Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Theoretical Study of Two Isomers of the Elusive C_{72} Family and the Chlorinated Derivative $C_{72}Cl_4$ in Core-excited and Ground States

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

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

Table of contents

1. Optimized coordinates of D_{6d}-$^{\#11190}C_{72}$ in gas phase:

Table S1. Coordinates of optimized structure of D_{6d}-$^{\#11190}C_{72}$ in gas phase at the B3LYP/6-311++G(3*df*, 3*pd*)//B3LYP/6-31G(*d*, *p*) level.

Atoms	Coordinates		
	X	Y	Z
C	0.000000	1.466441	2.907411
C	0.000000	2.808209	2.428672
C	1.157068	3.381420	1.783380
C	0.720201	4.099054	0.595577
C	1.425814	3.909986	-0.595577
C	0.688660	3.506929	-1.783380
C	1.404105	2.431980	-2.428672
C	0.733221	1.269975	-2.907411
C	1.466441	0.000000	-2.907411
C	0.733221	-1.269975	-2.907411
C	1.404105	-2.431980	-2.428672
C	0.688660	-3.506929	-1.783380
C	1.425814	-3.909986	-0.595577
C	0.720201	-4.099054	0.595577
C	1.157068	-3.381420	1.783380
C	0.000000	-2.808209	2.428672
C	0.000000	-1.466441	2.907411
C	-1.269975	-0.733221	2.907411
C	-1.269975	0.733221	2.907411
C	-2.431980	1.404105	2.428672
C	-2.349862	2.692760	1.783380
C	-3.189784	2.673240	0.595577
C	-2.673240	3.189784	-0.595577
C	-2.692760	2.349862	-1.783380
C	-1.404105	2.431980	-2.428672
C	-0.733221	1.269975	-2.907411
C	1.269975	0.733221	2.907411
C	1.269975	-0.733221	2.907411
C	2.431980	-1.404105	2.428672
C	2.349862	-2.692760	1.783380
C	3.189784	-2.673240	0.595577
C	2.673240	-3.189784	-0.595577
C	2.692760	-2.349862	-1.783380
C	3.381420	-1.157068	-1.783380
C	2.808209	0.000000	-2.428672
C	3.381420	1.157068	-1.783380
C	2.692760	2.349862	-1.783380

C	2.673240	3.189784	-0.595577
C	3.189784	2.673240	0.595577
C	2.349862	2.692760	1.783380
C	2.431980	1.404105	2.428672
C	3.506929	0.688660	1.783380
C	3.506929	-0.688660	1.783380
C	3.909986	-1.425814	0.595577
C	4.099054	-0.720201	-0.595577
C	4.099054	0.720201	-0.595577
C	3.909986	1.425814	0.595577
C	-1.466441	0.000000	-2.907411
C	-0.733221	-1.269975	-2.907411
C	-1.404105	-2.431980	-2.428672
C	-0.688660	-3.506929	-1.783380
C	-1.425814	-3.909986	-0.595577
C	-0.720201	-4.099054	0.595577
C	-1.157068	-3.381420	1.783380
C	-2.349862	-2.692760	1.783380
C	-2.431980	-1.404105	2.428672
C	-3.506929	-0.688660	1.783380
C	-3.506929	0.688660	1.783380
C	-3.909986	1.425814	0.595577
C	-4.099054	0.720201	-0.595577
C	-3.381420	1.157068	-1.783380
C	-2.808209	0.000000	-2.428672
C	-3.381420	-1.157068	-1.783380
C	-2.692760	-2.349862	-1.783380
C	-2.673240	-3.189784	-0.595577
C	-3.189784	-2.673240	0.595577
C	-3.909986	-1.425814	0.595577
C	-4.099054	-0.720201	-0.595577
C	-1.157068	3.381420	1.783380
C	-0.720201	4.099054	0.595577
C	-1.425814	3.909986	-0.595577
C	-0.688660	3.506929	-1.783380

2. Optimized coordinates of C_{2v}-$^{\#11188}C_{72}$ in gas phase:

Table S2. Coordinates of optimized structure of C_{2v}-$^{\#11188}C_{72}$ in gas phase at the B3LYP/6-311++G(3*df*, 3*pd*)//B3LYP/6-31G(*d*, *p*) level.

