2	6	9	8	A	5056.985	0.037	0.032
8	1	7	8	0	8	8	8	A	6094.041	0.009	0.020
8	1	7	8	0	8	9	9	A	6095.702	0.003	0.013
8	1	7	8	0	8	7	7	A	6095.885	-0.025	-0.015
8	2	6	8	1	7	7	7	E	7384.795	0.043	
8	2	6	8	1	7	7	7	A	7384.795	0.008	0.012
8	2	6	8	1	7	9	9	E	7384.795	0.031	
8	2	6	8	1	7	9	9	A	7384.795	-0.003	0.012
8	2	6	8	1	7	8	8	E	7384.885	0.028	
8	2	6	8	1	7	8	8	A	7384.885	-0.006	0.004
9	1	8	9	0	9	9	9	A	7040.700	-0.036	-0.032

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Table S1 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
9	2	7	9	1	8	9	9	E	7335.091	-0.004	
9	2	7	9	1	8	9	9	A	7335.091	-0.043	-0.033
9	2	7	9	1	8	10	10	E	7335.186	0.026	
9	2	7	9	1	8	10	10	A	7335.186	-0.013	-0.007
9	2	7	9	1	8	8	8	E	7335.186	0.019	
9	2	7	9	1	8	8	8	A	7335.186	-0.020	-0.007
9	9	0	8	8	0	9	8	E	62795.660	-0.052	
9	9	0	8	8	1	9	8	A	62795.110	-0.091	-0.100
9	9	1	8	8	0	9	8	A	62795.110	-0.091	-0.100
10	2	8	10	1	9	10	10	E	7392.054	-0.014	
10	2	8	10	1	9	10	10	A	7392.102	-0.013	-0.003
10	9	1	9	8	1	10	9	E	64241.390	-0.007	
10	9	1	9	8	2	10	9	A	64240.990	0.101	0.090
10	9	2	9	8	1	10	9	A	64240.990	0.101	0.090
10	10	0	9	9	0	10	9	E	70097.880	-0.167	
10	10	0	9	9	1	10	9	A	70097.630	0.054	0.022
10	10	1	9	9	0	10	9	A	70097.630	0.054	0.022
10	10	1	9	9	1	10	9	E	70096.310	-0.125	
11	8	3	10	7	3	11	10	E	59829.600	-0.027	
11	8	3	10	7	4	11	10	A	59829.140	0.055	0.058
11	8	4	10	7	3	11	10	A	59829.140	0.055	0.058
11	8	4	10	7	4	11	10	E	59828.000	0.000	
11	9	2	10	8	2	11	10	E	65686.950	0.003	
11	9	2	10	8	3	11	10	A	65686.470	0.028	0.015
11	9	3	10	8	2	11	10	A	65686.470	0.028	0.015
11	9	3	10	8	3	11	10	E	65685.300	-0.028	
11	10	1	10	9	1	11	10	E	71543.770	0.028	
11	10	1	10	9	2	11	10	A	71543.260	-0.014	-0.049
11	10	2	10	9	1	11	10	A	71543.260	-0.014	-0.049
11	10	2	10	9	2	11	10	E	71542.170	0.039	
11	11	0	10	10	0	11	10	E	77400.190	-0.107	
11	11	0	10	10	1	11	10	A	77399.890	0.025	-0.040
11	11	1	10	10	0	11	10	A	77399.890	0.025	-0.040
11	11	1	10	10	1	11	10	E	77398.660	-0.035	
12	8	4	11	7	4	12	11	E	61274.320	0.008	
12	8	4	11	7	5	12	11	A	61273.760	-0.013	-0.013
12	8	5	11	7	4	12	11	A	61273.760	-0.013	-0.013
12	8	5	11	7	5	12	11	E	61272.710	0.024	
12	9	3	11	8	3	12	11	E	67132.240	-0.018	
12	9	3	11	8	4	12	11	A	67131.820	0.064	0.048
12	9	4	11	8	3	12	11	A	67131.820	0.064	0.048
12	9	4	11	8	4	12	11	E	67130.660	0.020	
12	10	2	11	9	2	12	11	E	72989.370	0.039	
12	10	2	11	9	3	12	11	A	72988.900	0.034	-0.004
12	10	3	11	9	2	12	11	A	72988.900	0.034	-0.004
12	10	3	11	9	3	12	11	E	72987.780	0.058	
13	8	5	12	7	5	13	12	E	62718.260	-0.064	
13	8	5	12	7	6	13	12	A	62717.800	0.012	0.008
13	8	6	12	7	5	13	12	A	62717.800	0.012	0.008
13	8	6	12	7	6	13	12	E	62716.550	-0.150	
13	9	4	12	8	4	13	12	E	68577.170	-0.041	
13	9	4	12	8	5	13	12	A	68576.740	0.029	0.009
13	9	5	12	8	4	13	12	A	68576.740	0.029	0.009
13	9	5	12	8	5	13	12	E	68575.550	-0.044	
13	10	3	12	9	3	13	12	E	74434.670	-0.065	
13	10	3	12	9	4	13	12	A	74434.330	0.058	0.015
13	10	4	12	9	3	13	12	A	74434.330	0.058	0.015

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Table S1 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
13	10	4	12	9	4	13	12	E	74433.030	-0.097	
14	8	6	13	7	6	14	13	E	64161.380	-0.069	
14	8	6	13	7	7	14	13	A	64160.900	-0.016	-0.024
14	8	7	13	7	6	14	13	A	64160.900	-0.016	-0.024
14	8	7	13	7	7	14	13	E	64159.770	-0.056	
14	9	5	13	8	5	14	13	E	70021.630	-0.038	
14	9	5	13	8	6	14	13	A	70021.210	0.039	0.014
14	9	6	13	8	5	14	13	A	70021.210	0.039	0.014
14	9	6	13	8	6	14	13	E	70020.040	-0.013	
15	7	8	14	6	8	15	14	E	59734.980	-0.029	
15	7	8	14	6	9	15	14	A	59734.450	-0.023	0.006
15	7	9	14	6	8	15	14	A	59734.450	0.042	0.006
15	7	9	14	6	9	15	14	E	59733.340	-0.037	
15	8	7	14	7	7	15	14	E	65603.460	0.012	
15	8	7	14	7	8	15	14	A	65602.970	0.052	0.039
15	8	8	14	7	7	15	14	A	65602.970	0.053	0.039
15	8	8	14	7	8	15	14	E	65601.820	-0.006	
15	9	6	14	8	6	15	14	E	71465.360	-0.117	
15	9	6	14	8	7	15	14	A	71465.000	0.017	-0.013
15	9	7	14	8	6	15	14	A	71465.000	0.017	-0.013
15	9	7	14	8	7	15	14	E	71463.870	0.007	
15	10	5	14	9	5	15	14	E	77324.590	-0.020	
15	10	5	14	9	6	15	14	A	77324.240	0.087	0.034
15	10	6	14	9	5	15	14	A	77324.240	0.087	0.034
15	10	6	14	9	6	15	14	E	77323.040	0.035	
16	7	9	15	6	9	16	15	E	61170.840	-0.012	
16	7	9	15	6	10	16	15	A	61170.350	-0.011	0.054
16	7	10	15	6	9	16	15	A	61170.350	0.140	0.054
16	7	10	15	6	10	16	15	E	61169.210	-0.010	
16	8	8	15	7	8	16	15	E	67044.080	0.024	
16	8	8	15	7	9	16	15	A	67043.520	-0.009	-0.028
16	8	9	15	7	8	16	15	A	67043.520	-0.006	-0.028
16	8	9	15	7	9	16	15	E	67042.430	-0.004	
16	9	7	15	8	7	16	15	E	72908.430	-0.037	
16	9	7	15	8	8	16	15	A	72908.020	0.044	0.008
16	9	8	15	8	7	16	15	A	72908.020	0.044	0.008
16	9	8	15	8	8	16	15	E	72906.790	-0.064	
17	7	10	16	6	10	17	16	E	62603.670	-0.052	
17	7	10	16	6	11	17	16	A	62603.190	-0.135	0.013
17	7	11	16	6	10	17	16	A	62603.190	0.196	0.013
17	7	11	16	6	11	17	16	E	62602.100	0.006	
17	8	9	16	7	9	17	16	E	68482.970	-0.011	
17	8	9	16	7	10	17	16	A	68482.510	0.053	0.028
17	8	10	16	7	9	17	16	A	68482.510	0.059	0.028
17	8	10	16	7	10	17	16	E	68481.360	0.001	
17	9	8	16	8	8	17	16	E	74350.420	-0.032	
17	9	8	16	8	9	17	16	A	74350.030	0.068	0.023
17	9	9	16	8	8	17	16	A	74350.030	0.068	0.023
17	9	9	16	8	9	17	16	E	74348.830	-0.009	
18	7	11	17	6	11	18	17	E	64033.000	-0.076	
18	7	11	17	6	12	18	17	A	64032.460	-0.409	-0.089
18	7	12	17	6	11	18	17	A	64032.460	0.283	-0.089
18	7	12	17	6	12	18	17	E	64031.470	0.007	
18	8	10	17	7	10	18	17	E	69919.870	-0.032	
18	8	10	17	7	11	18	17	A	69919.430	0.045	0.016
18	8	11	17	7	10	18	17	A	69919.430	0.060	0.016
18	8	11	17	7	11	18	17	E	69918.250	-0.031	

