

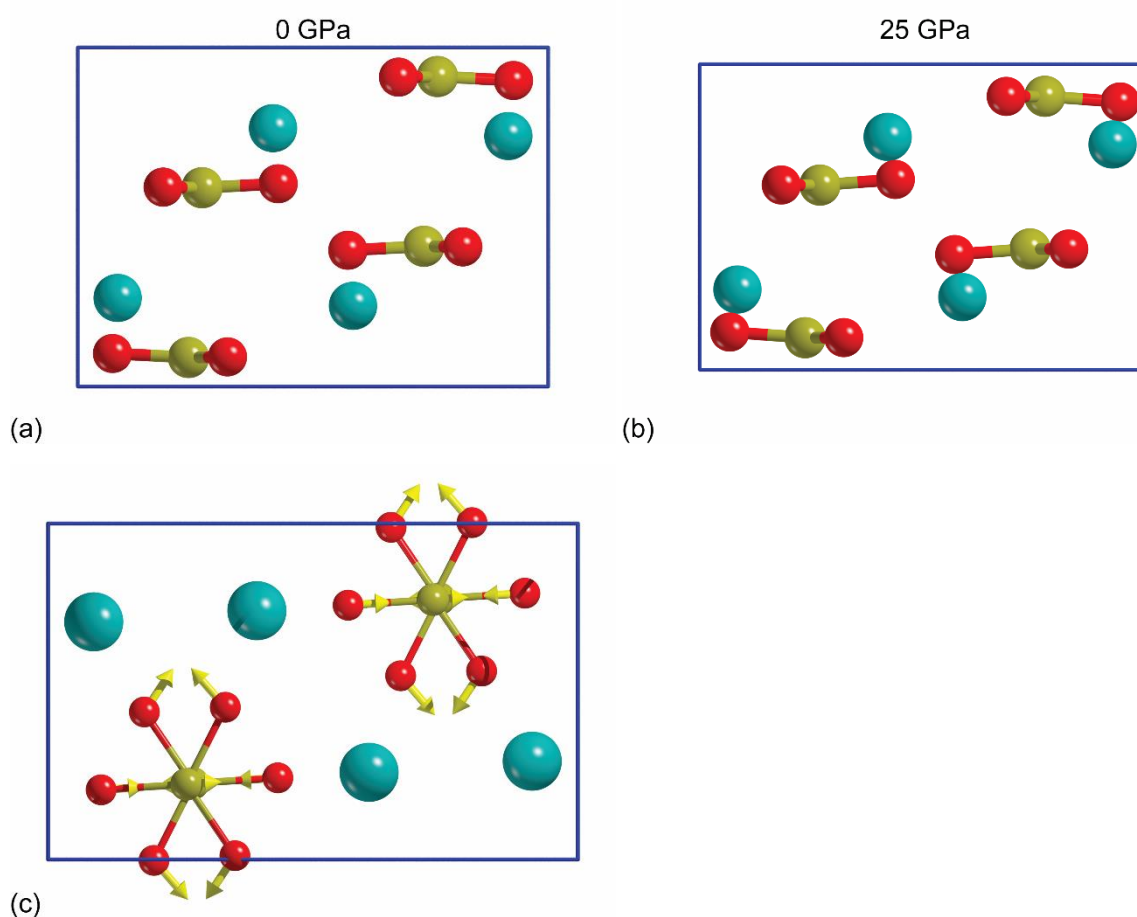
# The effect of long-range interactions on the infrared and Raman spectra of aragonite ( $\text{CaCO}_3$ , $Pm\bar{c}n$ ) up to 25 GPa

