Supporting Information

Theoretical studies on characterization of heterofullerene $C_{58}B_2$ isomers by X-ray spectroscopy

Jiayuan Qi *, Huanhuan Zhu, Mei Zheng, Xiaoying Hu

College of Chemistry, Fuzhou University, Fuzhou, Fujian, 350116, People's Republic of China

Table of contents

1. Optimized coordinates of the singlet 1,4-$C_{58}B_2$ in gas phase:

Table S1. Coordinates of optimized structure of the singlet 1,4-$C_{58}B_2$ in gas phase at the B3LYP/6-31G** level.

Atoms	Coordinates		
	X	Y	Z
C	1.887870	-3.020700	0.000000
C	2.404649	-2.341398	1.174322
C	1.592935	-2.182423	2.300667
C	0.237824	-2.693662	2.300179
C	-0.261445	-3.344377	1.170908
C	0.579331	-3.509911	0.000000
C	2.404649	-2.341398	-1.174322
C	3.241007	-1.243401	-0.725121
C	3.241007	-1.243401	0.725121
C	3.239188	-0.029889	1.423009
C	1.592604	-0.920612	3.025618
C	-0.603017	-1.756195	3.026018
C	-1.910282	-1.495849	2.603349
C	-2.449315	-2.201886	1.421379
C	-1.619353	-3.090857	0.725745
C	-1.619353	-3.090857	-0.725745
C	-0.261445	-3.344377	-1.170908
C	0.237824	-2.693662	-2.300179
C	1.592935	-2.182423	-2.300667
C	3.239188	-0.029889	-1.423009
C	2.403521	0.132838	-2.595971
C	1.592604	-0.920612	-3.025618
C	0.237137	-0.661020	-3.466699
C	-0.603017	-1.756195	-3.026018
C	-1.910282	-1.495849	-2.603349
C	-2.449315	-2.201886	-1.421379
C	-3.381885	-1.365732	-0.695805
C	-3.381885	-1.365732	0.695805
C	0.237137	-0.661020	3.466699
C	-2.422711	2.407630	1.167645
C	-1.608860	2.190181	2.278123
C	-0.248669	2.688712	2.286030
C	0.269521	3.356914	1.170864
C	-0.560825	3.544211	0.000000
C	-2.422711	2.407630	-1.167645
C	-3.355778	1.372596	-0.696244
C	-3.355778	1.372596	0.696244

C	-2.450994	-0.152215	2.667579
C	-1.610082	0.896439	3.024782
C	0.585590	1.742722	3.007766
C	1.891471	1.494210	2.593755
C	2.420803	2.173662	1.421869
C	1.627216	3.086190	0.726993
C	1.627216	3.086190	-0.726993
C	0.269521	3.356914	-1.170864
C	-0.248669	2.688712	-2.286030
C	-1.608860	2.190181	-2.278123
C	-2.450994	-0.152215	-2.667579
C	-1.610082	0.896439	-3.024782
C	-0.258304	0.649177	-3.455798
C	0.585590	1.742722	-3.007766
C	1.891471	1.494210	-2.593755
C	2.420803	2.173662	-1.421869
C	3.253241	1.229121	-0.697946
C	3.253241	1.229121	0.697946
C	-0.258304	0.649177	3.455798
C	2.403521	0.132838	2.595971
C	-1.876184	3.077485	0.000000
B	-3.397332	0.016295	-1.449504
B	-3.397332	0.016295	1.449504

2. Optimized coordinates of the singlet 1,16-$C_{58}B_2$ in gas phase:

Table S2. Coordinates of optimized structure of the singlet 1,16-$C_{58}B_2$ in gas phase at the B3LYP/6-31G** level.