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Table S1 – continued from previous page

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
18	9	9	17	8	9	18	17	E	75791.180	-0.044	
18	9	9	17	8	10	18	17	A	75790.770	0.032	-0.020
18	9	10	17	8	9	18	17	A	75790.770	0.033	-0.020
18	9	10	17	8	10	18	17	E	75789.580	-0.033	
19	7	12	18	6	12	19	18	E	65458.260	-0.042	
19	7	12	18	6	13	19	18	A	65458.540	0.068	0.032
19	7	13	18	6	13	19	18	E	65456.760	0.008	
19	8	11	18	7	11	19	18	E	71354.450	-0.022	
19	8	11	18	7	12	19	18	A	71353.950	-0.016	-0.045
19	8	12	18	7	11	19	18	A	71353.950	0.018	-0.045
19	8	12	18	7	12	19	18	E	71352.840	-0.010	
19	9	10	18	8	10	19	18	E	77230.520	-0.042	
19	9	10	18	8	11	19	18	A	77230.080	0.002	-0.060
19	9	11	18	8	10	19	18	A	77230.080	0.002	-0.060
19	9	11	18	8	11	19	18	E	77228.920	-0.032	
20	7	13	19	6	13	20	19	E	66878.620	-0.068	
20	7	14	19	6	14	20	19	E	66877.340	-0.024	

Table S2: Experimental rotational transition frequencies of 3'(Z)-aminoacetophenone (ν /MHz, $\Delta\nu = \nu_{obs} - \nu_{calc}$).

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
1	1	1	0	0	0	0	1	A	3302.708	-0.006	-0.003
1	1	1	0	0	0	0	1	E	3302.708	0.006	
1	1	1	0	0	0	2	1	A	3303.672	-0.006	-0.003
1	1	1	0	0	0	2	1	E	3303.672	0.006	
1	1	1	0	0	0	1	1	A	3304.312	-0.009	-0.005
1	1	1	0	0	0	1	1	E	3304.312	0.003	
2	0	2	1	0	1	1	1	A	3247.153	-0.001	0.001
2	0	2	1	0	1	1	1	E	3247.153	0.002	
2	0	2	1	0	1	3	2	A	3248.252	-0.001	0.002
2	0	2	1	0	1	3	2	E	3248.252	0.002	
2	0	2	1	0	1	2	1	A	3248.433	-0.001	0.001
2	0	2	1	0	1	2	1	E	3248.433	0.001	
2	0	2	1	0	1	1	0	A	3248.756	-0.001	0.001
2	0	2	1	0	1	1	0	E	3248.756	0.001	
2	0	2	1	0	1	2	2	A	3249.074	-0.002	0.001
2	0	2	1	0	1	2	2	E	3249.074	0.001	
2	1	2	1	1	1	1	1	A	3026.147	0.000	0.001
2	1	2	1	1	1	1	1	E	3026.147	0.000	
2	1	2	1	1	1	3	2	A	3027.553	-0.001	0.001
2	1	2	1	1	1	3	2	E	3027.553	-0.001	
2	1	2	1	1	1	1	0	A	3027.752	-0.002	0.000
2	1	2	1	1	1	1	0	E	3027.752	-0.001	
2	1	2	1	1	1	2	1	A	3028.287	0.000	0.002
2	1	2	1	1	1	2	1	E	3028.287	0.000	
2	1	2	1	1	1	2	2	A	3028.928	-0.002	0.000
2	1	2	1	1	1	2	2	E	3028.928	-0.002	
2	1	1	1	1	0	1	0	A	3517.754	-0.001	0.001
2	1	1	1	1	0	1	0	E	3517.754	0.004	
2	1	1	1	1	0	2	2	A	3518.608	-0.002	0.001
2	1	1	1	1	0	2	2	E	3518.608	0.003	
2	1	1	1	1	0	3	2	A	3519.298	-0.001	0.002
2	1	1	1	1	0	3	2	E	3519.298	0.004	
2	1	1	1	1	0	2	1	A	3519.890	-0.004	-0.001
2	1	1	1	1	0	2	1	E	3519.890	0.001	
2	1	1	1	1	0	1	1	A	3520.964	-0.001	0.001

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Table S2 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
2	1	1	1	1	0	1	1	E	3520.964	0.004	
2	1	2	1	0	1	1	1	A	4693.147	-0.008	-0.005
2	1	2	1	0	1	1	1	E	4693.147	0.003	
2	1	2	1	0	1	3	2	A	4694.553	-0.008	-0.004
2	1	2	1	0	1	3	2	E	4694.553	0.004	
2	1	2	1	0	1	1	0	A	4694.749	-0.010	-0.006
2	1	2	1	0	1	1	0	E	4694.749	0.002	
2	1	2	1	0	1	2	1	A	4695.286	-0.009	-0.006
2	1	2	1	0	1	2	1	E	4695.286	0.002	
2	1	2	1	0	1	2	2	A	4695.927	-0.010	-0.006
2	1	2	1	0	1	2	2	E	4695.927	0.002	
2	1	1	2	0	2	2	2	A	2182.661	-0.004	-0.003
2	1	1	2	0	2	2	2	E	2182.661	0.008	
2	1	1	2	0	2	3	3	A	2184.168	-0.009	-0.007
2	1	1	2	0	2	3	3	E	2184.168	0.003	
2	1	1	2	0	2	1	1	A	2185.015	-0.002	0.000
2	1	1	2	0	2	1	1	E	2185.015	0.010	
2	2	0	2	1	1	2	1	A	5025.075	0.005	0.010
2	2	0	2	1	1	2	1	E	5025.075	-0.008	
2	2	0	2	1	1	2	3	A	5025.453	0.001	0.005
2	2	0	2	1	1	2	3	E	5025.453	-0.012	
2	2	0	2	1	1	2	2	A	5026.144	0.003	0.007
2	2	0	2	1	1	2	2	E	5026.144	-0.010	
2	2	0	2	1	1	3	3	A	5026.278	0.002	0.007
2	2	0	2	1	1	3	3	E	5026.278	-0.010	
2	2	0	2	1	1	1	1	A	5026.350	0.000	0.004
2	2	0	2	1	1	1	1	E	5026.350	-0.013	
2	2	0	2	1	1	3	2	A	5026.970	0.006	0.010
2	2	0	2	1	1	3	2	E	5026.970	-0.007	
2	2	0	2	1	1	1	2	A	5027.427	0.005	0.010
2	2	0	2	1	1	1	2	E	5027.427	-0.007	
2	2	1	2	1	2	2	2	A	5736.826	0.003	0.007
2	2	1	2	1	2	2	2	E	5736.748	0.000	
2	2	1	2	1	2	3	2	A	5737.515	0.005	0.009
2	2	1	2	1	2	3	2	E	5737.438	0.002	
2	2	1	2	1	2	1	2	A	5737.897	0.005	0.009
2	2	1	2	1	2	1	2	E	5737.816	-0.002	
2	2	1	2	1	2	2	3	A	5738.201	0.002	0.007
2	2	1	2	1	2	2	3	E	5738.122	-0.002	
2	2	1	2	1	2	3	3	A	5738.886	0.000	0.005
2	2	1	2	1	2	3	3	E	5738.810	-0.002	
2	2	1	2	1	2	2	1	A	5738.966	0.003	0.008
2	2	1	2	1	2	2	1	E	5738.886	-0.003	
2	2	1	2	1	2	1	1	A	5740.035	0.003	0.008
2	2	1	2	1	2	1	1	E	5739.959	0.001	
3	0	3	2	0	2	2	2	A	4809.863	-0.004	-0.001
3	0	3	2	0	2	2	2	E	4809.863	0.000	
3	0	3	2	0	2	4	3	A	4811.055	-0.004	-0.001
3	0	3	2	0	2	4	3	E	4811.055	-0.001	
3	0	3	2	0	2	2	1	A	4811.142	-0.005	-0.002
3	0	3	2	0	2	2	1	E	4811.142	-0.002	
3	0	3	2	0	2	3	2	A	4811.288	-0.004	-0.001
3	0	3	2	0	2	3	2	E	4811.288	0.000	
3	0	3	2	0	2	3	3	A	4812.111	-0.004	-0.001
3	0	3	2	0	2	3	3	E	4812.111	-0.001	
3	1	3	2	1	2	2	2	A	4524.532	-0.006	-0.004
3	1	3	2	1	2	2	2	E	4524.532	-0.004	