Gianfranco Ulian<sup>1</sup>, Giovanni Valdrè<sup>1,\*</sup>

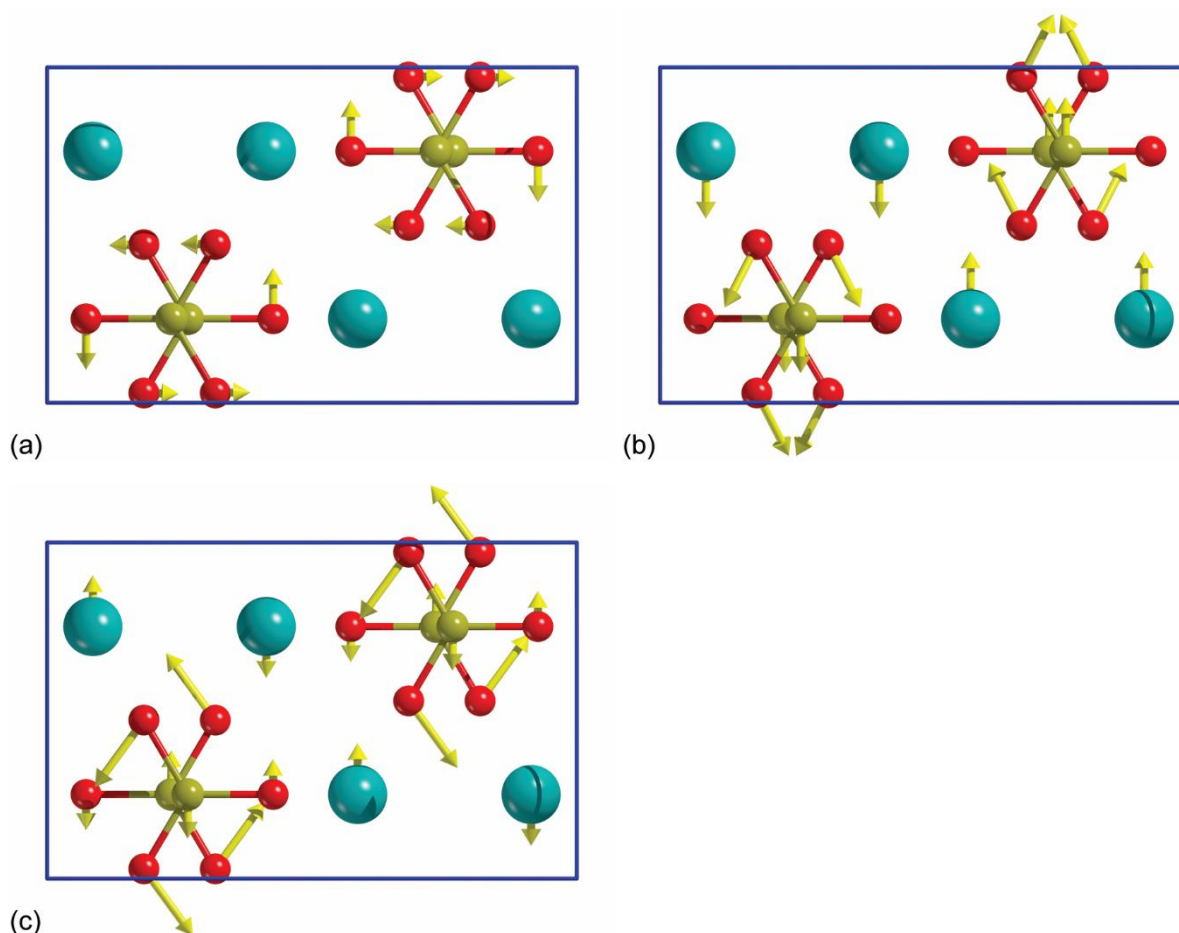
<sup>1</sup> Dipartimento di Scienze Biologiche, Geologiche e Ambientali, Centro di Ricerche

Interdisciplinari di Biomineralogia, Cristallografia e Biomateriali, Università di Bologna “Alma Mater Studiorum” Piazza di Porta San Donato 1, 40126 Bologna, Italy.

## Supplementary Materials



**Figure S1.** Views along the [100] direction of the configurations of aragonite (a) at 0 GPa and (b) at 25 GPa. It is worth noting the movements of the carbonate ions along the [001] direction (i.e., along the  $c$  axis). (c) The  $\nu_4$   $\text{CO}_3^{2-}$  normal mode as viewed from the [001] direction (see text for details).



**Figure S2.** Selected normal modes showing very high variation in the mode-Grüneisen's parameters between B3LYP-D\* and B3LYP-D3 methods. (a)  $A_u$  mode (silent), rotation of the carbonate ions around the C atom; (b)  $B_{3g}$  mode (Raman active), rotation of the carbonate ions around one of their O atoms; (c)  $B_{1g}$  mode (Raman active), rotation of the carbonate ions around one of their O atoms. In the three panels, Ca, C and O atoms are coloured in dark cyan, ochre and red, respectively, whereas the unit cell borders are represented with blue lines and the atom displacement vectors are shown as yellow arrows.

