Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Jahn-Teller Instability in Cationic Boron and Carbon Buckyballs B_{80}^{+} and C_{60}^{+}: A Comparative Study

Jules Tshishimbi Muya,[a] Harry Ramanantoanina,[b] Claude Daul,[b] Minh Tho Nguyen,[a] G. Gopakumar,[c] and Arnout Ceulemans*[a]

[a]*Department of Chemistry, University of Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium*

[b]*Department of Chemistry, University of Fribourg, Chemin du Musée 9, CH-1700 Fribourg, Switzerland*

[c]*Max-Planck Institut für Kohlenforschung Kaiser-Wilhelm-Platz 1 45470 Mülheim an der Ruhr, Germany*

SUPPLEMENTARY INFORMATION

*Corresponding author: arnout.ceulemans@chem.kuleuven.be

1 December 2012

Table S1. The multimode analysis of the descent in symmetry of B_{80}^{+} when the structure in I_h point group is taken as the reference point. The magnitudes of distortion vector q_k are given in Å; the contributions of the normal modes c_k are given as a percentage. The extent of the distortion is given as the norm of distortion vector.

For the detail of the method of calculations read M. Zlatar, M. Gruden-Pavlovi, C. Schläpfer, C. Daul, Chimia 64(3): 161-164, 2010.

Modes	**Freq***	$I_h \rightarrow D_{3d}$		$I_h \rightarrow S_6$		$I_h \rightarrow T_h 1$		$I_h \rightarrow T_h 2$	
		q_k	**c_k**	**q_k**	**c_k**	**q_k**	**c_k**	**q_k**	**c_k**
a_g #01	317	0.116	3.06	0.126	3.24	0.017	0.22	0.034	0.44
a_g #02	422	0.136	4.22	0.148	4.47	0.017	0.20	0.049	0.89
a_g #03	975	0.018	0.07	0.019	0.07	0.002	0.00	0.004	0.01
t_{1g} #01	474	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
t_{1g} #02	678	0.000	0.00	0.002	0.00	0.000	0.00	0.000	0.00
t_{1g} #03	788	0.000	0.00	0.001	0.00	0.000	0.00	0.000	0.00
t_{1g} #04	986	0.000	0.00	0.001	0.00	0.000	0.00	0.000	0.00
t_{2g} #01	349	0.000	0.00	0.003	0.00	0.000	0.00	0.000	0.00
t_{2g} #02	479	0.000	0.00	0.001	0.00	0.000	0.00	0.000	0.00
t_{2g} #03	624	0.000	0.00	0.001	0.00	0.000	0.00	0.000	0.00
t_{2g} #04	694	0.000	0.00	0.003	0.00	0.000	0.00	0.000	0.00
t_{2g} #05	1084	0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
g_g #01	-121	0.630	90.41	0.668	90.52	0.372	99.02	0.517	98.61
g_g #02	303	0.047	0.49	0.050	0.51	0.028	0.55	0.004	0.01
g_g #03	430	0.003	0.00	0.007	0.01	0.003	0.01	0.005	0.01
g_g #04	578	0.011	0.03	0.014	0.04	0.002	0.00	0.007	0.02
g_g #05	705	0.015	0.05	0.015	0.05	0.002	0.00	0.004	0.00
g_g #06	867	0.017	0.07	0.017	0.06	0.002	0.00	0.001	0.00
g_g #07	1012	0.009	0.02	0.009	0.02	0.002	0.00	0.003	0.00
g_g #08	1053	0.001	0.00	0.004	0.00	0.002	0.00	0.005	0.01
h_g #01	175	0.025	0.15	0.019	0.07	0.000	0.00	0.000	0.00
h_g #02	270	0.055	0.69	0.044	0.39	0.000	0.00	0.000	0.00
h_g #03	319	0.049	0.56	0.045	0.40	0.000	0.00	0.000	0.00
h_g #04	498	0.009	0.02	0.010	0.02	0.000	0.00	0.000	0.00
h_g #05	572	0.012	0.03	0.008	0.01	0.000	0.00	0.000	0.00
h_g #06	647	0.002	0.00	0.003	0.00	0.000	0.00	0.000	0.00
h_g #07	731	0.004	0.00	0.001	0.00	0.000	0.00	0.000	0.00
h_g #08	860	0.020	0.09	0.019	0.07	0.000	0.00	0.000	0.00
h_g #09	961	0.007	0.01	0.006	0.01	0.000	0.00	0.000	0.00
h_g #10	1051	0.008	0.01	0.007	0.01	0.000	0.00	0.000	0.00
h_g #11	1099	0.007	0.01	0.007	0.01	0.000	0.00	0.000	0.00
Total	-	0.663	100.00	0.702	100.00	0.374	100.00	0.521	100.00