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Table S2 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
3	1	3	2	1	2	4	3	A	4526.487	-0.003	0.000
3	1	3	2	1	2	4	3	E	4526.487	-0.001	
3	1	3	2	1	2	2	1	A	4526.676	-0.002	0.001
3	1	3	2	1	2	2	1	E	4526.676	0.000	
3	1	3	2	1	2	3	2	A	4526.758	-0.002	0.001
3	1	3	2	1	2	3	2	E	4526.758	0.000	
3	1	3	2	1	2	3	3	A	4528.133	-0.003	0.000
3	1	3	2	1	2	3	3	E	4528.133	-0.001	
3	1	2	2	1	1	3	3	A	5261.854	-0.004	0.000
3	1	2	2	1	1	3	3	E	5261.854	0.002	
3	1	2	2	1	1	2	1	A	5262.130	-0.004	0.000
3	1	2	2	1	1	2	1	E	5262.130	0.002	
3	1	2	2	1	1	4	3	A	5262.342	-0.004	0.000
3	1	2	2	1	1	4	3	E	5262.342	0.002	
3	1	2	2	1	1	3	2	A	5262.542	-0.004	-0.001
3	1	2	2	1	1	3	2	E	5262.542	0.002	
3	1	2	2	1	1	2	2	A	5263.201	-0.004	-0.001
3	1	2	2	1	1	2	2	E	5263.201	0.002	
3	2	2	2	2	1	2	1	A	4909.789	-0.010	-0.006
3	2	2	2	2	1	2	1	E	4909.838	0.010	
3	2	2	2	2	1	4	3	A	4910.172	-0.008	-0.005
3	2	2	2	2	1	4	3	E	4910.217	0.007	
3	2	2	2	2	1	3	2	A	4910.862	-0.006	-0.002
3	2	2	2	2	1	3	2	E	4910.903	0.006	
3	2	1	2	2	0	2	2	A	5010.357	-0.016	-0.012
3	2	1	2	2	0	2	2	E	5010.357	0.023	
3	2	1	2	2	0	2	1	A	5009.074	-0.018	-0.015
3	2	1	2	2	0	2	1	E	5009.074	0.020	
3	2	1	2	2	0	4	3	A	5009.411	-0.018	-0.015
3	2	1	2	2	0	4	3	E	5009.411	0.020	
3	2	1	2	2	0	3	2	A	5009.891	-0.018	-0.015
3	2	1	2	2	0	3	2	E	5009.891	0.020	
3	0	3	2	1	2	2	2	A	3363.007	0.002	0.003
3	0	3	2	1	2	2	2	E	3363.007	-0.004	
3	0	3	2	1	2	3	2	A	3364.432	0.001	0.003
3	0	3	2	1	2	3	2	E	3364.432	-0.004	
3	0	3	2	1	2	4	3	A	3364.752	0.001	0.003
3	0	3	2	1	2	4	3	E	3364.752	-0.004	
3	0	3	2	1	2	2	1	A	3365.144	-0.002	0.000
3	0	3	2	1	2	2	1	E	3365.144	-0.007	
3	0	3	2	1	2	3	3	A	3365.808	0.001	0.003
3	0	3	2	1	2	3	3	E	3365.808	-0.004	
3	1	3	2	0	2	2	2	A	5971.390	-0.009	-0.006
3	1	3	2	0	2	2	2	E	5971.390	0.002	
3	1	3	2	0	2	2	1	A	5972.670	-0.009	-0.005
3	1	3	2	0	2	2	1	E	5972.670	0.001	
3	1	3	2	0	2	4	3	A	5972.790	-0.008	-0.004
3	1	3	2	0	2	4	3	E	5972.790	0.002	
3	1	3	2	0	2	3	2	A	5973.613	-0.008	-0.004
3	1	3	2	0	2	3	2	E	5973.613	0.002	
3	1	3	2	0	2	3	3	A	5974.436	-0.008	-0.004
3	1	3	2	0	2	3	3	E	5974.436	0.002	
3	1	2	3	0	3	3	3	A	2633.914	-0.006	-0.003
3	1	2	3	0	3	3	3	E	2633.914	0.009	
3	1	2	3	0	3	4	4	A	2635.455	-0.009	-0.006
3	1	2	3	0	3	4	4	E	2635.455	0.006	
3	1	2	3	0	3	2	2	A	2636.002	-0.002	0.001

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Table S2 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
3	1	2	3	0	3	2	2	E	2636.002	0.013	
3	2	1	3	1	2	3	2	A	4772.833	-0.012	-0.007
3	2	1	3	1	2	3	2	E	4772.833	0.007	
3	2	1	3	1	2	3	4	A	4773.004	-0.012	-0.008
3	2	1	3	1	2	3	4	E	4773.004	0.008	
3	2	1	3	1	2	4	4	A	4773.376	0.017	0.021
3	2	1	3	1	2	4	4	E	4773.376	0.037	
3	2	1	3	1	2	3	3	A	4773.495	-0.009	-0.005
3	2	1	3	1	2	3	3	E	4773.495	0.010	
3	2	1	3	1	2	4	3	A	4773.836	-0.011	-0.007
3	2	1	3	1	2	4	3	E	4773.836	0.008	
3	2	1	3	1	2	2	3	A	4773.958	-0.009	-0.005
3	2	1	3	1	2	2	3	E	4773.958	0.010	
3	2	2	3	1	3	3	3	A	6120.911	-0.020	-0.014
3	2	2	3	1	3	3	3	E	6120.911	0.024	
3	2	2	3	1	3	4	4	A	6122.554	-0.023	-0.017
3	2	2	3	1	3	4	4	E	6122.554	0.020	
3	2	2	3	1	3	2	2	A	6123.133	-0.020	-0.014
3	2	2	3	1	3	2	2	E	6123.133	0.023	
4	0	4	3	0	3	3	3	A	6307.874	-0.003	-0.001
4	0	4	3	0	3	3	3	E	6307.874	0.001	
4	0	4	3	0	3	5	4	A	6309.265	-0.009	-0.007
4	0	4	3	0	3	5	4	E	6309.265	-0.005	
4	0	4	3	0	3	4	3	A	6309.541	-0.003	0.000
4	0	4	3	0	3	4	3	E	6309.541	0.002	
4	0	4	3	0	3	4	4	A	6310.599	0.000	0.002
4	0	4	3	0	3	4	4	E	6310.599	0.004	
4	1	4	3	1	3	3	3	A	6007.384	-0.003	-0.001
4	1	4	3	1	3	3	3	E	6007.384	0.000	
4	1	4	3	1	3	5	4	A	6009.498	-0.001	0.000
4	1	4	3	1	3	5	4	E	6009.498	0.001	
4	1	4	3	1	3	3	2	A	6009.606	-0.003	-0.001
4	1	4	3	1	3	3	2	E	6009.606	-0.001	
4	1	4	3	1	3	4	3	A	6009.666	-0.002	0.000
4	1	4	3	1	3	4	3	E	6009.666	0.000	
4	1	4	3	1	3	4	4	A	6011.309	-0.005	-0.003
4	1	4	3	1	3	4	4	E	6011.309	-0.003	
4	1	3	3	1	2	4	4	A	6982.701	-0.005	-0.002
4	1	3	3	1	2	4	4	E	6982.701	0.003	
4	1	3	3	1	2	3	2	A	6982.964	-0.006	-0.002
4	1	3	3	1	2	3	2	E	6982.964	0.002	
4	1	3	3	1	2	5	4	A	6983.049	-0.003	0.001
4	1	3	3	1	2	5	4	E	6983.049	0.005	
4	1	3	3	1	2	4	3	A	6983.190	-0.004	-0.001
4	1	3	3	1	2	4	3	E	6983.190	0.004	
4	1	3	3	1	2	3	3	A	6983.624	-0.005	-0.002
4	1	3	3	1	2	3	3	E	6983.624	0.003	
4	2	3	3	2	2	3	2	A	6527.267	0.001	0.004
4	2	3	3	2	2	3	2	E	6527.267	0.001	
4	2	3	3	2	2	5	4	A	6527.351	0.001	0.005
4	2	3	3	2	2	5	4	E	6527.351	0.001	
4	2	3	3	2	2	4	3	A	6527.675	0.000	0.004
4	2	3	3	2	2	4	3	E	6527.675	0.000	
4	2	2	3	2	1	4	4	A	6764.810	-0.001	0.002
4	2	2	3	2	1	4	4	E	6764.810	0.011	
4	2	2	3	2	1	3	2	A	6765.067	0.036	0.039
4	2	2	3	2	1	3	2	E	6765.067	0.048	