**Table S1.** Unit cell parameters (lattice constants and cell volume and mean relevant bond lengths and angles of aragonite as obtained from theoretical and experimental determinations.

	B3LYP <sup>1</sup>	B3LYP-D* <sup>2</sup>	B3LYP-D3 <sup>2</sup>	XRD <sup>3</sup>
a (Å)	5.008	5.0177	4.9544	4.96183
b (Å)	8.029	7.9005	7.8836	7.96914
c (Å)	5.861	5.7901	5.7091	5.74285
V (Å <sup>3</sup> )	235.666	229.535	222.987	227.081
<C-O> (Å)	1.2847	1.2829	1.2857	1.289
<O-C-O> (°)	119.95	119.95	-	2.5272
<Ca --- O> (Å)	2.5402	2.5135	-	119.89

**Table S2.** Infrared vibrational modes  $\nu$  ( $\text{cm}^{-1}$ ) and oscillator strengths  $f$  ( $\times 10^3$ , dimensionless) from simulations and from experimental measurements and fittings.

		$\nu_{\text{calc-D3}^1}$	$\nu_{\text{calc-D}^*2}$	$\nu_{\text{calc}^3}$	$\nu_{\text{exp}^3}$	$\Delta\nu_{\text{D3}}$	$\Delta\nu_{\text{D2}}$	$f_{\text{calc-D3}^1}$	$f_{\text{calc-D}^*2}$	$f_{\text{calc}^3}$	$f_{\text{exp}^3}$	$\Delta f_{\text{D3}}$	$\Delta f_{\text{D}^*}$
$B_{1u}$	L	197.0	180.4	174.1	183.1	13.9	-2.7	52.9	36.9	91.8	60.4	-7.5	-23.5
	L	232.7	213.6	210.1	207.8	24.9	5.8	3306.3	3795.6	3920.2	4105.6	-799.4	-310.0
	L	276.7	267.2	269.1	259.2	17.5	8.0	116.6	186.1	62.4	77.4	39.2	108.7
	L	309.9	291.0	288.9	286.9	23.0	4.1	21.7	18.8	35.0	43.5	-21.8	-24.7
	$\nu_4$	726.8	719.3	719.2	718.3	8.5	1.0	0.3	0.2	0.1	0.4	-0.1	-0.2
	$\nu_2$	860.2	862.1	861.9	852.2	8.0	9.9	128.7	117.2	113.1	116.1	12.6	1.1
	$\nu_1$	1100.9	1091.6	1092.9	1082.8	18.1	8.8	2.9	2.7	2.4	1.9	1.0	0.8
	$\nu_3$	1491.0	1485.7	1469.9	-	-	-	0.1	0.0	0.0	-	-	-
	$F[\Delta F]$							3629.4	4157.5	4225.0	4405.3	-775.9	-247.8
$B_{2u}$	L	90.0	27.8	65.4	105.4	-15.4	-77.6	4525.4	54048.2	6554.9	2228.3	2297.1	51819.9
	L	175.9	163.0	158.7	164.2	11.7	-1.2	1.2	1.0	62.1	53.4	-52.2	-52.4
	L	229.6	202.0	198	219.9	9.7	-17.9	4635.0	5675.7	5838.5	4862.0	-227.0	813.7
	$\nu_4$	703.5	697.7	697.4	699.8	3.7	-2.1	6.7	4.1	5.2	6.7	0.0	-2.6
	$\nu_3$	1461.3	1443.4	1445.1	1444.5	16.8	-1.1	479.5	478.7	467.1	458.0	21.5	20.7
	$F[\Delta F]$							9647.8	60207.7	12927.8	7608.4	2039.4	52599.3
$B_{3u}$	L	155.0	152.5	147.3	144.4	10.6	8.1	127.9	94.0	16.2	59.3	68.6	34.7
	L	221.3	199.0	200.7	208.6	12.7	-9.6	1911.1	2633.8	2617.5	1829.6	81.5	804.2
	L	274.4	248.7	245.5	249.5	24.9	-0.8	2147.7	2322.5	2286.7	2423.0	-275.3	-100.5
	L	316.5	304.8	293.1	298	18.5	6.8	0.0	0.1	7.0	164.9	-164.9	-164.8
	$\nu_4$	719.1	711.7	712.2	712.4	6.7	-0.7	20.7	17.9	15.5	16.6	4.1	1.3
	$\nu_2$	917.6	915.2	913.1	908.8	8.8	6.4	0.3	0.3	0.1	0.2	0.1	0.1
	$\nu_1$	1101.8	1092.5	1092.9	1082.8	19.0	9.7	1.8	3.4	1.3	1.1	0.7	2.3
	$\nu_3$	1493.4	1486.7	1474.1	1466.6	26.8	20.1	481.6	472.9	469.2	461.2	20.4	11.7
	$F[\Delta F]$							4691.1	5544.8	5413.5	4955.9	-264.8	588.9

