Electronic Supplementary Material for PCCP

Structure, dipole moment and large amplitude motions of 1-benzofuran

Assimo Maris, B. Michela Giuliano, Sonia Melandri, Paolo Ottaviani and Walther Caminati*

Dipartimento di Chimica "G. Ciamician" dell' Università, Via Selmi 2, I-40126 Bologna, Italy

Laura B. Favero

Istituto per lo Studio dei Materiali Nanostrutturati (ISMN, Sezione di Bologna), CNR, Via Gobetti 101, I-40129 Bologna (Italy).

Biagio Velino

Dipartimento di Chimica Fisica e Inorganica dell'Università, Viale Risorgimento 4, I-40136 Bologna, Italy.

---

*Corresponding author: Ph. +39-051-2099480; fax +39-051-2099456; E-mail *walther.caminati@ciam.unibo.it*

ESI file: One table of rotational transitions.

Table S1: Wave guide conventional MW measured transition frequencies (MHz) for 7 vibrational states of BF.

Table S1: Wave guide conventional MW measured transition frequencies (MHz) for 7 vibrational states of BF.

J' (K_a', K_c') - J" (K_a'', K_c'')	ground state	butterfly v=1	twist v=1	bending v=1	butterfly v=1 twist v=1	butterfly v=2	twist v=2
4 (4, 1) - 3 (3, 0)	28837.04	28776.85	28824.20	28887.00	28764.38	28718.03	28811.03
4 (4, 0) - 3 (3, 1)	28844.33	28784.15	28831.40	28894.20	28771.70	28725.43	28818.35
5 (4, 2) - 4 (3, 1)	31658.20	31600.00	31645.05	31708.40	31587.60	31543.27	31631.92
5 (4, 1) - 4 (3, 2)	31709.70	31651.80	31696.00	31759.95	31638.55	31595.53	31682.27
6 (4, 2) - 5 (3, 3)	34609.64						
6 (4, 3) - 5 (3, 2)	34404.15						
6 (5, 2) - 5 (4, 1)	39519.25	39443.65	39502.15	39583.65	39427.35	39370.12	39485.27
6 (5, 1) - 5 (4, 2)	39524.25	39448.85	39507.15	39588.75	39432.45		39490.31
7 (6, 2) - 7 (5, 3)	27306.36	27197.38	27289.98	27382.44	27181.94	27090.72	27273.94
7 (6, 1) - 7 (5, 2)	27304.04	27194.90	27287.58	27380.08	27179.30	27088.50	27271.74
7 (7) - 7 (6)[a]		32215.96					
9 (7, 3) - 9 (6, 4)	32226.50						32188.52
9 (7, 2) - 9 (6, 3)	32225.32						32187.30
10 (7, 3) - 10 (6, 4)	32127.30	31997.82	32108.66	32216.92	31980.22	31871.21	32090.28
10 (7, 4) - 10 (6, 5)	32131.30	32001.87	32112.66	32220.96	31984.30		32094.27
10 (3, 8) - 9 (2, 7)		33747.06					
11 (6, 6) - 10 (6, 5)	31700.20						
11 (1, 10) - 10 (2, 9)	28842.60						
11 (7, 5) - 11 (6, 6)	32005.46						
11 (7, 4) - 11 (6, 5)	31992.26						
12 (3, 9) - 11 (3, 8)	36656.84						
12 (8) - 11 (8)[a]	34409.76						
12 (1, 11) - 11 (2, 10)	31334.70		31340.10				
12 (2, 11) - 11 (1, 10)	31726.48		31735.48	31729.44			
12 (2, 10) - 11 (3, 9)			31737.32				
12 (3, 10) - 11 (2, 9)	36204.88	36189.30	36219.85				
13 (7, 7) - 13 (6, 8)	31650.54	31519.76	31634.34	31739.76	31504.72	31391.57	31618.44
13 (7, 6) - 13 (6, 7)	31550.92	31418.34	31536.24	31640.50	31404.64	31288.44	31522.24
13 (1, 12) - 12 (1, 11)	33888.09						
13 (2, 12) - 12 (2, 11)	33822.22						
13 (3, 10) - 12 (3, 9)	39375.46						
13 (7, 7) - 12 (7, 6)	37477.65		37468.35				
13 (7, 6) - 12 (7, 5)	37481.40		37472.20				
13 (8) - 12 (8)[a]	37341.42						
13 (1, 12) - 12 (2, 11)	33753.42		33760.70				
13 (2, 12) - 12 (1, 11)	33956.87						
14 (1, 13) - 13 (1, 12)	36199.06						
14 (2, 13) - 13 (2, 12)	36164.70						
14 (0, 14) - 13 (1, 13)	33826.26	33854.34	33840.42	33821.54	33868.52		
14 (1, 14) - 13 (0, 13)	33828.72	33856.84	33842.94	33824.02	33870.96		

14 (2, 13) - 14 (1, 14)	30380.40			
14 (7, 8) - 14 (6, 9)	31425.77			
14 (1, 13) - 13 (2, 12)		36155.05		
14 (2, 13) - 13 (1, 12)	36233.52			
15 (2, 14) - 15 (1, 15)	32722.16			
15 (0, 15) - 14 (1, 14)	36159.42	36189.62	36174.86	36154.16
15 (1, 15) - 14 (0, 14)	36160.53	36190.54		
16 (2, 15) - 16 (1, 16)	35065.10			
16 (2, 14) - 16 (1, 15)	31231.20			
16 (3, 14) - 16 (2, 15)			31331.82	
17 (2, 16) - 17 (1, 17)		37345.14		
17 (3, 15) - 17 (2, 16)	33754.98			
17 (5, 12) - 16 (6, 11)	31734.36			
18 (4, 15) - 18 (3, 16)	32221.06			
18 (8, 10) - 18 (7, 11)		35068.34		
22 (6, 17) - 22 (5, 18)	33806.66	33757.74		
24 (5, 19) - 24 (4, 20)			36186.14	
24 (9, 15) - 24 (8, 16)	36660.70			
24 (7, 18) - 23 (8, 15)	33815.02			
28 (9, 20) - 28 (8, 21)	39412.80		39368.50	
28 (10, 18) - 27 (11, 17)			33877.28	
29 (11, 19) - 28 (12, 16)	30518.64	30832.18	30508.22	
29 (11, 18) - 28 (12, 17)	30652.34	30970.62	30638.40	
30 (11, 20) - 29 (12, 17)				33963.76
32 (8, 25) - 31 (9, 22)				36229.04
34 (14, 21) - 33 (15, 18)	29493.35			
34 (14, 20) - 33 (15, 19)	29497.05			
36 (10, 26) - 36 (9, 27)		31343.66		
38 (11, 27) - 38 (10, 28)	31461.10	36215.70		
39 (12, 27) - 39 (11, 28)				
39 (16, 24) - 38 (17, 21)	34607.28			
39 (16, 23) - 38 (17, 22)	34608.44			