Atoms	Coordinates		
	X	Y	Z
C	-1.115012	2.268758	2.661028
C	-1.826297	-0.254662	3.130420
C	-0.506954	-0.532558	3.486924
C	0.506954	0.532558	3.486924
C	0.171610	1.916306	3.030676
C	-1.324646	3.021636	1.438478
C	-2.486815	2.476352	0.703895
C	-3.064509	1.358104	1.434368
C	-3.460531	0.223892	0.731977
C	-2.338075	-1.380117	2.330258
C	-0.171610	-1.916306	3.030676
C	1.115012	-2.268758	2.661028
C	1.826297	0.254662	3.130420
C	2.338075	1.380117	2.330258
C	1.318657	2.410023	2.304407
C	1.119771	3.197483	1.168124
C	-0.225354	3.503419	0.717749
C	-2.466278	2.468947	-0.694066
C	-1.318657	2.980602	-1.427230
C	-0.220008	3.486832	-0.735837
C	1.126025	3.170010	-1.179843
C	1.951767	2.984776	-0.000308
C	2.922811	1.977084	0.019759
C	3.120355	1.153483	1.202301
C	3.460531	-0.223892	0.731977
C	3.064509	-1.358104	1.434368
C	-1.318657	-2.410023	2.304407
C	1.318657	-2.980602	-1.427230
C	0.220008	-3.486832	-0.735837
C	-1.126025	-3.170010	-1.179843
C	-1.317433	-2.365795	-2.306155
C	-0.173140	-1.844597	-3.031468
C	2.138697	-1.112248	-2.585686
C	2.965018	-1.311523	-1.411862
C	2.466278	-2.468947	-0.694066
C	2.486815	-2.476352	0.703895
C	1.324646	-3.021636	1.438478

C	0.225354	-3.503419	0.717749
C	-1.951767	-2.984776	-0.000308
C	-2.922811	-1.977084	0.019759
C	-3.115836	-1.145896	-1.151634
C	-2.341362	-1.337832	-2.294517
C	-1.832344	-0.183445	-3.019406
C	-0.494573	-0.497361	-3.469844
C	0.494573	0.497361	-3.469844
C	1.832344	0.183445	-3.019406
C	3.441968	-0.201067	-0.705622
C	3.115836	1.145896	-1.151634
C	2.341362	1.337832	-2.294517
C	1.317433	2.365795	-2.306155
C	0.173140	1.844597	-3.031468
C	-1.119771	2.145746	-2.598405
C	-2.138697	1.112248	-2.585686
C	-2.965018	1.311523	-1.411862
C	-3.441968	0.201067	-0.705622
C	-1.119771	-3.197483	1.168124
C	-3.120355	-1.153483	1.202301
C	1.119771	-2.145746	-2.598405
B	-2.206932	1.165979	2.701820
B	2.206932	-1.165979	2.701820

3. Optimized coordinates of the singlet I_h-C_{60} in gas phase:

Table S3. Coordinates of optimized structure of the singlet I_h-C_{60} in gas phase at the B3LYP/6-31G** level.

Atoms	Coordinates		
	X	Y	Z
C	0.726688	-1.000200	3.327513
C	-0.726688	-1.000200	3.327513
C	-1.424393	-1.960508	2.593903
C	-0.697705	-2.960708	1.829818
C	0.697705	-2.960708	1.829818
C	1.424393	-1.960508	2.593903
C	1.175806	0.382042	3.327513
C	0.000000	1.236315	3.327513
C	-1.175806	0.382042	3.327513
C	-2.304716	0.748848	2.593903
C	-2.600198	-1.578466	1.829818
C	-1.424393	-3.196823	0.593503
C	-0.726688	-3.423522	-0.593503
C	0.726688	-3.423522	-0.593503
C	1.424393	-3.196823	0.593503
C	2.600198	-2.342551	0.593503
C	2.600198	-1.578466	1.829818
C	3.031404	-0.251352	1.829818
C	2.304716	0.748848	2.593903
C	0.000000	2.423322	2.593903
C	1.175806	2.805364	1.829818
C	2.304716	1.985163	1.829818
C	3.031404	1.749047	0.593503
C	3.480521	0.366805	0.593503
C	3.480521	-0.366805	-0.593503
C	3.031404	-1.749047	-0.593503
C	2.304716	-1.985163	-1.829818
C	1.175806	-2.805364	-1.829818
C	-2.600198	-2.342551	0.593503
C	-1.175806	-0.382042	-3.327513
C	-2.304716	-0.748848	-2.593903
C	-3.031404	0.251352	-1.829818
C	-2.600198	1.578466	-1.829818
C	-1.424393	1.960508	-2.593903
C	0.726688	1.000200	-3.327513
C	1.175806	-0.382042	-3.327513
C	0.000000	-1.236315	-3.327513