Notes: 1 – present work, B3LYP-D3; 2 – present work, B3LYP-D\*; 3 – B3LYP (calc) and experimental data from the work of Carter et al.<sup>1</sup>.  $\Delta\nu$  and  $\Delta f$  is the difference between the vibrational frequencies and oscillator strengths, respectively, simulated in the present work and the reported experimental ones.  $F = \sum_n f_n$  is the sum of the oscillator strengths, whereas  $\Delta F = \sum_n |\Delta f_n|$  is the sum of the absolute differences between the calculated and the experimental oscillator strengths.

**Table S3.** Silent vibrational modes  $\nu$  ( $A_u$ ,  $\text{cm}^{-1}$ ) obtained from simulations at the DFT/B3LYP level of theory with and without corrections for the long-range interactions.

		<b>B3LYP-D3<sup>1</sup></b>	<b>B3LYP-D*<sup>1</sup></b>	<b>B3LYP<sup>2</sup></b>	<b>B3LYP<sup>3</sup></b>
$A_u$	L	106.8	49.5	70.8	69
	L	151.2	138.5	132.6	134
	L	170.9	150.2	147.6	143
	L	281.9	273.5	265.4	261
	$\nu_4$	696.9	691.2	686.8	692
	$\nu_3$	1404.5	1388.1	1420.1	1393

Notes: 1 – present work, 2 – theoretical study performed by Ungureanu et al.<sup>4</sup>; 3 – DFT simulations of Carteret and co-workers<sup>1</sup>.

**Table S4.** Vibrational modes  $\nu$  (cm<sup>-1</sup>) of aragonite, subdivided in irreducible representations (IRREPs), simulated at the DFT/B3LYP-D3 level of theory between about -3 GPa and 25 GPa.

