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Quantum-Chemical *Ab Initio* Calculations on Borabenzene (C_5H_5B) and its Adducts with Ne, Ar, Kr, and N_2. Could Free Borabenzene be Observed in Rare Gas Matrices?*

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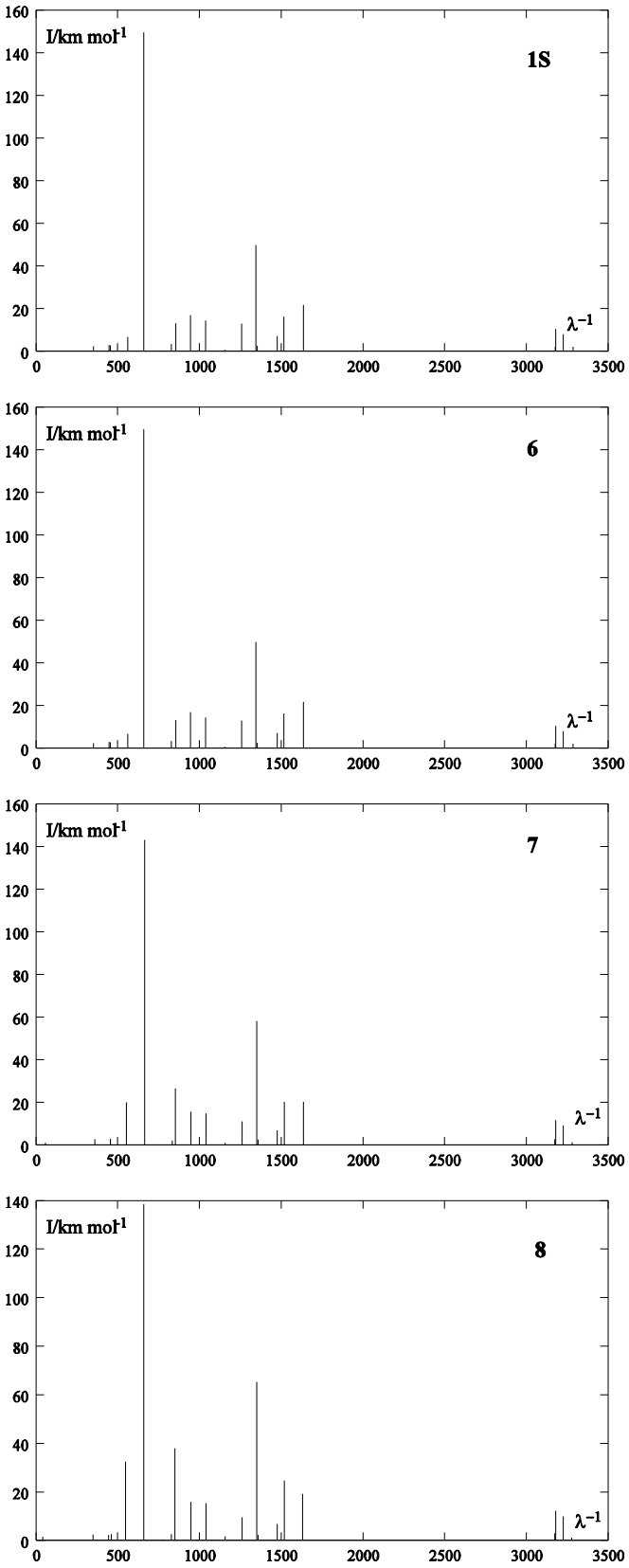

Figure S1. The most intense normal modes of C_5H_5B (**1S**), $C_5H_5B\cdots Ne$ (**6**), $C_5H_5B\cdots Ar$ (**7**), and $C_5H_5B\cdots Kr$ (**9**) calculated at the MP2/6-311++G** level of theory. Intensities in $km\cdot mol^{-1}$ and wavenumbers in cm^{-1}.