C	0.000000	-2.423322	-2.593903
C	-1.175806	-2.805364	-1.829818
C	-2.304716	-1.985163	-1.829818
C	-3.480521	-0.366805	-0.593503
C	-3.480521	0.366805	0.593503
C	-3.031404	1.749047	0.593503
C	-2.600198	2.342551	-0.593503
C	-1.424393	3.196823	-0.593503
C	-0.697705	2.960708	-1.829818
C	0.697705	2.960708	-1.829818
C	1.424393	1.960508	-2.593903
C	2.304716	-0.748848	-2.593903
C	3.031404	0.251352	-1.829818
C	2.600198	1.578466	-1.829818
C	2.600198	2.342551	-0.593503
C	1.424393	3.196823	-0.593503
C	0.726688	3.423522	0.593503
C	-0.726688	3.423522	0.593503
C	-1.175806	2.805364	1.829818
C	-2.304716	1.985163	1.829818
C	-3.031404	-1.749047	-0.593503
C	-3.031404	-0.251352	1.829818
C	-0.726688	1.000200	-3.327513

4. The details of calculations:

Table S4. Statistics over bond lengths (Å) of I_h-C_{60}, 1,4-$C_{58}B_2$ and 1,16-$C_{58}B_2$.

I_h-C_{60}		1,4-$C_{58}B_2$		1,16-$C_{58}B_2$	
R(1,2)	1.4534	R(1,2)	1.4517	R(1,5)	1.3843
R(1,6)	1.3951	R(1,6)	1.3970	R(1,6)	1.4510
R(1,7)	1.4534	R(1,7)	1.4517	R(1,59)	1.5524
R(2,3)	1.3951	R(2,3)	1.3974	R(2,3)	1.3946
R(2,9)	1.4534	R(2,9)	1.4515	R(2,10)	1.4727
R(3,4)	1.4534	R(3,4)	1.4483	R(2,59)	1.5319
R(3,11)	1.4534	R(3,11)	1.4552	R(3,4)	1.4705
R(4,5)	1.3951	R(4,5)	1.3957	R(3,11)	1.4951
R(4,12)	1.4534	R(4,12)	1.4535	R(4,5)	1.4951
R(5,6)	1.4534	R(5,6)	1.4510	R(4,13)	1.3946
R(5,15)	1.4534	R(5,15)	1.4513	R(5,15)	1.4446
R(6,17)	1.4534	R(6,17)	1.4510	R(6,7)	1.4790
R(7,8)	1.4534	R(7,8)	1.4515	R(6,17)	1.4000
R(7,19)	1.3951	R(7,19)	1.3974	R(7,8)	1.4553
R(8,9)	1.4534	R(8,9)	1.4502	R(7,18)	1.3981
R(8,20)	1.3951	R(8,20)	1.3999	R(8,9)	1.3916
R(9,10)	1.3951	R(9,10)	1.3999	R(8,59)	1.5423
R(10,57)	1.4534	R(10,55)	1.4529	R(9,55)	1.4379
R(10,59)	1.4534	R(10,57)	1.4494	R(9,57)	1.4947
R(11,29)	1.4534	R(11,29)	1.4489	R(10,27)	1.4493
R(11,59)	1.3951	R(11,57)	1.3971	R(10,57)	1.3913
R(12,13)	1.3951	R(12,13)	1.3983	R(11,12)	1.3843
R(12,29)	1.4534	R(12,29)	1.4490	R(11,27)	1.4446
R(13,14)	1.4534	R(13,14)	1.4785	R(12,37)	1.4510
R(13,39)	1.4534	R(13,38)	1.4498	R(12,60)	1.5524
R(14,15)	1.3951	R(14,15)	1.4011	R(13,14)	1.4727
R(14,28)	1.4534	R(14,28)	1.4475	R(13,60)	1.5319
R(15,16)	1.4534	R(15,16)	1.4515	R(14,15)	1.4493
R(16,17)	1.4534	R(16,17)	1.4513	R(14,24)	1.3913
R(16,26)	1.3951	R(16,26)	1.4011	R(15,16)	1.3967
R(17,18)	1.3951	R(17,18)	1.3957	R(16,17)	1.4511
R(18,19)	1.4534	R(18,19)	1.4483	R(16,22)	1.4501
R(18,24)	1.4534	R(18,24)	1.4535	R(17,20)	1.4537
R(19,22)	1.4534	R(19,22)	1.4552	R(18,19)	1.4548
R(20,21)	1.4534	R(20,21)	1.4494	R(18,54)	1.4504
R(20,56)	1.4534	R(20,54)	1.4529	R(19,20)	1.3933
R(21,22)	1.3951	R(21,22)	1.3971	R(19,52)	1.4520
R(21,54)	1.4534	R(21,52)	1.4545	R(20,21)	1.4524