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Table S2 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
4	2	2	3	2	1	5	4	A	6765.067	-0.015	-0.012
4	2	2	3	2	1	5	4	E	6765.067	-0.003	
4	2	2	3	2	1	4	3	A	6765.151	-0.003	0.000
4	2	2	3	2	1	4	3	E	6765.151	0.009	
4	2	2	3	2	1	3	3	A	6765.494	-0.001	0.002
4	2	2	3	2	1	3	3	E	6765.494	0.011	
4	3	2	3	3	1	3	2	A	6592.670	0.003	0.007
4	3	2	3	3	1	5	4	A	6592.907	0.005	
4	3	2	3	3	1	4	3	A	6593.480	0.002	0.009
4	3	1	3	3	0	3	2	A	6602.383	0.002	
4	3	1	3	3	0	5	4	A	6602.612	0.001	0.006
4	3	1	3	3	0	4	3	A	6603.166	0.001	
4	1	3	4	1	4	4	4	A	2445.107	-0.009	0.005
4	1	3	4	1	4	4	4	E	2445.107	0.004	
4	1	3	4	1	4	5	5	A	2447.268	-0.009	0.005
4	1	3	4	1	4	5	5	E	2447.268	0.004	
4	1	3	4	1	4	3	3	A	2447.838	0.006	0.004
4	1	3	4	1	4	3	3	E	2447.838	0.019	
4	0	4	3	1	3	3	3	A	5145.549	0.001	-0.006
4	0	4	3	1	3	3	3	E	5145.549	-0.002	
4	0	4	3	1	3	4	3	A	5147.214	0.000	-0.006
4	0	4	3	1	3	4	3	E	5147.214	-0.003	
4	0	4	3	1	3	5	4	A	5147.535	0.000	0.009
4	0	4	3	1	3	5	4	E	5147.535	-0.003	
4	0	4	3	1	3	3	2	A	5147.772	0.002	0.002
4	0	4	3	1	3	3	2	E	5147.772	-0.001	
4	0	4	3	1	3	4	4	A	5148.858	-0.003	0.001
4	0	4	3	1	3	4	4	E	5148.858	-0.005	
4	1	4	3	0	3	3	3	A	7169.712	-0.004	0.001
4	1	4	3	0	3	3	3	E	7169.712	0.006	
4	1	4	3	0	3	3	2	A	7171.136	-0.005	0.003
4	1	4	3	0	3	3	2	E	7171.136	0.004	
4	1	4	3	0	3	5	4	A	7171.233	-0.005	-0.001
4	1	4	3	0	3	5	4	E	7171.233	0.004	
4	1	4	3	0	3	4	3	A	7171.991	-0.006	-0.001
4	1	4	3	0	3	4	3	E	7171.991	0.003	
4	1	4	3	0	3	4	4	A	7173.043	-0.010	-0.002
4	1	4	3	0	3	4	4	E	7173.043	-0.001	
4	1	3	4	0	4	4	4	A	3307.562	-0.008	-0.003
4	1	3	4	0	4	4	4	E	3307.562	0.011	
4	1	3	4	0	4	5	5	A	3309.231	-0.010	-0.004
4	1	3	4	0	4	5	5	E	3309.231	0.008	
4	1	3	4	0	4	3	3	A	3309.662	-0.009	-0.007
4	1	3	4	0	4	3	3	E	3309.662	0.009	
4	2	3	4	1	4	4	4	A	6638.919	-0.019	-0.004
4	2	3	4	1	4	4	4	E	6638.919	0.022	
4	2	3	4	1	4	5	5	A	6640.408	-0.019	-0.006
4	2	3	4	1	4	5	5	E	6640.408	0.021	
4	2	3	4	1	4	3	3	A	6640.795	-0.015	-0.005
4	2	3	4	1	4	3	3	E	6640.795	0.025	
4	2	2	4	1	3	3	3	A	4555.361	-0.009	-0.011
4	2	2	4	1	3	5	5	A	4555.419	0.030	
4	2	2	4	1	3	5	5	E	4555.361	-0.005	-0.011
4	2	2	4	1	3	4	4	A	4555.474	0.009	
4	2	2	4	1	3	4	4	E	4555.419	-0.022	-0.008
5	0	5	4	0	4	4	4	A	7741.938	-0.002	
5	0	5	4	0	4	4	4	E	7741.938	0.003	-0.005

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Table S2 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
5	0	5	4	0	4	6	5	A	7743.590	0.000	
5	0	5	4	0	4	6	5	E	7743.590	0.004	0.034
5	0	5	4	0	4	4	3	A	7743.590	-0.016	
5	0	5	4	0	4	4	3	E	7743.590	-0.011	0.014
5	0	5	4	0	4	5	4	A	7743.859	-0.003	
5	0	5	4	0	4	5	4	E	7743.859	0.002	-0.003
5	0	5	4	0	4	5	5	A	7745.190	0.003	
5	0	5	4	0	4	5	5	E	7745.190	0.007	0.000
5	1	5	4	1	4	4	4	A	7472.427	0.005	
5	1	5	4	1	4	4	4	E	7472.427	0.008	-0.017
5	1	5	4	1	4	6	5	A	7474.636	0.003	
5	1	5	4	1	4	6	5	E	7474.636	0.006	-0.004
5	1	5	4	1	4	4	3	A	7474.713	0.010	
5	1	5	4	1	4	4	3	E	7474.713	0.013	0.002
5	1	5	4	1	4	5	4	A	7474.765	-0.001	
5	1	5	4	1	4	5	4	E	7474.765	0.002	0.005
5	1	5	4	1	4	5	5	A	7476.590	0.009	
5	1	5	4	1	4	5	5	E	7476.590	0.012	0.002
5	2	4	4	2	3	6	5	A	8127.821	0.009	
5	2	4	4	2	3	6	5	E	8127.821	0.014	0.010
5	2	4	4	2	3	4	3	A	8127.821	0.034	
5	2	4	4	2	3	5	4	E	8128.023	0.009	-0.001
5	0	5	4	1	4	4	4	A	6879.494	0.008	
5	0	5	4	1	4	4	4	E	6879.494	0.008	0.009
5	0	5	4	1	4	5	4	A	6881.409	0.001	
5	0	5	4	1	4	5	4	E	6881.409	0.000	0.009
5	0	5	4	1	4	6	5	A	6881.628	0.002	
5	0	5	4	1	4	6	5	E	6881.628	0.001	0.035
5	0	5	4	1	4	4	3	A	6881.770	0.003	
5	0	5	4	1	4	4	3	E	6881.770	0.002	0.006
5	0	5	4	1	4	5	5	A	6883.228	0.005	
5	0	5	4	1	4	5	5	E	6883.228	0.004	-0.001
5	1	5	4	0	4	4	3	A	8336.580	0.039	
5	1	5	4	0	4	4	3	E	8336.580	0.047	0.001
5	1	5	4	0	4	6	5	A	8336.580	-0.017	
5	1	5	4	0	4	6	5	E	8336.580	-0.009	0.001
5	1	5	4	0	4	5	4	A	8337.214	-0.006	
5	1	5	4	0	4	5	4	E	8337.214	0.002	0.004
5	1	4	4	2	3	5	4	A	4476.536	0.006	
5	1	4	4	2	3	5	4	E	4476.536	-0.012	0.039
5	1	4	4	2	3	6	5	A	4477.060	0.006	
5	1	4	4	2	3	6	5	E	4477.060	-0.012	-0.017
5	1	4	4	2	3	4	3	A	4477.183	0.005	
5	1	4	4	2	3	4	3	E	4477.183	-0.013	-0.006
5	1	4	5	0	5	5	5	A	4234.071	0.012	
5	1	4	5	0	5	5	5	E	4234.026	-0.010	0.002
5	1	4	5	0	5	6	6	A	4235.855	-0.001	
5	1	4	5	0	5	6	6	E	4235.824	-0.008	0.002
5	1	4	5	0	5	4	4	A	4236.227	0.006	
5	1	4	5	0	5	4	4	E	4236.191	-0.007	0.002
5	2	4	5	1	5	5	5	A	7292.178	-0.012	
5	2	4	5	1	5	5	5	E	7292.178	0.030	0.017
5	2	4	5	1	5	6	6	A	7293.591	-0.015	
5	2	4	5	1	5	6	6	E	7293.591	0.027	0.005
5	2	4	5	1	5	4	4	A	7293.883	-0.012	
5	2	4	5	1	5	4	4	E	7293.883	0.031	0.012
5	2	3	5	1	4	5	5	A	4452.466	0.004	

