Supporting Information

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

Frederic Mauguiere,*,† Michael Rey,† Vladimir Tyuterev,† Jaime Suarez,‡ and Stavros C. Farantos‡

University of Reims, GSMA, Moulin de la Housse, B.P. 1039, 51067 Reims, France, Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (FORTH), PO Box 1527, Vasilika Vouton, Heraklion 71110, Crete, Greece, and Department of Chemistry, University of Crete, PO Box 2208, Vasilika Vouton, Heraklion 71305, Crete, Greece

E-mail: fredmaug@iesl.forth.gr

[†]University of Reims, GSMA, Moulin de la Housse, B.P. 1039, 51067 Reims, France

[‡]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (FORTH), PO Box 1527, Vasilika Vouton, Heraklion 71110, Crete, Greece

Department of Chemistry, University of Crete, PO Box 2208, Vasilika Vouton, Heraklion 71305, Crete, Greece

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)
	No.	and a	OH)	OHIO	MIL	MILE
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)
	9	20	200	210	of the	CLAP .
	2499.85	3629.77	4751.80	5865.90	6972.05	8070.19
(0,0,8)	(9,0,0)	(10,0,0)	(11,0,0)	(12,0,0)	(13,0,0)	(14,0,0)
Mills	Mino	Miller	Mine	Miles	Mine	Miller
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)
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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)
Milita	Miller	Miller	Marie	Millians	Million	a to Marie
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)
CHIEF.	ALL STREET	Olive.	Office.		All I	William .
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 .

(0,0,1)	(2,0,0)	(0,0,8)	(4,0,0)	(5,0,0)	(6,0,0)
	1	N.	OHL	OHIO	OHIO
1123.91	2240.35	3349.29	4450.66	5544:42	6630.48
(7,0,0)	(0,0,8)	(0,0,0)	(10,0,0)	(11,0,0)	(12,0,0)
PHIL	OHIO	PHILL	OHINO .	GHIND.	Him
7708.74	8779.06	9841.27	10895.16	11940.45	12976.80
(13,0,0)	(14,0,0)	(15,0,0)	(16,0,0)	(17,0,0)	(19,0,0)
Quilly.	annil 1	Juni	Milmo	Quunty)	Minne
14003.80	15020.95	16027.73	17023.56	18007.94	19940.48
(20,0,0)	(0,0,1)	(0,0,2)	(0,0,3)	(0,0,4)	(0,0,5)
20888.10	1342.82	2674.80	3996.01	5306.47	6606.24
(0,0,6)	(0,0,7)	(0,0,8)	(0,0,9)	(0,0,10)	(0,0,11)
M	Me	N/B	OMB	1/6	
7895.35	9173.82	10441.66	11698.82	12944.97	14184.51
(0,0,12)	(0,0,13)	(0,0,14)	(0,0,15)	(0,0,16)	(0,0,17)
Wills			MILLE		MARKE
15408.80	16625.74	17829.89	19024.73	20209.04	21382.73

. . . .

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.

(2,0,0) / [2,0]+,0	(3,0,0) / [3,0]+,0	(4,0,0) / [4,0]+,0	(5,0,0) / [5,0]+,0	(7,0,0) / [7,0]+,0
	0	8		
7201.55	10599.70	13828.16	16897.85	22526.79
(1,0,1)/[2,0] _{-,0}	(2,0,1) / [3,0].,0	(3,0,1) / [4,0].,0	(4,0,1) / [5,0].,0	(6,0,1) / [7,0],,
			20	
7249.85	10613.40	13830.85	16898.28	22526.94
(8,0,0) / (8,0)+,0	(10,0,0) / [10,0]+,0	(11,0,0) / [11,0]+,0	(12,0,0) / [12,0]+,0	(14,0,0) / [14,0]+,0
25116.02	29803.55	9 1110 31900.54	33819.90	37014.72
(7,0,1) / [8,0].,0	(9,0,1) / [10,0], ₀	(10,0,1) / (11,0),0	(11,0,1) / [12,0].,0	(13,0,1) / [14,0].,0
25116.03	29803.56	31900.53	33819.90	37014.73

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.

(1,0,0)	(2,0,0)	(3,0,0)	(4,0,0)	(5,0,0)
6)	00>	CSD	\$20	(1)11(0)
2723.41	5363.29	7917.47	10378.13	12765.94
(6,0,0)	(7,0,0)	(0,0,8)	(0,0,9)	(11,0,0)
(nn)	JEHA)	JUNUA	(mm)	Финица.
15064.29	17280.14	19412.30	21461.47	25312.00
(12,0,0)	(0,0,181)	(14',0,0)	(15',0,0)	(16',0,0)
OHERA D	annull ((postt ice)	OMMERCE (I)	AMMILIA O
27120.66	28816.47	30448.61	31992.43	33444.83
(17',0,0)	(13",0,0)	(14",0,0)	(15",0,0)	(0,0,1)
Control & Control		Sinning.	mues	3
34804.66	28950.07	30743.02	32467.85	3707.91
(0,0,2)	(0,0,3)	(0,0,4)	(0,0,5)	(6,0,0)
2	2	2	2	9
7251.35	10632.74	13854.68	16920.68	19836.57
(0,0,7)	('8,0,0)	(0,0,9')	(0,0,10')	(0,0,11')
9				9/4
22623.73	25329.61	27966.12	30538.71	33048.71