- The calculated frequencies are given in cm^{-1} and calculated for the neutral B_{80} within the Ih point group at B3LYP/6.31G(D) level of theory

Table S2. The multimode analysis of the descent in symmetry of B_{80}^{+} when the structure in T_h point group is taken as the reference point. The magnitudes of distortion vector q_k are given in Å; the contributions of the normal modes c_k are given as a percentage. The extent of the distortion is given as the norm of distortion vector. For the detail of the method of calculations read M. Zlatar, M. Gruden-Pavlovi, C. Schläpfer, C. Daul, Chimia 64(3): 161-164, 2010.

Modes	$T_h 1 \rightarrow D_{2h}$			$T_h 2 \rightarrow S_6$		
	Freq*	q_k	c_k	**Freq***	q_k	c_k
ag #01	177	0.153	57.74	115	0.078	4.01
ag #02	304	0.045	5.03	304	0.054	1.96
ag #03	324	0.045	5.10	324	0.064	2.70
ag #04	432	0.049	6.01	431	0.015	0.15
ag #05	433	0.038	3.52	433	0.091	5.51
ag #06	583	0.006	0.08	576	0.001	0.00
ag #07	698	0.004	0.04	719	0.001	0.00
ag #08	876	0.002	0.01	875	0.005	0.02
ag #09	974	0.012	0.35	968	0.010	0.06
ag #10	1005	0.015	0.55	1027	0.012	0.10
ag #11	1071	0.005	0.06	1043	0.005	0.01
eg #01	179	0.031	2.30	177	0.000	0.00
eg #02	306	0.021	1.08	262	0.000	0.00
eg #03	330	0.081	16.18	329	0.000	0.00
eg #04	498	0.013	0.41	500	0.000	0.00
eg #05	580	0.013	0.44	565	0.000	0.00
eg #06	639	0.005	0.06	660	0.000	0.00
eg #07	734	0.005	0.06	729	0.000	0.00
eg #08	859	0.007	0.12	866	0.000	0.00
eg #09	962	0.015	0.58	972	0.000	0.00
eg #10	1046	0.011	0.30	1048	0.000	0.00
eg #11	1107	0.001	0.00	1102	0.000	0.00
tg #01	101	0.000	0.00	106	0.352	81.78
tg #02	182	0.000	0.00	179	0.051	1.70
tg #03	279	0.000	0.00	294	0.009	0.06
tg #04	312	0.000	0.00	310	0.039	0.99
tg #05	325	0.000	0.00	331	0.026	0.44
tg #06	351	0.000	0.00	351	0.000	0.00
tg #07	431	0.000	0.00	430	0.002	0.00
tg #08	473	0.000	0.00	469	0.002	0.00
tg #09	482	0.000	0.00	480	0.005	0.02
tg #10	502	0.000	0.00	498	0.012	0.10
tg #11	569	0.000	0.00	578	0.002	0.00
tg #12	579	0.000	0.00	579	0.015	0.14
tg #13	626	0.000	0.00	623	0.001	0.00
tg #14	653	0.000	0.00	637	0.003	0.01
tg #15	681	0.000	0.00	677	0.002	0.00
tg #16	691	0.000	0.00	687	0.001	0.00
tg #17	712	0.000	0.00	708	0.002	0.00
tg #18	737	0.000	0.00	737	0.007	0.04
tg #19	788	0.000	0.00	785	0.003	0.01
tg #20	865	0.000	0.00	856	0.012	0.10
tg #21	874	0.000	0.00	873	0.001	0.00
tg #22	964	0.000	0.00	956	0.001	0.00
tg #23	987	0.000	0.00	981	0.003	0.01

tg #24	1015	0.000	0.00	1007	0.003	0.01
tg #25	1052	0.000	0.00	1044	0.009	0.06
tg #26	1054	0.000	0.00	1063	0.005	0.02
tg #27	1088	0.000	0.00	1088	0.004	0.01
tg #28	1098	0.000	0.00	1101	0.001	0.00
Total	-	0.201	100.00	-	0.390	100.00