Continued on next page

Table S2 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
5	2	3	5	1	4	5	5	E	4452.431	-0.006	-0.004
5	2	3	5	1	4	6	6	A	4452.587	0.001	
5	2	3	5	1	4	6	6	E	4452.548	-0.013	-0.007
5	2	3	5	1	4	4	4	A	4452.587	-0.024	
5	2	3	5	1	4	4	4	E	4452.587	0.000	-0.003
6	1	5	5	2	4	6	5	A	6658.710	0.006	
6	1	5	5	2	4	6	5	E	6658.710	-0.006	0.009
6	1	5	5	2	4	7	6	A	6659.266	0.004	
6	1	5	5	2	4	7	6	E	6659.266	-0.008	0.006
6	1	5	5	2	4	5	4	A	6659.376	0.001	
6	1	5	5	2	4	5	4	E	6659.376	-0.011	-0.019
6	1	5	6	0	6	6	6	A	5411.257	0.003	
6	1	5	6	0	6	7	7	A	5413.124	0.007	-0.001
6	1	5	6	0	6	5	5	A	5413.437	0.006	
6	2	4	6	1	5	7	7	A	4535.261	-0.012	-0.003
6	2	4	6	1	5	7	7	E	4535.261	0.014	
6	2	4	6	1	5	5	5	A	4535.310	-0.024	-0.005
6	2	4	6	1	5	5	5	E	4535.310	0.001	
7	1	6	7	0	7	7	7	A	6797.324	-0.022	0.010
7	1	6	7	0	7	7	7	E	6797.324	0.015	
7	1	6	7	0	7	8	8	A	6799.168	-0.027	0.014
7	1	6	7	0	7	8	8	E	6799.168	0.011	
7	1	6	7	0	7	6	6	A	6799.444	-0.017	0.013
7	1	6	7	0	7	6	6	E	6799.444	0.020	
7	2	5	7	1	6	7	7	A	4857.000	-0.018	-0.006
7	2	5	7	1	6	7	7	E	4857.000	0.009	
7	2	5	7	1	6	8	8	A	4857.618	-0.010	-0.019
7	2	5	7	1	6	8	8	E	4857.618	0.017	
7	2	5	7	1	6	6	6	A	4857.692	-0.024	-0.013
7	2	5	7	1	6	6	6	E	4857.692	0.003	
8	2	6	8	1	7	8	8	A	5458.481	0.011	-0.018
8	2	6	8	1	7	9	9	A	5459.304	-0.005	-0.008
8	2	6	8	1	7	7	7	A	5459.421	0.007	-0.012
12	12	0	11	11	0	12	11	E	60812.530	0.196	
12	12	0	11	11	1	12	11	A	60812.060	-0.029	-0.003
12	12	1	11	11	0	12	11	A	60812.060	-0.029	-0.017
12	12	1	11	11	1	12	11	E	60811.210	-0.133	
13	12	2	12	11	1	13	12	A	62457.070	-0.051	0.019
13	12	1	12	11	2	13	12	A	62457.070	-0.051	0.003
14	12	2	13	11	2	14	13	E	64101.990	-0.047	
14	12	3	13	11	2	14	13	A	64101.840	0.045	0.015
14	12	2	13	11	3	14	13	A	64101.840	0.045	-0.003
14	12	3	13	11	3	14	13	E	64101.080	0.033	
14	11	3	13	10	3	14	13	E	60529.360	-0.088	
14	11	3	13	10	4	14	13	A	60529.150	-0.033	-0.003
14	11	4	13	10	3	14	13	A	60529.150	-0.033	-0.036
14	11	4	13	10	4	14	13	E	60528.390	-0.061	
15	12	4	14	11	3	15	14	A	65745.900	0.057	-0.036
15	12	3	14	11	4	15	14	A	65745.900	0.057	0.045
15	11	4	14	10	5	15	14	A	62171.860	0.023	0.045
15	11	5	14	10	4	15	14	A	62171.860	0.023	-0.044
15	11	5	14	10	5	15	14	E	62171.100	-0.005	
16	11	5	15	10	6	16	15	A	63812.970	0.052	-0.044
16	11	6	15	10	5	16	15	A	63812.970	0.052	0.037
16	11	6	15	10	6	16	15	E	63812.170	-0.015	
16	10	6	15	9	6	16	15	E	60232.020	0.041	
16	10	6	15	9	7	16	15	A	60231.750	0.057	0.037

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Table S2 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Sym	ν_{obs}	$\Delta\nu_{XIAM}$	$\Delta\nu_{SPFIT}$
16	10	7	15	9	6	16	15	A	60231.750	0.059	-0.010
16	10	7	15	9	7	16	15	E	60230.960	-0.015	
17	10	7	16	9	7	17	16	E	61865.950	-0.070	
17	10	7	16	9	8	17	16	A	61865.700	-0.038	-0.010
17	10	8	16	9	7	17	16	A	61865.700	-0.031	-0.006
17	10	8	16	9	8	17	16	E	61864.960	-0.056	

Table S3: Experimental rotational transition frequencies of 3'(E)-aminoacetophenone (ν /MHz, $\Delta\nu = \nu_{obs} - \nu_{calc}$).

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}	$\Delta\nu$
1	1	1	0	0	0	0	1	3219.925	-0.002
1	1	1	0	0	0	2	1	3220.881	-0.002
1	1	1	0	0	0	1	1	3221.518	-0.003
2	0	2	1	0	1	1	1	3269.015	0.001
2	0	2	1	0	1	3	2	3270.113	0.000
2	0	2	1	0	1	2	1	3270.306	-0.001
2	0	2	1	0	1	1	0	3270.606	-0.002
2	0	2	1	0	1	2	2	3270.942	-0.002
2	1	2	1	1	1	1	1	3040.196	-0.004
2	1	2	1	1	1	3	2	3041.594	-0.002
2	1	2	1	1	1	1	0	3041.789	-0.004
2	1	2	1	1	1	2	1	3042.322	-0.003
2	1	2	1	1	1	2	2	3042.963	0.001
2	1	1	1	1	0	1	0	3555.263	-0.001
2	1	1	1	1	0	2	2	3556.115	0.001
2	1	1	1	1	0	3	2	3556.798	0.001
2	1	1	1	1	0	2	1	3557.387	-0.002
2	1	1	1	1	0	1	1	3558.454	0.002
2	1	2	1	0	1	1	1	4611.524	-0.002
2	1	2	1	0	1	3	2	4612.919	-0.004
2	1	2	1	0	1	1	0	4613.114	-0.006
2	1	2	1	0	1	2	1	4613.649	-0.003
2	1	2	1	0	1	2	2	4614.284	-0.005
2	1	1	2	0	2	3	3	2115.858	-0.003
2	2	0	2	1	1	2	1	4741.931	-0.002
2	2	0	2	1	1	2	3	4742.308	-0.006
2	2	0	2	1	1	2	2	4742.995	-0.002
2	2	0	2	1	1	3	3	4743.142	-0.003
2	2	0	2	1	1	1	1	4743.226	0.000
2	2	0	2	1	1	3	2	4743.827	-0.001
2	2	0	2	1	1	1	2	4744.289	-0.001
2	2	1	2	1	2	2	2	5484.980	-0.001
2	2	1	2	1	2	3	2	5485.659	-0.005
2	2	1	2	1	2	1	2	5486.047	0.004
2	2	1	2	1	2	2	3	5486.346	-0.001
2	2	1	2	1	2	3	3	5487.026	-0.004
2	2	1	2	1	2	2	1	5487.106	0.000
2	2	1	2	1	2	1	1	5488.167	-0.001
3	0	3	2	0	2	2	2	4833.551	-0.002
3	0	3	2	0	2	4	3	4834.760	-0.002
3	0	3	2	0	2	2	1	4834.843	-0.002
3	0	3	2	0	2	3	2	4835.008	-0.003
3	0	3	2	0	2	3	3	4835.838	-0.004
3	1	3	2	1	2	2	2	4543.359	-0.002
3	1	3	2	1	2	4	3	4545.297	-0.003
3	1	3	2	1	2	2	1	4545.485	-0.001