Table S1. Total energies of molecules 1S – 9. The numbers in parentheses are the zero point vibrational energies calculated at the MP2/6-311++G level**

All energies in Hartrees

Molecule	MP2/6-311++G**	CCSD(T)/aug-cc-pVTZ//MP2/6-311++G**
1S	-217.684732 (0.083911)	-217.905018[A] -218.031678[B]
1T	-217.599048[C] (0.085173) -217.613781[D]	
2	-327.018937 (0.093708)	-327.313853
3	-326.984020 (0.092529)	-327.278612
4	-326.988224 (0.089007)	-327.286959
5	-326.988978 (0.089744)	
6	-346.424871 (0.084181)	-346.718721 -346.910262[B]
7	-744.642424 (0.084449)	-744.956533 -745.140033[B]
8	-2969.783198 (0.084258)	-2970.222013 -2970.456197[B]
N_2	-109.301556 (0.004957)	-109.380183
Ne	-128.739166	-128.812648 -128.877527[B]
Ar	-526.954671	-527.048758 -527.105534[B]
Kr	-2752.095449	-2752.311680 -2752.418602[B]

t_1=0.014. [B]extrapolation to infinite basis set limit (See ref [30]). [C]UMP2, $\langle \boldsymbol{S}^2 \rangle$=2.342. [D]PMP2, $\langle \boldsymbol{S}^2 \rangle$=2.048.

Table S2. Calculated (MP2/6-311++G) normal frequencies of S1, 6, 7, and 8.**
Frequencies in cm^{-1}, intensities in $kmmol^{-1}$.

1S		6		7		8	
		20.0	0.0 B_2	54.8	0.0 B_1	40.8	1.6 A_1
		33.0	0.1 B_1	57.2	1.2 A_1	45.4	0.1 B_1
		39.9	0.1 A_1	57.8	0.0 B_2	56.1	0.0 B_2
352.0	2.5 B_1	352.7	2.3 B_1	359.1	2.8 B_1	349.8	2.5 B_1
377.2	0.0 A_2	377.6	0.0 A_2	377.9	0.0 A_2	374.2	0.0 A_2
445.3	3.0 B_2	447.0	2.9 B_2	454.6	3.1 B_1	444.2	2.3 B_1
448.3	2.0 B_1	456.2	2.9 B_1	456.0	2.7 B_2	459.8	2.7 B_2
563.4	5.1 A_1	562.7	6.8 A_1	554.4	20.0 A_1	547.9	32.4 A_1
658.4	151.0 B_1	660.1	149.5 B_1	665.0	143.0 B_1	658.6	138.5 B_1
668.3	0.0 A_2	671.1	0.0 A_2	680.6	0.0 A_2	677.9	0.0 A_2
776.6	0.0 B_1	777.2	0.0 B_1	777.9	0.0 B_1	777.1	0.1 B_1
822.0	4.5 B_1	827.3	3.4 B_1	832.9	2.2 B_1	827.2	2.7 B_1
846.0	0.0 A_2	849.6	0.0 A_2	852.1	26.5 A_1	847.1	0.0 A_2
854.7	11.5 A_1	854.4	13.3 A_1	854.0	0.0 A_2	849.9	38.0 A_1
945.9	17.2 A_1	946.0	16.9 A_1	948.3	15.8 A_1	948.9	15.9 A_1
990.4	0.7 B_2	990.6	0.6 A_1	990.6	0.3 A_1	989.8	0.2 A_1
1036.8	14.3 B_2	1036.6	14.4 B_2	1039.1	14.9 B_2	1040.2	15.4 A_1
1153.7	0.1 B_2	1154.1	0.1 B_2	1156.7	1.2 A_1	1157.1	1.7 B_2
1155.8	0.6 A_1	1155.8	0.7 A_1	1156.9	0.2 B_2	1157.8	0.4 B_2
1257.3	13.4 B_2	1258.0	13.1 B_2	1260.2	11.1 B_2	1260.2	9.5 B_2
1345.5	48.4 A_1	1346.4	49.8 A_1	1351.6	58.2 A_1	1352.3	65.2 A_1
1352.8	2.6 B_2	1353.9	2.6 B_2	1358.4	2.6 B_2	1359.6	2.4 B_2
1476.3	7.2 B_2	1476.4	7.2 B_2	1475.7	7.0 B_2	1474.8	6.8 B_2
1515.8	16.3 A_1	1516.5	16.2 A_1	1519.3	20.3 A_1	1519.7	24.7 A_1
1635.8	22.0 B_2	1636.8	21.8 B_2	1635.4	20.3 B_2	1632.3	19.2 B_2
3176.6	2.0 A_1	3176.0	2.2 A_1	3175.5	2.7 A_1	3174.9	3.1 A_1
3181.1	10.3 B_2	3180.5	10.6 B_2	3179.9	:11.7 B_2	3179.3	12.2 B_2
3227.3	7.8 A_1	3226.8	8.1 A_1	3225.9	9.2 A_1	3225.1	9.9 A_1
3283.5	0.4 A_1	3283.0	0.3 A_1	3279.6	0.2 A_1	3277.6	0.1 A_1
3285.3	2.3 B_2	3284.9	2.2 B_2	3281.6	1.4 B_2	3279.5	1.1 B_2