R(22,23)	1.4534	R(22,23)	1.4489	R(21,22)	1.4517
R(23,24)	1.4534	R(23,24)	1.4490	R(21,50)	1.3971
R(23,52)	1.3951	R(23,50)	1.4008	R(22,23)	1.3996
R(24,25)	1.3951	R(24,25)	1.3983	R(23,24)	1.4546
R(25,26)	1.4534	R(25,26)	1.4785	R(23,48)	1.4492
R(25,50)	1.4534	R(25,48)	1.4498	R(24,25)	1.4947
R(26,27)	1.4534	R(26,27)	1.4475	R(25,26)	1.3916
R(27,28)	1.3951	R(27,28)	1.3916	R(25,47)	1.4379
R(27,49)	1.4534	R(27,59)	1.5743	R(26,36)	1.4553
R(28,38)	1.4534	R(28,60)	1.5743	R(26,60)	1.5423
R(29,58)	1.3951	R(29,56)	1.4008	R(27,56)	1.3967
R(30,31)	1.3951	R(30,31)	1.3938	R(28,29)	1.3933
R(30,37)	1.4534	R(30,37)	1.4711	R(28,35)	1.4548
R(30,60)	1.4534	R(30,58)	1.4529	R(28,58)	1.4520
R(31,32)	1.4534	R(31,32)	1.4487	R(29,30)	1.4524
R(31,40)	1.4534	R(31,39)	1.4937	R(29,38)	1.4537
R(32,33)	1.3951	R(32,33)	1.3995	R(30,31)	1.3971
R(32,41)	1.4534	R(32,40)	1.4532	R(30,39)	1.4517
R(33,34)	1.4534	R(33,34)	1.4476	R(31,32)	1.4516
R(33,44)	1.4534	R(33,43)	1.4538	R(31,42)	1.4510
R(34,46)	1.4534	R(34,45)	1.4476	R(32,44)	1.4528
R(34,60)	1.3951	R(34,58)	1.3957	R(32,58)	1.3964
R(35,36)	1.4534	R(35,36)	1.4711	R(33,34)	1.4493
R(35,48)	1.3951	R(35,47)	1.3938	R(33,46)	1.4003
R(35,60)	1.4534	R(35,58)	1.4529	R(33,58)	1.4514
R(36,37)	1.4534	R(36,37)	1.3925	R(34,35)	1.4504
R(36,49)	1.3951	R(36,59)	1.5520	R(34,47)	1.3998
R(37,38)	1.3951	R(37,60)	1.5520	R(35,36)	1.3981
R(38,39)	1.4534	R(38,39)	1.3908	R(36,37)	1.4790
R(39,40)	1.3951	R(38,60)	1.5517	R(37,38)	1.4000
R(40,58)	1.4534	R(39,56)	1.4402	R(38,56)	1.4511
R(41,42)	1.3951	R(40,41)	1.3923	R(39,40)	1.3996
R(41,58)	1.4534	R(40,56)	1.4521	R(39,56)	1.4501
R(42,43)	1.4534	R(41,42)	1.4544	R(40,41)	1.4492
R(42,59)	1.4534	R(41,57)	1.4545	R(40,57)	1.4546
R(43,44)	1.3951	R(42,43)	1.3948	R(41,42)	1.3939
R(43,57)	1.4534	R(42,55)	1.4523	R(41,55)	1.4559
R(44,45)	1.4534	R(43,44)	1.4540	R(42,43)	1.4551
R(45,46)	1.4534	R(44,45)	1.4538	R(43,44)	1.4461
R(45,55)	1.3951	R(44,53)	1.3948	R(43,53)	1.4003
R(46,47)	1.3951	R(45,46)	1.3995	R(44,45)	1.4028
R(47,48)	1.4534	R(46,47)	1.4487	R(45,46)	1.4461

