Supporting Information

A periodic orbit bifurcation analysis of vibrationally excited isotopologues of sulphur dioxide and water molecules: symmetry breaking substitutions

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Figure 1: Vibrational overtone and combination states of SO_2. States (21,0,0) and (20,0,1) are superimposed with the corresponding POs.

(1,0,0)	(2,0,0)	(3,0,0)	(4,0,0)	(5,0,0)	(6,0,0)	(7,0,0)
1151.69	2295.81	3432.36	4561.32	5682.69	6796.45	7902.60
	(1,0,1)	(2,0,1)	(3,0,1)	(4,0,1)	(5,0,1)	(6,0,1)
	2499.85	3629.77	4751.80	5865.90	6972.05	8070.19
(8,0,0)	(9,0,0)	(10,0,0)	(11,0,0)	(12,0,0)	(13,0,0)	(14,0,0)
9001.10	10091.93	11175.04	12250.38	13317.86	14377.38	15428.79
(7,0,1)	(8,0,1)	(9,0,1)	(10,0,1)	(11,0,1)	(12,0,1)	(13,0,1)
9160.27	10242.23	11315.97	12381.38	13438.34	14486.67	15526.15
(15,0,0)	(16,0,0)	(17,0,0)	(18,0,0)	(19,0,0)	(20,0,0)	(21,0,0)
16471.79	17506.04	18530.91	19545.41	20547.95	21536.35	22508.47
(14,0,1)	(15,0,1)	(16,0,1)	(17,0,1)	(18,0,1)	(19,0,1)	(20,0,1)
16556.48	17577.30	18588.09	19587.72	20577.73	21554.41	22518.15

Figure 2: Vibrational overtone stretching states of $^{16}OS^{18}O$. States (20,0,0) and (0,0,17) are superimposed with the corresponding periodic orbits .

Figure 3: Vibrational doublet states of H_2O. States $(8,0,0)/[8,0]_{+,0}$, $(14,0,0)/[14,0]_{+,0}$ and $(13,0,1)/[14,0]_{-,0}$ are superimposed with the corresponding periodic orbits.
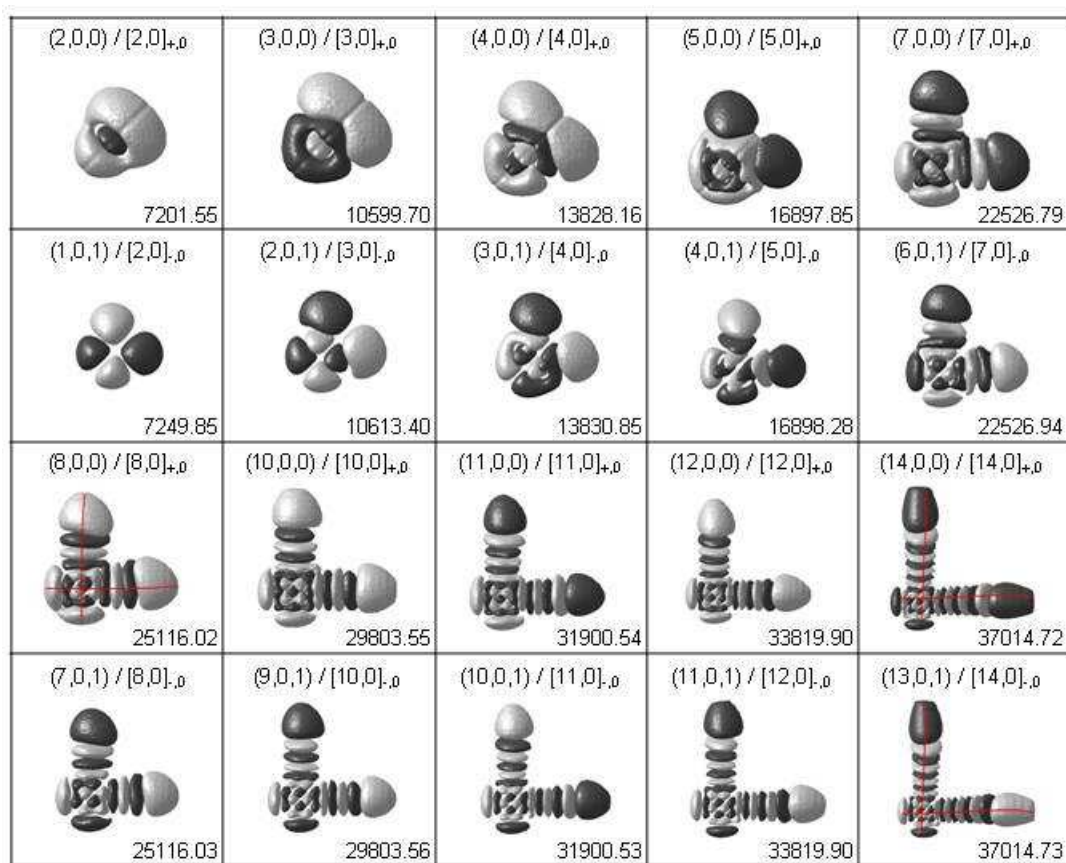
Figure 4: Vibrational overtone stretching states of HOD. States (12,0,0), (16′,0,0), (17′,0,0), (13″,0,0), (14″,0,0), (15″,0,0) and (0,0,11′) are superimposed with the corresponding periodic orbits.