IRREP	Pressure (GPa)														
	-3.1	-2	-1	0	1	3.1	5.1	7.1	9.2	11.2	13.3	15.4	20.6	24.9	
<i>B<sub>1u</sub></i>	177.8	184.6	190.9	197.0	202.7	213.5	224.1	233.9	243.6	252.6	261.3	269.8	289.2	302.6	
	214.0	220.8	227.3	233.0	238.4	248.4	257.7	266.0	272.8	278.5	284.7	290.7	303.2	310.8	
	269.2	271.6	274.0	276.5	279.1	284.5	289.9	295.5	300.8	306.0	311.2	316.6	330.4	340.8	
	291.9	298.4	304.6	310.2	315.5	325.5	335.2	344.8	354.0	362.8	371.6	380.4	401.6	417.1	
	718.7	721.4	724.1	726.4	729.1	733.6	738.6	743.0	747.4	752.0	756.3	760.5	769.8	777.5	
	862.1	861.6	861.0	860.4	859.9	858.7	857.7	856.5	855.2	853.5	852.0	850.7	847.7	845.2	
	1091.1	1094.3	1097.4	1100.0	1103.3	1109.1	1114.5	1119.7	1124.7	1129.7	1134.4	1138.4	1148.9	1157.4	
	1475.3	1480.5	1485.6	1490.1	1494.8	1503.3	1510.7	1518.5	1525.2	1531.9	1538.0	1543.6	1555.9	1565.6	
	<i>B<sub>2u</sub></i>	62.8	73.7	82.7	90.2	96.6	107.9	116.9	124.4	130.8	137.0	142.0	146.5	154.9	160.1
		160.1	165.6	171.0	176.1	181.2	191.6	201.8	211.6	221.0	229.6	238.3	246.6	265.1	279.3
201.9		211.7	221.0	229.7	237.7	253.1	267.3	280.4	292.3	303.4	313.8	323.5	344.3	360.3	
698.2		700.0	701.7	703.5	705.2	708.4	711.7	714.9	718.0	721.1	724.1	727.2	734.4	739.7	
1445.4		1450.8	1455.9	1461.0	1465.9	1475.3	1484.1	1492.6	1501.1	1509.1	1517.0	1524.6	1541.9	1557.2	
<i>B<sub>3u</sub></i>		149.7	151.6	153.5	155.1	156.5	159.4	162.3	165.3	167.8	170.1	172.3	174.5	178.3	179.8
		202.3	209.3	215.5	221.2	226.5	236.3	246.1	255.4	263.6	270.9	278.2	285.7	301.5	310.3
		250.3	258.7	267.0	274.6	281.6	294.9	307.7	319.6	330.7	341.3	351.7	361.9	386.9	404.5
		297.0	303.6	310.0	316.3	322.4	334.7	346.3	357.4	367.9	378.0	387.7	397.3	419.1	435.9
		711.4	714.0	716.5	719.0	721.3	725.9	730.5	735.1	739.6	744.0	748.4	752.6	762.4	770.3
	914.7	915.8	916.6	917.6	918.6	920.6	922.6	924.4	926.1	927.5	929.1	930.6	934.3	938.0	
	1091.4	1094.8	1098.3	1101.3	1104.8	1111.0	1116.6	1122.5	1128.2	1133.7	1139.1	1144.1	1156.1	1165.6	
	1478.9	1483.6	1488.2	1492.7	1496.9	1504.6	1511.5	1518.6	1525.2	1531.6	1537.8	1543.6	1557.6	1568.0	
	<i>A<sub>g</sub></i>	149.8	150.4	150.4	150.5	150.2	149.6	148.5	148.0	146.3	143.3	141.4	133.2	107.5	82.6
		162.8	167.4	171.4	175.1	178.3	184.6	189.4	193.1	195.6	196.2	198.1	196.1	191.5	199.7
199.4		204.0	207.4	210.1	212.6	216.6	220.8	225.7	230.2	235.2	239.6	248.1	261.4	281.9	
208.9		215.6	222.3	228.7	235.0	246.5	257.6	268.7	279.1	289.0	298.0	307.7	330.3	337.6	
283.8		291.3	299.1	306.4	313.2	326.9	340.1	352.1	363.5	373.2	383.0	394.6	420.6	445.1	
703.6		706.0	708.1	710.6	713.0	717.2	721.7	726.2	730.8	735.1	739.8	747.3	767.6	760.5	
863.0		862.4	861.8	861.3	860.8	859.6	858.5	857.3	856.0	853.1	853.3	853.1	849.6	847.3	