Table S3. The 30 lowest states of borabenzene and the rare gas adducts 6-8 calculated at the TDDFT/B3LYP/6-311++G(3df,3pd)//MP2/6-311++G level. λ is the wavelengths in nm and *f* is the oscillator strength. The entries i → j indicate that the leading transition for this state occurs from KS orbital i to KS orbital j.**

No.	**1S**			**6**			**7**			**8**		
		λ	*f*		λ	*f*		λ	*f*		λ	*f*
1	B_1	408.74	0.0052	B_1	399.63	0.0051	B_1	381.68	0.0039	B_1	382.22	0.0032
		20 → 21			25 → 26			29 → 30			38 → 39	
2	A_2	303.31	0.0000	A_2	298.60	0.0000	A_2	288.94	0.0000	A_2	289.41	0.0000
		19 → 21			24 → 26			28 → 30			37 → 39	
3	**B_2**	**253.44**	**0.1012**	**B_2**	**253.40**	**0.1001**	**B_2**	**253.47**	**0.0941**	**B_2**	**253.78**	**0.0901**
		20 → 22			25 → 27			29 → 31			38 → 40	
4	B_1	236.77	0.0024	B_1	237.74	0.0029	B_1	239.21	0.0032	B_1	241.41	0.0032
		20 → 23			25 → 28			29 → 32			38 → 41	
5	A_2	216.17	0.0000	A_2	216.64	0.0000	A_2	217.88	0.0000	A_2	218.59	0.0000
		20 → 25			25 → 30			29 → 33			38 → 42	
6	A_1	214.96	0.0081	A_1	215.07	0.0090	A_1	215.64	0.0122	B_1	218.46	0.0128
		20 → 24			25 → 29			29 → 34			38 → 44	
7	B_1	208.94	0.0271	B_1	211.09	0.0247	B_1	214.98	0.0197	A_1	216.21	0.0154
		20 → 26			25 → 31			29 → 35			38 → 43	
8	A_2	200.19	0.0000	A_2	200.95	0.0000	A_2	202.25	0.0000	A_2	203.83	0.0000
		19 → 23			24 → 28			28 → 32			37 → 41	
9	B_2	198.35	0.0033	**A_1**	**198.03**	**0.2302**	**A_1**	**198.26**	**0.2345**	**A_1**	**198.71**	**0.2276**
		18 → 21			24 → 27			28 → 31			37 → 40	
10	**A_1**	**197.92**	**0.2269**	B_2	196.60	0.0055	A_2	195.99	0.0000	B_1	198.18	0.0117
		19 → 22			23 → 26			29 → 36			38 → 45	
11	A_2	194.35	0.0000	A_2	195.10	0.0000	B_1	194.25	0.0048	A_2	196.81	0.0000
		20 → 27			25 → 32			29 → 37			38 → 46	
12	B_1	188.50	0.0020	B_1	190.41	0.0025	B_2	193.18	0.0135	B_2	193.44	0.0134