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Table S3 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν	$\Delta\nu$
3	1	3	2	1	2	3	2	4545.568	-0.004
3	1	3	2	1	2	3	3	4546.934	-0.005
3	1	2	2	1	1	3	3	5315.415	-0.001
3	1	2	2	1	1	2	1	5315.683	0.001
3	1	2	2	1	1	4	3	5315.895	0.001
3	1	2	2	1	1	3	2	5316.099	0.000
3	1	2	2	1	1	2	2	5316.745	-0.001
3	2	2	2	2	1	2	1	4948.457	0.001
3	2	2	2	2	1	4	3	4948.837	0.002
3	2	2	2	2	1	3	2	4949.520	0.001
3	2	1	2	2	0	2	1	5062.701	-0.003
3	2	1	2	2	0	4	3	5063.034	-0.001
3	2	1	2	2	0	3	2	5063.493	-0.002
3	2	1	2	2	0	2	2	5063.997	0.000
3	0	3	2	1	2	2	2	3490.207	-0.001
3	0	3	2	1	2	3	2	3491.667	0.001
3	0	3	2	1	2	4	3	3491.952	0.000
3	0	3	2	1	2	2	1	3492.334	0.001
3	0	3	2	1	2	3	3	3493.036	0.004
3	1	3	2	0	2	2	2	5886.700	-0.005
3	1	3	2	0	2	2	1	5887.992	-0.006
3	1	3	2	0	2	4	3	5888.104	-0.006
3	1	3	2	0	2	3	2	5888.907	-0.010
3	1	2	3	0	3	3	3	2595.439	0.004
3	1	2	3	0	3	4	4	2596.995	0.001
3	1	2	3	0	3	2	2	2597.546	0.006
3	2	1	3	1	2	4	4	4490.277	-0.009
3	2	1	3	1	2	3	3	4490.389	-0.004
3	2	2	3	1	3	4	4	5890.566	0.001
3	2	2	3	1	3	2	2	5891.139	0.000
4	0	4	3	0	3	3	3	6325.770	-0.004
4	0	4	3	0	3	5	4	6327.194	-0.012
4	0	4	3	0	3	4	3	6327.488	-0.001
4	0	4	3	0	3	4	4	6328.564	-0.005
4	1	4	3	1	3	3	3	6028.854	-0.002
4	1	4	3	1	3	5	4	6030.959	-0.001
4	1	4	3	1	3	3	2	6031.067	0.000
4	1	4	3	1	3	4	3	6031.132	0.000
4	1	4	3	1	3	4	4	6032.767	-0.004
4	1	3	3	1	2	4	4	7048.449	-0.002
4	1	3	3	1	2	3	2	7048.695	-0.001
4	1	3	3	1	2	5	4	7048.782	0.002
4	1	3	3	1	2	4	3	7048.932	0.002
4	1	3	3	1	2	3	3	7049.340	-0.003
4	2	3	3	2	2	3	2	6575.746	0.001
4	2	3	3	2	2	5	4	6575.832	0.003
4	2	2	3	2	1	4	4	6846.828	0.008
4	2	2	3	2	1	3	2	6847.135	-0.001
4	2	2	3	2	1	5	4	6847.135	-0.001
4	2	2	3	2	1	4	3	6847.135	-0.001
4	2	2	3	2	1	3	3	6847.598	0.013
4	3	2	3	3	1	3	2	6650.844	0.014
4	3	2	3	3	1	5	4	6651.070	0.008
4	3	2	3	3	1	4	3	6651.639	0.009
4	3	1	3	3	0	3	2	6663.197	0.004
4	3	1	3	3	0	5	4	6663.421	0.002
4	3	1	3	3	0	4	3	6663.960	-0.001

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Table S3 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν	$\Delta\nu$
4	0	4	3	1	3	3	3	5271.868	0.000
4	0	4	3	1	3	4	3	5273.583	0.000
4	0	4	3	1	3	5	4	5273.857	-0.001
4	0	4	3	1	3	3	2	5274.079	-0.001
4	0	4	3	1	3	4	4	5275.220	-0.001
4	1	4	3	0	3	3	3	7082.771	0.009
4	1	4	3	0	3	4	4	7086.117	-0.002
4	1	4	3	0	3	3	2	7084.214	-0.006
4	1	4	3	0	3	5	4	7084.304	-0.004
4	1	4	3	0	3	4	3	7085.034	-0.005
4	1	3	4	0	4	4	4	3316.882	0.006
4	1	3	4	0	4	5	5	3318.570	0.002
4	1	3	4	0	4	3	3	3319.009	0.005
4	2	2	4	1	3	4	3	4288.234	-0.007
4	2	2	4	1	3	4	5	4288.322	-0.004
4	2	2	4	1	3	3	3	4288.627	-0.010
4	2	2	4	1	3	5	5	4288.627	-0.010
4	2	2	4	1	3	5	4	4288.968	0.001
4	2	2	4	1	3	3	4	4289.050	0.002
4	2	3	4	0	4	5	5	7192.528	-0.008
4	2	3	4	1	4	4	4	6433.958	0.008
4	2	3	4	1	4	5	5	6435.441	0.007
4	2	3	4	1	4	3	3	6435.822	0.006
5	0	5	4	0	4	6	5	7752.210	-0.002
5	0	5	4	0	4	4	3	7752.210	-0.002
5	0	5	4	0	4	5	4	7752.478	-0.003
5	1	5	4	1	4	6	5	7496.741	0.000
5	1	5	4	1	4	4	3	7496.809	-0.001
5	1	5	4	1	4	5	4	7496.876	-0.002
5	0	5	4	1	4	5	4	6994.935	0.003
5	0	5	4	1	4	6	5	6995.104	0.003
5	0	5	4	1	4	4	3	6995.235	0.002
5	1	4	4	2	3	5	4	4867.509	0.002
5	1	4	4	2	3	6	5	4868.007	0.005
5	1	4	4	2	3	4	3	4868.122	0.002
5	1	4	5	0	5	5	5	4306.522	-0.003
5	1	4	5	0	5	6	6	4308.334	-0.001
5	1	4	5	0	5	4	4	4308.700	-0.003
5	1	5	4	0	4	5	4	8254.408	-0.019
5	1	5	4	0	4	6	5	8253.820	-0.001
5	1	5	4	0	4	4	3	8253.820	-0.001
5	2	4	5	1	5	5	5	7120.864	0.007
5	2	4	5	1	5	6	6	7122.275	0.007
5	2	4	5	1	5	4	4	7122.565	0.010
5	2	3	5	1	4	5	5	4225.160	-0.003
5	2	3	5	1	4	6	6	4225.371	-0.009
5	2	3	5	1	4	4	4	4225.371	-0.009
5	3	2	5	2	3	5	5	7885.373	0.004
5	3	2	5	2	3	6	6	7885.183	0.011
6	1	5	6	0	6	6	6	5551.151	-0.010
6	1	5	6	0	6	7	7	5553.001	-0.015
6	1	5	6	0	6	5	5	5553.318	-0.011
6	1	5	5	2	4	6	5	7062.982	0.009
6	1	5	5	2	4	7	6	7063.496	0.009
6	1	5	5	2	4	5	4	7063.613	0.020
6	2	4	6	1	5	7	7	4373.505	-0.002
6	2	4	6	1	5	5	5	4373.584	0.001

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Table S3 – *continued from previous page*

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν	$\Delta\nu$
6	2	4	6	1	5	6	6	4373.056	-0.005
6	3	3	6	2	4	5	5	7474.031	0.035
6	3	3	6	2	4	7	7	7474.031	-0.019
6	3	3	6	2	4	6	6	7474.372	0.000
7	1	6	7	0	7	7	7	6993.604	-0.008
7	1	6	7	0	7	8	8	6995.426	0.002
7	1	6	7	0	7	7	8	6995.693	0.017
7	2	5	7	1	6	7	7	4787.097	-0.002
7	2	5	7	1	6	8	8	4787.794	0.002
7	2	5	7	1	6	6	6	4787.891	-0.001
7	3	4	7	2	5	8	8	7027.686	0.001
7	3	4	7	2	5	7	7	7027.990	-0.005
8	2	6	8	1	7	8	8	5505.108	-0.009
8	2	6	8	1	7	9	9	5506.025	-0.011
8	2	6	8	1	7	7	7	5506.146	-0.006
13	12	1	12	11	2	13	12	60560.640	-0.064
13	12	2	12	11	1	13	12	60560.640	-0.064
14	12	2	13	11	3	14	13	62219.620	0.113
14	12	3	13	11	2	14	13	62219.620	0.113
15	11	4	14	10	5	15	14	60484.080	-0.016
15	11	5	14	10	4	15	14	60484.080	-0.016
16	11	5	15	10	6	16	15	62138.670	-0.074
16	11	6	15	10	5	16	15	62138.670	-0.074
17	10	7	16	9	8	17	16	60383.350	0.015
17	10	8	16	9	7	17	16	60383.350	0.031

Table S4: Experimental rotational transition frequencies of $^{13}\text{C1-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4310.524	0.004
3	1	2	2	1	1	4	3	4532.792	-0.009
4	0	4	3	0	3	5	4	5725.150	0.007
4	0	4	3	0	3	4	3	5725.263	0.004
4	1	3	3	1	2	5	4	6037.869	-0.002
4	1	3	3	1	2	3	2	6037.809	0.001
4	1	3	3	1	2	4	3	6037.967	-0.002
4	1	4	3	1	3	5	4	5488.966	-0.002
5	0	5	4	0	4	6	5	7121.516	-0.012
5	0	5	4	0	4	5	4	7121.665	0.004
5	1	4	4	1	3	6	5	7537.603	0.006
5	1	4	4	1	3	5	4	7537.603	0.006
5	1	5	4	1	4	6	5	6852.887	-0.001

Table S5: Experimental rotational transition frequencies of $^{13}\text{C2-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4308.816	0.001
3	1	2	2	1	1	4	3	4533.744	0.003
4	0	4	3	0	3	5	4	5722.134	0.001
4	0	4	3	0	3	4	3	5722.254	0.003
4	1	3	3	1	2	3	2	6038.852	-0.004
4	1	3	3	1	2	5	4	6038.918	-0.001
4	1	3	3	1	2	4	3	6039.024	0.007
4	1	4	3	1	3	5	4	5484.457	0.003
5	0	5	4	0	4	6	5	7116.645	-0.003
5	0	5	4	0	4	5	4	7116.786	0.003
5	1	4	4	1	3	6	5	7538.553	-0.005
5	1	4	4	1	3	5	4	7538.553	-0.005
5	1	5	4	1	4	6	5	6846.975	-0.004