1093.7		1097.1	1100.4	1104.1	1107.0	1113.2	1118.9	1125.0	1130.7	1137.0	1141.3	1153.3	1178.5	1189.3	
1478.2		1482.2	1486.1	1489.7	1493.4	1499.7	1505.4	1511.5	1517.0	1522.0	1527.1	1533.8	1546.8	1554.4	
<i>B<sub>1g</sub></i>		105.4	113.0	119.7	125.2	129.9	138.1	144.9	150.5	155.1	158.9	162.3	165.3	171.6	172.4
	170.9	177.2	182.0	186.2	190.2	197.8	205.3	212.3	218.6	224.7	230.4	235.7	247.5	256.1	
	179.5	185.1	191.6	198.2	204.6	216.9	228.6	239.6	249.7	259.3	268.4	277.1	296.2	309.1	
	275.2	281.5	287.8	293.8	299.6	311.2	322.2	332.6	342.0	351.0	359.4	367.3	384.6	396.9	
	702.2	704.0	705.8	707.6	709.3	712.7	716.1	719.5	722.7	726.0	729.1	732.2	739.0	744.4	
	1414.0	1418.4	1422.5	1426.7	1430.7	1438.4	1445.7	1452.7	1459.6	1466.4	1472.9	1478.9	1495.3	1505.4	
	<i>B<sub>2g</sub></i>	186.5	191.5	195.6	198.8	201.4	205.4	209.4	212.8	215.9	218.8	222.0	225.6	236.8	247.2
		209.2	213.2	217.3	221.4	225.8	234.9	244.5	254.3	263.4	272.3	280.6	289.2	307.4	318.1
		251.1	256.1	260.8	265.1	268.8	275.7	281.5	287.1	292.1	296.8	302.0	307.0	319.0	328.1
		265.3	272.2	278.4	283.7	288.5	296.7	304.5	311.8	318.4	324.2	330.1	336.0	349.3	358.3
283.0		288.5	294.3	300.7	307.2	321.5	335.0	348.6	361.2	373.4	385.0	396.1	421.7	440.7	
714.4		717.5	720.5	723.3	726.1	731.5	737.0	742.2	747.5	752.5	757.5	762.3	773.8	782.4	
913.5		914.5	915.3	916.3	917.4	919.1	921.1	922.8	924.4	925.8	927.3	928.7	932.2	935.5	
1090.0		1093.2	1096.3	1099.3	1102.4	1108.0	1113.1	1118.3	1123.3	1128.1	1132.7	1136.9	1145.9	1154.7	
1596.4		1601.4	1606.2	1611.1	1615.3	1623.5	1630.7	1638.5	1645.4	1652.4	1659.0	1665.3	1680.7	1692.3	
<i>B<sub>3g</sub></i>		101.1	107.8	113.3	117.8	121.7	128.3	134.0	139.3	144.0	148.4	152.3	156.0	165.6	168.5
	151.9	155.3	158.8	161.9	165.3	171.8	178.0	184.0	189.4	194.4	199.2	203.5	211.6	217.1	
	204.3	212.7	220.6	227.9	234.7	247.7	260.0	271.5	281.9	291.7	301.0	309.6	325.7	340.0	
	217.3	224.2	230.9	237.5	243.9	256.9	269.1	280.5	290.9	300.8	310.2	319.2	340.5	356.7	
	706.6	708.6	710.5	712.4	714.2	717.7	721.1	724.4	727.5	730.4	733.3	736.1	742.3	746.5	
	1463.8	1468.8	1473.4	1478.2	1482.7	1491.5	1499.7	1507.6	1515.8	1523.0	1530.3	1537.2	1552.9	1567.6	
	<i>A<sub>u</sub></i>	71.7	85.8	97.1	106.8	115.3	130.2	142.3	152.2	160.2	166.9	172.4	177.1	185.3	190.0
		136.3	141.5	146.6	151.2	155.4	163.5	171.1	178.7	186.1	193.8	201.3	209.0	227.5	242.9
		148.6	156.7	164.0	170.9	177.3	189.4	201.2	212.2	222.4	232.1	241.6	250.4	269.1	283.2
		264.4	270.3	276.1	281.9	287.5	299.0	309.9	320.3	330.0	339.3	347.9	356.3	374.8	387.9
692.6		694.1	695.5	696.9	698.3	701.1	703.7	706.3	708.8	711.4	713.9	716.4	722.0	725.9	
1391.7		1396.2	1400.3	1404.5	1408.6	1416.4	1423.7	1430.6	1437.4	1444.5	1451.0	1457.2	1471.1	1483.9	

