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SUPPLEMENTARY MATERIAL

Supplementary material 1

Resonance Integrals

R/A	(a _{1u})/cm-1	(a _{2u})/cm-1	(e _g)/cm-1
2.5	13392.9	2101.46	2927.05
2.6	11930.2	1844	2601.84
2.7	10554	1604.53	2296.32
2.8	9277.45	1385.22	2013.45
2.9	8107.79	1187.09	1754.81
3.0	7047.38	1010.19	1520.87
3.1	6094.95	853.953	1311.28
3.2	5246.64	717.274	1125.12
3.3	4496.68	598.776	961.038
3.4	3838.17	496.88	817.411
3.5	3263.52	409.93	692.486
3.6	2764.88	336.264	584.463
3.7	2334.45	274.28	491.553
3.8	1964.68	222.467	412.039
3.9	1648.44	179.417	344.297
4.0	1379.12	143.875	286.838
4.1	1150.64	114.699	238.293
4.2	957.505	90.8876	197.43
4.3	794.818	71.5651	163.157
4.4	658.215	55.9761	134.508
4.5	543.863	43.4722	110.631
4.6	448.41	33.5017	90.7922
4.7	368.951	25.5982	74.3534
4.8	302.976	19.3736	60.7689
4.9	248.33	14.5027	49.5702
5.0	203.174	10.7185	40.3608

Supplementary material 2

Resonance Integrals

R/A	(a _{1ueg})/cm-1	(a _{2ueg})/cm-1
2.5	16319.9	5028.51
2.6	14532	4445.84
2.7	12850.3	3900.85
2.8	11290.9	3398.67
2.9	9862.6	2941.9
3.0	8568.25	2531.06
3.1	7406.23	2165.23
3.2	6371.76	1842.39
3.3	5457.72	1559.81
3.4	4655.58	1314.29
3.5	3956.01	1102.42
3.6	3349.34	920.727
3.7	2826	765.833
3.8	2376.72	634.506
3.9	1992.74	523.714
4.0	1665.96	430.713
4.1	1388.93	352.992
4.2	1154.94	288.318
4.3	957.975	234.722
4.4	792.723	190.484
4.5	654.494	154.103
4.6	539.202	124.294
4.7	443.304	99.9516
4.8	363.745	80.1425
4.9	297.9	64.0729
5.0	243.535	51.0793

Supplementary material 3

Interplanar Coulombic Integrals

R/A	(a1ueg)/cm-1	(a2ueg)/cm-1
2.5	25945.1	26983.6
2.6	25672.8	26694
2.7	25400.8	26405.7
2.8	25129.5	26119
2.9	24859	25834.1
3.0	24589.6	25551.2
3.1	24321.4	25270.4
3.2	24054.6	24992
3.3	23789.4	24716
3.4	23525.9	24442.6
3.5	23264.2	24171.9
3.6	23004.4	23903.8
3.7	22746.7	23638.6
3.8	22491.2	23376.2
3.9	22237.9	23116.8
4.0	21986.9	22860.3
4.1	21738.2	22606.8
4.2	21492	22356.3
4.3	21248.2	22108.8
4.4	21007	21864.5
4.5	20768.3	21623.1
4.6	20532.2	21384.9
4.7	20298.8	21149.7
4.8	20068	20917.6
4.9	19839.8	20688.6
5.0	19614.4	20462.6

Supplementary material 4

Energy Differences between The EX and CR States

R/A	(a _{1ueg})/cm-1	(a _{2ueg})/cm-1
2.5	5083.73	7292.95
2.6	5356.04	7582.61
2.7	5627.98	7870.92
2.8	5899.32	8157.63
2.9	6169.79	8442.54
3.0	6439.24	8725.43
3.1	6707.43	9006.17
3.2	6974.19	9284.58
3.3	7239.43	9560.56
3.4	7502.95	9833.98
3.5	7764.64	10104.8
3.6	8024.37	10372.8
3.7	8282.07	10638
3.8	8537.6	10900.4
3.9	8790.91	11159.8
4.0	9041.95	11416.3
4.1	9290.59	11669.8
4.2	9536.82	11920.3
4.3	9780.58	12167.8
4.4	10021.8	12412.1
4.5	10260.5	12653.5
4.6	10496.6	12891.7
4.7	10730	13126.9
4.8	10960.8	13359
4.9	11189	13588
5.0	11414.4	13814