Table S6: Experimental rotational transition frequencies of $^{13}\text{C3-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4296.036	-0.002
3	1	3	2	1	2	4	3	4105.762	-0.003
4	0	4	3	0	3	5	4	5705.409	0.003
4	0	4	3	0	3	4	3	5705.525	0.002
4	1	3	3	1	2	3	2	6019.858	0.002
4	1	3	3	1	2	5	4	6019.924	0.005
4	1	3	3	1	2	4	3	6020.010	-0.007
4	1	4	3	1	3	5	4	5468.927	-0.007
5	0	5	4	0	4	6	5	7096.199	-0.010
5	0	5	4	0	4	5	4	7096.351	0.007
5	1	4	4	1	3	6	5	7514.950	-0.001
5	1	4	4	1	3	5	4	7514.950	-0.001
5	1	5	4	1	4	6	5	6827.691	0.000
5	1	5	4	1	4	5	4	6827.795	0.007

Table S7: Experimental rotational transition frequencies of $^{13}\text{C4-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4285.017	-0.002
3	1	2	2	1	1	4	3	4504.443	0.002
3	1	3	2	1	2	4	3	4097.274	0.000
3	1	3	2	1	2	3	2	4097.542	0.001
4	0	4	3	0	3	5	4	5691.680	-0.001
4	1	3	3	1	2	3	2	6000.143	0.000
4	1	3	3	1	2	5	4	6000.203	-0.003
4	1	3	3	1	2	4	3	6000.305	0.001
4	1	4	3	1	3	5	4	5457.846	0.002
5	0	5	4	0	4	6	5	7080.529	0.001
5	1	4	4	1	3	6	5	7490.766	0.001
5	1	4	4	1	3	5	4	7490.766	0.001
5	1	5	4	1	4	6	5	6814.178	-0.002

Table S8: Experimental rotational transition frequencies of $^{13}\text{C5-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4296.408	-0.001
3	1	2	2	1	1	4	3	4519.968	0.001
3	1	2	2	1	1	3	2	4520.158	-0.004
3	1	3	2	1	2	4	3	4106.029	0.000
4	0	4	3	0	3	5	4	5705.863	0.006
4	0	4	3	0	3	4	3	5705.979	0.005
4	1	3	3	1	2	3	2	6020.568	0.005
4	1	3	3	1	2	5	4	6020.624	-0.002
4	1	3	3	1	2	4	3	6020.721	-0.003
4	1	4	3	1	3	5	4	5469.279	0.003
5	0	5	4	0	4	6	5	7096.697	-0.011
5	0	5	4	0	4	5	4	7096.849	0.006
5	1	4	4	1	3	6	5	7515.816	0.001
5	1	4	4	1	3	5	4	7515.816	0.001
5	1	5	4	1	4	6	5	6828.099	-0.004
5	1	5	4	1	4	5	4	6828.200	0.000

Table S9: Experimental rotational transition frequencies of $^{13}\text{C6-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4308.951	0.004
3	1	2	2	1	1	4	3	4533.816	-0.007
4	0	4	3	0	3	5	4	5722.332	0.008
4	0	4	3	0	3	4	3	5722.441	-0.002
4	1	3	3	1	2	5	4	6039.024	-0.009
4	1	3	3	1	2	4	3	6039.132	0.001
4	1	4	3	1	3	5	4	5484.671	0.000
5	0	5	4	0	4	6	5	7116.904	-0.005
5	0	5	4	0	4	5	4	7117.045	0.000
5	1	4	4	1	3	6	5	7538.718	0.010
5	1	4	4	1	3	5	4	7538.718	0.010
5	1	5	4	1	4	6	5	6847.255	-0.001

Table S10: Experimental rotational transition frequencies of $^{13}\text{C7-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4285.057	0.009
3	1	2	2	1	1	4	3	4504.510	-0.006
3	1	3	2	1	2	4	3	4097.227	-0.006
3	1	3	2	1	2	3	2	4097.498	-0.003
4	0	4	3	0	3	4	3	5691.855	0.004
4	1	3	3	1	2	3	2	6000.254	0.007
4	1	3	3	1	2	5	4	6000.305	-0.005
4	1	3	3	1	2	4	3	6000.400	-0.007
4	1	4	3	1	3	5	4	5457.790	-0.004
5	0	5	4	0	4	5	4	7080.746	-0.006
5	1	4	4	1	3	6	5	7490.909	0.006
5	1	4	4	1	3	5	4	7490.909	0.006
5	1	5	4	1	4	6	5	6814.130	0.007

Table S11: Experimental rotational transition frequencies of $^{13}\text{C8-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4256.445	0.004
3	1	2	2	1	1	4	3	4475.343	0.006
3	1	2	2	1	1	3	2	4475.530	-0.002
3	1	3	2	1	2	4	3	4069.365	0.009
3	1	3	2	1	2	3	2	4069.627	0.003
4	0	4	3	0	3	5	4	5653.487	-0.001
4	0	4	3	0	3	4	3	5653.613	0.010
4	1	3	3	1	2	5	4	5961.372	-0.002
4	1	3	3	1	2	3	2	5961.314	0.002
4	1	3	3	1	2	4	3	5961.465	-0.007
4	1	4	3	1	3	5	4	5420.607	0.007
5	0	5	4	0	4	6	5	7032.648	-0.010
5	0	5	4	0	4	5	4	7032.798	0.008
5	1	5	4	1	4	6	5	6767.598	0.003
5	1	5	4	1	4	5	4	6767.673	-0.019

Table S12: Experimental rotational transition frequencies of $^{15}\text{N-4AA}$

J'	K'_a	K'_c	J''	K''_a	K''_c	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4238.414	-0.004
3	1	2	2	1	1	4452.696	0.004
4	0	4	3	0	3	5630.510	-0.003
4	1	4	3	1	3	5400.849	-0.003
4	1	3	3	1	2	5931.450	-0.004
5	0	5	4	0	4	7005.571	0.002
5	1	5	4	1	4	6743.268	0.004
5	1	4	4	1	3	7405.239	0.002

Table S13: Experimental rotational transition frequencies of $^{13}\text{C1-3AA-Z}$.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4808.965	0.001
3	0	3	2	0	2	2	1	4809.050	-0.002
3	0	3	2	0	2	3	2	4809.195	-0.002
3	1	3	2	1	2	3	2	4524.826	-0.004
4	1	4	3	1	3	5	4	6006.971	-0.002
4	1	4	3	1	3	3	2	6007.076	-0.005
4	1	4	3	1	3	4	3	6007.146	0.005
3	1	2	2	1	1	2	1	5259.574	0.001
3	1	2	2	1	1	4	3	5259.786	0.001
4	0	4	3	0	3	5	4	6306.647	-0.010
4	0	4	3	0	3	4	3	6306.923	-0.003
2	0	2	1	0	1	3	2	3246.785	0.003
4	1	3	3	1	2	5	4	6979.709	0.004
5	1	5	4	1	4	6	5	7471.547	0.010
5	1	5	4	1	4	5	4	7471.676	0.006
2	1	2	1	0	1	3	2	4693.602	-0.003
4	0	4	3	1	3	5	4	5144.241	0.003
4	0	4	3	1	3	4	3	5143.911	-0.005
4	0	4	3	1	3	3	2	5144.471	-0.002

Table S14: Experimental rotational transition frequencies of $^{13}\text{C2-3AA-Z}$.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4806.606	-0.003
3	0	3	2	0	2	2	1	4806.698	0.001
3	0	3	2	0	2	3	2	4806.843	0.000
3	1	3	2	1	2	4	3	4522.015	-0.002
3	1	3	2	1	2	3	2	4522.291	0.003
4	1	4	3	1	3	5	4	6003.325	-0.003
4	1	4	3	1	3	4	3	6003.500	0.003
3	1	2	2	1	1	2	1	5259.162	0.002
3	1	2	2	1	1	3	2	5259.574	0.001
3	1	2	2	1	1	4	3	5259.372	0.000
4	0	4	3	0	3	5	4	6302.538	-0.006
4	0	4	3	0	3	4	3	6302.817	0.002
2	0	2	1	0	1	3	2	3245.635	-0.003
4	1	3	3	1	2	5	4	6978.752	-0.006
5	1	5	4	1	4	5	4	7466.780	-0.002
2	1	2	1	0	1	3	2	4682.674	0.006
4	0	4	3	1	3	5	4	5150.108	0.003
4	0	4	3	1	3	4	3	5149.790	0.002
4	0	4	3	1	3	3	2	5150.342	0.003
3	1	3	2	0	2	4	3	5959.053	0.006
3	1	3	2	0	2	3	2	5959.874	0.004
3	1	3	2	0	2	2	1	5958.921	-0.008