**Table S5.** DFT/B3LYP-D\* vibrational modes  $\nu$  (cm<sup>-1</sup>) of aragonite, subdivided in irreducible representations (IRREPs), between about -3 GPa and 25 GPa. Frequency marked with an asterisk are soft modes.

IRREP	Pressure (GPa)													
	-3.1	-2.0	-1.0	0.1	1.1	3.1	5.2	7.2	9.2	11.2	13.2	15.2	20.3	24.4
$B_{1u}$	155.2	164.6	172.9	180.4	187.4	200.1	211.9	222.7	232.3	241.1	249.4	257.1	274.8	289.1
	187.4	197.2	205.8	213.6	220.3	232.5	244.3	254.9	264.8	273.0	280.4	287.5	304.6	308.8
	259.2	261.8	264.4	267.2	269.7	275.2	280.9	287.0	292.8	297.8	302.9	307.1	319.6	330.0
	269.1	276.7	284.2	291.0	297.3	309.1	320.3	330.9	340.9	349.8	358.7	367.1	386.8	402.3
	710.8	713.6	716.5	719.3	721.8	726.9	731.9	736.6	741.1	745.3	750.2	754.0	764.1	772.1
	864.2	863.5	862.9	862.1	861.8	860.3	859.3	858.2	857.2	855.7	854.0	851.7	848.8	844.5
	1081.5	1085.1	1088.3	1091.6	1094.1	1100.6	1106.4	1111.9	1117.3	1122.2	1127.6	1131.6	1142.4	1150.5
	1467.4	1473.9	1479.9	1485.7	1491.0	1500.9	1510.3	1518.6	1526.7	1533.6	1540.3	1546.1	1560.7	1569.1
$B_{2u}$	-56.3*	-40.9*	-18.4*	27.8	44.0	63.2	75.6	87.1	96.2	104.0	111.5	117.7	130.2	140.9
	145.7	151.9	157.3	163.0	168.5	179.2	190.0	200.4	210.2	218.8	227.5	235.6	254.8	267.1
	167.4	180.0	191.5	202.0	212.1	230.1	246.8	261.7	275.5	288.2	300.1	310.6	335.6	350.9
	692.0	694.0	695.9	697.7	699.5	703.0	706.3	709.6	712.8	715.8	718.7	721.5	728.6	734.4
$B_{3u}$	1426.8	1432.5	1438.3	1443.4	1448.6	1458.2	1467.1	1476.4	1485.1	1493.1	1501.0	1509.0	1527.2	1542.5
	143.6	147.4	150.2	152.5	154.5	157.8	161.4	164.7	167.8	170.1	172.7	174.4	180.5	182.9
	173.4	182.5	191.2	199.0	205.7	217.9	229.9	241.4	251.9	260.8	269.0	276.8	295.6	304.9
	219.7	230.1	239.6	248.7	257.0	272.5	287.0	300.2	312.6	323.4	333.9	343.5	366.7	385.1
	283.8	290.8	297.9	304.8	311.4	324.6	337.5	349.5	360.8	371.4	381.5	391.1	413.0	428.2
	703.5	706.3	709.1	711.7	714.2	719.1	723.9	728.6	733.2	737.6	742.0	746.2	756.7	764.6
	911.7	912.8	914.3	915.2	916.7	918.5	920.8	922.8	924.8	926.4	927.4	928.5	931.0	932.5
	1081.7	1085.3	1089.0	1092.5	1095.6	1102.4	1108.8	1115.0	1120.8	1126.3	1131.7	1136.6	1148.8	1158.1
$A_g$	1470.8	1476.4	1481.6	1486.7	1491.3	1500.1	1508.3	1515.9	1523.0	1529.4	1535.5	1541.0	1554.8	1564.6
	139.6	144.0	146.2	146.9	147.0	146.7	146.5	146.4	145.8	144.6	142.6	140.8	138.6	130.3
	154.9	156.3	160.3	164.9	168.3	175.4	180.5	184.0	186.9	189.0	190.8	193.4	194.0	195.4
	174.1	183.8	191.5	197.7	202.1	210.3	218.1	224.9	231.6	237.1	241.2	245.3	258.5	263.9
	186.0	193.5	200.5	207.6	214.2	227.8	240.5	252.8	264.3	274.7	284.3	292.5	318.2	327.4
	261.3	269.8	278.2	285.9	293.6	308.1	322.7	336.3	349.1	360.5	372.1	382.0	405.5	423.2
	696.0	698.8	701.4	703.8	706.1	710.6	715.4	720.1	724.3	728.7	729.5	737.6	745.8	762.1