		$20 \rightarrow 30$			$25 \rightarrow 33$			$27 \rightarrow 30$			$36 \rightarrow 39$	
13	B_1	186.36	0.0015	B_1	188.39	0.0006	B_1	189.83	0.0014	B_1	190.99	0.0017
		$20 \rightarrow 29$			$25 \rightarrow 35$			$29 \rightarrow 39$			$38 \rightarrow 48$	
14	B_1	186.23	0.0189	B_1	186.51	0.0230	B_1	187.58	0.0245	B_1	188.18	0.0238
		$19 \rightarrow 25$			$24 \rightarrow 30$			$28 \rightarrow 33$			$37 \rightarrow 42$	
15	A_1	185.96	0.0057	A_1	186.20	0.0113	A_1	186.70	0.0280	A_1	187.57	0.0380
		$20 \rightarrow 28$			$25 \rightarrow 34$			$28 \rightarrow 31$			$38 \rightarrow 47$	
16	B_1	183.05	0.0094	B_1	181.55	0.0061	A_2	183.39	0.0000	A_2	186.07	0.0000
		$17 \rightarrow 21$			$22 \rightarrow 26$			$28 \rightarrow 35$			$37 \rightarrow 44$	
17	A_2	178.80	0.0000	A_2	180.34	0.0000	B_1	178.15	0.0029	B_1	178.44	0.0023
		$19 \rightarrow 26$			$24 \rightarrow 31$			$26 \rightarrow 30$			$35 \rightarrow 39$	
18	$\boldsymbol{B_2}$	**174.47**	**0.4169**	$\boldsymbol{B_2}$	**174.30**	**0.4172**	$\boldsymbol{B_2}$	**174.38**	**0.4069**	B_1	177.14	0.0004
		$19 \rightarrow 24$			$24 \rightarrow 29$			$28 \rightarrow 34$			$38 \rightarrow 49$	
19	B_1	170.44	0.0012	B_1	171.07	0.0000	B_1	173.38	0.0000	$\boldsymbol{B_2}$	**175.02**	**0.3890**
		$18 \rightarrow 22$			$25 \rightarrow 36$			$29 \rightarrow 40$			$37 \rightarrow 43$	
20	B_1	168.99	0.0002	B_1	170.35	0.0018	B_1	170.50	0.0013	A_2	172.09	0.0000
		$19 \rightarrow 27$			$23 \rightarrow 27$			$27 \rightarrow 31$			$37 \rightarrow 45$	
21	B_1	167.73	0.0015	B_1	169.34	0.0001	B_1	170.21	0.0004	B_1	171.07	0.0005
		$20 \rightarrow 31$			$24 \rightarrow 32$			$28 \rightarrow 36$			$37 \rightarrow 46$	
22	B_2	165.34	0.0194	B_2	165.91	0.0190	A_2	169.02	0.0000	A_1	170.70	0.0068
		$19 \rightarrow 28$			$24 \rightarrow 34$			$28 \rightarrow 37$			$38 \rightarrow 50$	
23	A_2	163.89	0.0000	A_2	165.77	0.0000	B_2	166.89	0.0144	B_1	170.43	0.0013
		$19 \rightarrow 30$			$24 \rightarrow 33$			$28 \rightarrow 38$			$36 \rightarrow 40$	
24	A_2	162.79	0.0000	A_2	164.12	0.0000	A_2	165.23	0.0000	B_2	167.75	0.0152
		$19 \rightarrow 29$			$24 \rightarrow 35$			$28 \rightarrow 39$			$37 \rightarrow 47$	
25	$\boldsymbol{A_1}$	**162.59**	**0.1904**	A_2	162.89	0.0000	A_1	163.94	0.0095	A_2	167.26	0.0000
		$16 \rightarrow 21$			$25 \rightarrow 37$			$29 \rightarrow 42$			$38 \rightarrow 51$	
26	A_2	161.56	0.0000	A_1	161.56	0.0002	A_2	163.41	0.0000	A_2	166.09	0.0000
		$20 \rightarrow 32$			$25 \rightarrow 38$			$29 \rightarrow 41$			$37 \rightarrow 48$	
27	B_2	161.34	0.0023	B_2	161.49	0.0028	B_2	162.28	0.0056	B_1	164.20	0.0189
		$20 \rightarrow 33$			$25 \rightarrow 39$			$29 \rightarrow 43$			$38 \rightarrow 52$	
28	A_1	160.91	0.0068	$\boldsymbol{A_1}$	**161.45**	**0.1983**	$\boldsymbol{A_1}$	**160.02**	**0.2639**	B_2	163.07	0.0086

		$20 \rightarrow 34$			$21 \rightarrow 26$			$25 \rightarrow 30$			$38 \rightarrow 53$	
29	A_2	154.59	0.0000	A_2	154.66	0.0000	A_2	155.25	0.0000	$\boldsymbol{A_1}$	**161.76**	**0.4222**
		$16 \rightarrow 22$			$21 \rightarrow 27$			$25 \rightarrow 31$			$34 \rightarrow 39$	
30	A_2	150.71	0.0000	A_2	151.10	0.0000	A_2	153.03	0.0000	A_2	160.14	0.0000
		$18 \rightarrow 24$			$24 \rightarrow 36$			$28 \rightarrow 40$			$38 \rightarrow 54$	