Table S15: Experimental rotational transition frequencies of $^{13}\text{C3-3AA-Z}$.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4786.224	0.000
3	0	3	2	0	2	2	1	4786.308	-0.004
3	0	3	2	0	2	3	2	4786.453	-0.002
3	1	3	2	1	2	4	3	4503.553	0.002
3	1	3	2	1	2	3	2	4503.818	-0.003
4	1	4	3	1	3	5	4	5979.403	-0.003
4	1	4	3	1	3	3	2	5979.518	0.004
4	1	4	3	1	3	4	3	5979.566	-0.007
3	1	2	2	1	1	2	1	5232.100	-0.001
3	1	2	2	1	1	3	2	5232.519	0.006
3	1	2	2	1	1	4	3	5232.307	-0.007
4	0	4	3	0	3	5	4	6278.065	-0.003
4	0	4	3	0	3	4	3	6278.327	-0.009
2	0	2	1	0	1	3	2	3230.890	-0.001
4	1	3	3	1	2	5	4	6943.738	0.008
5	1	5	4	1	4	6	5	7437.682	0.004
5	1	5	4	1	4	5	4	7437.812	0.002
5	1	5	4	1	4	4	3	7437.756	0.008
2	1	2	1	0	1	3	2	4682.118	-0.008
4	0	4	3	1	3	5	4	5109.508	0.002
4	0	4	3	1	3	4	3	5109.171	-0.009
4	0	4	3	1	3	3	2	5109.747	0.005
3	1	3	2	0	2	4	3	5954.794	0.008

Table S16: Experimental rotational transition frequencies of $^{13}\text{C4-3AA-Z}$.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4774.367	0.001
3	0	3	2	0	2	2	1	4774.458	0.004
3	0	3	2	0	2	3	2	4774.598	0.001
3	1	3	2	1	2	4	3	4492.300	0.001
3	1	3	2	1	2	3	2	4492.567	-0.002
3	1	3	2	1	2	2	1	4492.492	0.005
4	1	4	3	1	3	5	4	5964.395	-0.001
4	1	4	3	1	3	3	2	5964.515	0.009
4	1	4	3	1	3	4	3	5964.561	-0.003
3	1	2	2	1	1	2	1	5219.700	-0.006
3	1	2	2	1	1	3	2	5220.122	0.004
3	1	2	2	1	1	4	3	5219.919	0.001
4	0	4	3	0	3	5	4	6262.245	-0.005
4	0	4	3	0	3	4	3	6262.521	0.004
2	0	2	1	0	1	3	2	3222.996	-0.005
4	1	3	3	1	2	5	4	6927.178	0.001
5	1	5	4	1	4	6	5	7418.914	-0.002
5	1	5	4	1	4	5	4	7419.047	-0.002
5	1	5	4	1	4	4	3	7418.987	0.001
2	1	2	1	0	1	3	2	4668.319	0.002
4	0	4	3	1	3	5	4	5098.998	-0.001
4	0	4	3	1	3	4	3	5098.672	-0.003
3	1	3	2	0	2	4	3	5937.611	-0.005

Table S17: Experimental rotational transition frequencies of $^{13}\text{C5-3AA-Z}$.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4786.946	0.002
3	0	3	2	0	2	2	1	4787.033	0.002
3	0	3	2	0	2	3	2	4787.185	0.002
3	1	3	2	1	2	3	2	4502.740	0.002
4	1	4	3	1	3	5	4	5976.455	-0.002
4	1	4	3	1	3	4	3	5976.625	-0.003
3	1	2	2	1	1	3	2	5245.363	0.000
3	1	2	2	1	1	4	3	5245.162	0.001
4	0	4	3	0	3	5	4	6273.298	-0.006
4	0	4	3	0	3	4	3	6273.572	-0.007
2	0	2	1	0	1	3	2	3233.875	-0.004
4	1	3	3	1	2	5	4	6958.535	0.000
5	1	5	4	1	4	6	5	7432.024	-0.001
5	1	5	4	1	4	5	4	7432.168	0.008
5	1	5	4	1	4	4	3	7432.090	-0.005
2	1	2	1	0	1	3	2	4635.141	-0.009
4	0	4	3	1	3	5	4	5156.518	0.008
4	0	4	3	1	3	4	3	5156.208	0.003
4	0	4	3	1	3	3	2	5156.736	-0.006
3	1	3	2	0	2	4	3	5903.736	-0.001
3	1	3	2	0	2	3	2	5904.564	0.007
3	1	3	2	0	2	2	1	5903.628	0.008

Table S18: Experimental rotational transition frequencies of $^{13}\text{C6-3AA-Z}$.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4801.203	0.001
3	0	3	2	0	2	2	1	4801.290	0.001
3	0	3	2	0	2	3	2	4801.442	0.002
3	1	3	2	1	2	4	3	4516.251	0.004
3	1	3	2	1	2	3	2	4516.518	0.000
3	1	3	2	1	2	2	1	4516.439	0.004
4	1	4	3	1	3	5	4	5995.076	-0.001
4	1	4	3	1	3	3	2	5995.190	0.003
4	1	4	3	1	3	4	3	5995.247	0.000
3	1	2	2	1	1	2	1	5257.959	0.003
3	1	2	2	1	1	3	2	5258.374	0.004
3	1	2	2	1	1	4	3	5258.169	0.000
4	0	4	3	0	3	5	4	6293.226	0.001
4	0	4	3	0	3	4	3	6293.508	0.009
2	0	2	1	0	1	3	2	3242.964	-0.002
4	1	3	3	1	2	5	4	6976.281	-0.002
5	1	5	4	1	4	6	5	7455.616	0.005
5	1	5	4	1	4	5	4	7455.746	0.002
5	1	5	4	1	4	4	3	7455.670	-0.010
2	1	2	1	0	1	3	2	4658.933	-0.005
4	0	4	3	1	3	5	4	5162.203	-0.006
4	0	4	3	1	3	4	3	5161.892	-0.007
3	1	3	2	0	2	4	3	5932.214	-0.004
3	1	3	2	0	2	3	2	5933.036	-0.003

Table S19: Experimental rotational transition frequencies of $^{13}\text{C7-3AA-Z}$.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4782.138	0.001
3	0	3	2	0	2	2	1	4782.226	0.000
3	0	3	2	0	2	3	2	4782.368	0.000
3	1	3	2	1	2	4	3	4499.835	0.005
4	1	4	3	1	3	5	4	5974.566	0.000
4	1	4	3	1	3	4	3	5974.729	-0.004
3	1	2	2	1	1	3	2	5227.233	-0.001
3	1	2	2	1	1	4	3	5227.027	-0.007
4	0	4	3	0	3	5	4	6273.094	0.002
4	0	4	3	0	3	4	3	6273.365	0.005
2	0	2	1	0	1	3	2	3227.973	0.009
4	1	3	3	1	2	5	4	6936.870	-0.002
5	1	5	4	1	4	6	5	7431.771	-0.020
5	1	5	4	1	4	5	4	7431.929	0.006
2	1	2	1	0	1	3	2	4681.498	0.000
4	0	4	3	1	3	5	4	5101.876	0.009
4	0	4	3	1	3	4	3	5101.540	0.000
3	1	3	2	0	2	4	3	5953.365	0.001
3	1	3	2	0	2	3	2	5954.186	-0.001
3	1	3	2	0	2	2	1	5953.251	0.007

Table S20: Experimental rotational transition frequencies of $^{13}\text{C8-3AA-Z}$.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$
3	0	3	2	0	2	4	3	4739.611	-0.002
3	0	3	2	0	2	2	1	4739.697	-0.004
3	0	3	2	0	2	3	2	4739.841	0.001
3	1	3	2	1	2	4	3	4460.614	0.000
3	1	3	2	1	2	3	2	4460.880	-0.003
4	1	4	3	1	3	3	2	5923.226	-0.003
4	1	4	3	1	3	4	3	5923.292	0.006
4	1	4	3	1	3	5	4	5923.111	-0.008
3	1	2	2	1	1	2	1	5175.313	-0.002
3	1	2	2	1	1	3	2	5175.728	0.003
3	1	2	2	1	1	4	3	5175.525	-0.001
4	0	4	3	0	3	5	4	6219.683	-0.005
4	0	4	3	0	3	4	3	6219.954	0.003
2	0	2	1	0	1	3	2	3198.241	0.010
5	1	5	4	1	4	6	5	7368.627	0.003
5	1	5	4	1	4	5	4	7368.754	-0.001
5	1	5	4	1	4	4	3	7368.700	0.006
2	1	2	1	0	1	3	2	4660.950	0.001
4	0	4	3	1	3	5	4	5035.961	-0.007
4	0	4	3	1	3	4	3	5035.633	0.000
4	0	4	3	1	3	3	2	5036.213	0.006
3	1	3	2	0	2	3	2	5924.156	-0.002