	865.2	864.5	863.9	863.1	862.8	861.4	860.5	859.3	858.3	856.9	855.2	849.3	850.1	844.7
	1084.1	1087.8	1091.6	1095.1	1098.9	1105.2	1111.9	1117.6	1123.4	1128.9	1133.1	1140.8	1151.5	1156.1
	1472.2	1477.0	1481.5	1485.9	1489.9	1497.6	1504.8	1511.4	1517.6	1523.0	1528.8	1532.8	1546.8	1552.8
$B_{1g}$	70.9	85.4	96.1	104.3	111.4	122.9	132.2	139.6	146.4	151.7	156.1	161.0	170.4	174.2
	136.1	146.6	155.9	163.9	171.2	183.1	191.6	198.9	205.3	211.3	217.1	222.2	234.1	243.1
	172.9	176.3	179.8	184.1	188.6	199.1	211.2	223.3	235.0	245.8	255.9	265.9	288.2	302.4
	262.5	270.2	277.6	284.9	291.7	305.0	317.8	329.4	340.4	350.1	359.5	367.9	387.2	399.2
	697.0	699.2	701.1	703.1	705.0	708.7	712.3	715.9	719.4	722.6	725.8	728.9	736.6	741.9
	1397.3	1402.1	1406.6	1410.4	1414.3	1422.6	1429.9	1437.6	1444.2	1451.4	1458.5	1464.6	1479.6	1492.7
$B_{2g}$	163.4	172.4	179.6	185.7	190.3	197.6	204.0	209.3	214.0	217.2	219.6	221.3	225.8	229.8
	199.0	203.7	208.5	213.7	218.9	229.5	240.9	251.3	261.2	269.4	277.8	285.4	302.9	310.8
	234.1	240.8	246.8	252.4	257.2	265.7	273.0	279.0	284.5	289.3	293.6	298.2	310.7	321.8
	245.5	252.5	258.9	264.9	270.3	280.2	289.5	298.4	306.9	314.0	321.1	327.6	344.0	354.2
	267.7	273.9	280.3	286.7	293.2	306.9	320.7	334.3	347.6	360.5	372.5	384.1	410.2	429.0
	705.4	709.0	712.3	715.5	718.5	724.2	730.0	735.4	740.7	745.8	751.0	755.8	767.7	776.8
	910.8	911.8	913.0	913.9	915.1	917.0	919.2	921.1	923.0	924.5	925.6	926.7	929.1	930.5
	1081.2	1084.5	1087.9	1091.1	1093.8	1100.0	1105.7	1111.2	1116.3	1121.3	1126.2	1130.3	1140.9	1148.6
$B_{3g}$	1586.8	1592.6	1598.2	1603.4	1608.3	1617.4	1625.9	1633.6	1641.0	1647.7	1654.1	1660.1	1674.8	1686.1
	62.6	75.8	85.9	93.8	100.1	110.0	118.3	125.5	132.1	138.1	143.5	149.2	160.1	166.8
	143.6	147.9	151.3	155.1	158.5	165.2	171.6	177.7	183.4	187.9	192.4	196.6	205.9	212.7
	173.5	184.0	193.6	202.8	211.5	227.6	242.5	256.1	268.3	279.3	289.4	298.9	319.9	333.0
	203.4	210.4	217.6	224.2	230.9	243.7	255.8	267.4	278.5	288.6	298.3	308.1	329.5	345.4
	701.0	703.2	705.2	707.2	709.1	712.8	716.4	719.8	723.2	726.3	729.3	732.2	738.9	744.1
$A_u$	1446.5	1451.7	1457.0	1461.7	1466.5	1475.3	1483.1	1492.0	1500.0	1507.3	1514.9	1522.1	1538.9	1553.6
	-63.8*	-41.6*	20.0	49.5	66.2	91.3	109.7	126.0	139.2	150.7	161.2	170.1	186.7	193.2
	115.2	125.8	132.9	138.5	143.5	151.8	159.2	165.7	171.6	176.8	181.9	187.8	202.3	217.1
	124.8	132.7	141.5	150.2	158.4	173.4	187.3	199.6	211.4	221.8	231.9	241.1	263.0	276.6
	253.8	260.3	266.8	273.5	279.8	292.3	304.9	316.3	327.2	337.0	346.6	355.5	375.4	388.4
	686.8	688.4	689.8	691.2	692.6	695.3	697.9	700.6	703.2	705.7	708.4	710.8	717.2	721.8
	1374.7	1379.5	1384.1	1388.1	1392.2	1400.5	1407.9	1415.8	1422.6	1429.9	1436.7	1443.3	1458.2	1471.6

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