R(47,53)	1.4534	R(46,51)	1.4532	R(45,51)	1.4528
R(48,51)	1.4534	R(47,49)	1.4937	R(46,49)	1.4551
R(49,50)	1.4534	R(48,49)	1.3908	R(47,48)	1.4559
R(50,51)	1.3951	R(48,59)	1.5517	R(48,49)	1.3939
R(51,52)	1.4534	R(49,50)	1.4402	R(49,50)	1.4510
R(52,53)	1.4534	R(50,51)	1.4521	R(50,51)	1.4516
R(53,54)	1.3951	R(51,52)	1.3923	R(51,52)	1.3964
R(54,55)	1.4534	R(52,53)	1.4544	R(52,53)	1.4514
R(55,56)	1.4534	R(53,54)	1.4523	R(53,54)	1.4493
R(56,57)	1.3951	R(54,55)	1.3959	R(54,55)	1.3998

Table S5. Total energies (a.u.) and the relative energies (kcal/mol) at the B97D/6-311++G**// B97D/6-31G** level of all the 23 isomers of $C_{58}B_2$ (atom numbering according to IUPAC rules) in the singlet and triplet states.

Labels	Isomers	Singlet		Triplet	
		E_{total}	ΔE	E_{total}	ΔE
a	1,4-$C_{58}B_2$	-2258.01809443	0.00	-2257.55783792	37.96
b	1,16-$C_{58}B_2$	-2258.00528363	8.04	-2257.55560442	39.36
c	1,35-$C_{58}B_2$	-2258.00263668	9.70	-2257.55566287	39.32
d	1,53-$C_{58}B_2$	-2258.00148865	10.42	-2257.55488932	39.81
e	1,55-$C_{58}B_2$	-2257.99988930	11.42	-2257.55557389	39.38
f	1,7-$C_{58}B_2$	-2257.99965757	11.57	-2257.55844797	37.58
g	1,60-$C_{58}B_2$	-2257.99871501	12.16	-2257.55394063	40.40
h	1,18-$C_{58}B_2$	-2257.99720116	13.11	-2257.55533707	39.53
i	1,38-$C_{58}B_2$	-2257.99608165	13.81	-2257.55578442	39.25
j	1,51-$C_{58}B_2$	-2257.99492185	14.54	-2257.55806213	37.82
k	1,52-$C_{58}B_2$	-2257.99475931	14.64	-2257.55776825	38.00
l	1,19-$C_{58}B_2$	-2257.99389989	15.18	-2257.55074167	42.41
m	1,34-$C_{58}B_2$	-2257.99377412	15.26	-2257.55776096	38.01
n	1,49-$C_{58}B_2$	-2257.99219152	16.25	-2257.55781691	37.97
o	1,13-$C_{58}B_2$	-2257.99217563	16.26	-2257.55442661	40.10
p	1,33-$C_{58}B_2$	-2257.99215166	16.28	-2257.55793427	37.90
q	1,3-$C_{58}B_2$	-2257.99209873	16.31	-2257.55749837	38.17
r	1,31-$C_{58}B_2$	-2257.99209022	16.32	-2257.55737573	38.25
s	1,15-$C_{58}B_2$	-2257.99182427	16.48	-2257.55560472	39.36
t	1,2-$C_{58}B_2$	-2257.99072047	17.18	-2257.61832830	0.00
u	1,17-$C_{58}B_2$	-2257.99039897	17.38	-2257.55654080	38.77
v	1,39-$C_{58}B_2$	-2257.98927996	18.08	-2257.55648398	38.81
w	1,6-$C_{58}B_2$	-2257.97949937	24.22	-2257.53412951	52.84

The two $C_{58}B_2$ isomers and the corresponding pure carbon counterpart I_h-C_{60} have been optimized at the B3LYP/6-31G** level by using the Gaussian 09 program, with eight-cores CPU (Intel Xeon X5450, 3.0GHz) and 6000MB memory. Then, the single point calculations with 6-311++G** basis set were employed. The total CPU times are listed in Table S6. The potential pitfall of the optimization process is that the hybrid density functional method (B3LYP) has problems with describing the weak interaction. But according to our calculations, the slight effects on the systems of the present work can be safely neglected.

Table S6. The total CPU times (hour) for the optimization and single point calculations of the two $C_{58}B_2$ isomers and the corresponding pure carbon counterpart I_h-C_{60}.

Molecule	CPU time (h)
1,4-$C_{58}B_2$	111.4
1,16-$C_{58}B_2$	112.4
I_h-C_{60}	1.8