Atoms	Coordinates		
	X	Y	Z
C	0.711964	0.000000	4.128752
C	1.158608	1.224178	3.561381
C	1.158608	-1.224178	3.561381
C	-0.711964	0.000000	4.128752
C	2.305655	1.268776	2.705325
C	0.000000	2.051984	3.315016
C	0.000000	-2.051984	3.315016
C	2.305655	-1.268776	2.705325
C	2.367827	2.369875	1.812700
C	2.954048	0.000000	2.318398
C	0.000000	3.001420	2.265375
C	-1.158608	1.224178	3.561381
C	0.000000	-3.001420	2.265375
C	-1.158608	-1.224178	3.561381
C	2.367827	-2.369875	1.812700
C	3.144567	2.318505	0.605773
C	1.214173	3.214823	1.560988
C	3.750666	0.000000	1.148609
C	-1.214173	3.214823	1.560988
C	-1.214173	-3.214823	1.560988
C	1.214173	-3.214823	1.560988
C	-2.305655	-1.268776	2.705325
C	3.144567	-2.318505	0.605773
C	2.427378	3.049075	-0.418911
C	3.839421	1.161973	0.287354
C	1.210688	3.558672	0.170832
C	3.839421	-1.161973	0.287354
C	-2.367827	2.369875	1.812700
C	-1.210688	3.558672	0.170832
C	-2.367827	-2.369875	1.812700
C	-1.210688	-3.558672	0.170832
C	-2.954048	0.000000	2.318398
C	2.427378	-3.049075	-0.418911
C	1.210688	-3.558672	0.170832
C	2.433366	2.592875	-1.727414
C	3.908214	0.721128	-1.097103
C	0.000000	3.637836	-0.580739

C	-3.144567	2.318505	0.605773
C	-2.305655	1.268776	2.705325
C	-2.427378	3.049075	-0.418911
C	-3.144567	-2.318505	0.605773
C	-2.427378	-3.049075	-0.418911
C	0.000000	-3.637836	-0.580739
C	2.433366	-2.592875	-1.727414
C	3.205396	1.418559	-2.082024
C	1.206101	2.594603	-2.494980
C	0.000000	3.128007	-1.957026
C	-2.433366	2.592875	-1.727414
C	-3.839421	-1.161973	0.287354
C	-2.433366	-2.592875	-1.727414
C	0.000000	-3.128007	-1.957026
C	3.908214	-0.721128	-1.097103
C	3.205396	-1.418559	-2.082024
C	2.440276	0.694050	-3.072165
C	1.205059	1.418403	-3.314636
C	-1.206101	2.594603	-2.494980
C	-3.205396	1.418559	-2.082024
C	-3.839421	1.161973	0.287354
C	-3.750666	0.000000	1.148609
C	-3.908214	-0.721128	-1.097103
C	-3.205396	-1.418559	-2.082024
C	-1.206101	-2.594603	-2.494980
C	1.206101	-2.594603	-2.494980
C	2.440276	-0.694050	-3.072165
C	0.000000	0.735200	-3.632621
C	-1.205059	1.418403	-3.314636
C	-3.908214	0.721128	-1.097103
C	-2.440276	0.694050	-3.072165
C	-2.440276	-0.694050	-3.072165
C	-1.205059	-1.418403	-3.314636
C	1.205059	-1.418403	-3.314636
C	0.000000	-0.735200	-3.632621

3. Optimized coordinates of C_2-$^{\#11188}C_{72}Cl_4$ in gas phase:

Table S3. Coordinates of optimized structure of C_2-$^{\#11188}C_{72}Cl_4$ in gas phase at the B3LYP/6-311++G(3*df*, 3*pd*)//B3LYP/6-31G(*d*, *p*) level.

Atoms	Coordinates		
	X	Y	Z
C	-0.482829	0.633378	3.654328
C	-1.559735	0.205143	2.704856
C	0.345529	1.840244	3.058115
C	0.482829	-0.633378	3.654328
C	-2.328224	1.111981	1.901710
C	-1.553597	-1.147737	2.482661
C	1.553597	1.147737	2.482661
C	-0.357639	2.641368	1.946702
C	-3.271937	0.523373	1.041301
C	-1.729584	2.401635	1.546128
C	-2.361991	-1.738623	1.465829
C	-0.345529	-1.840244	3.058115
C	2.361991	1.738623	1.465829
C	1.559735	-0.205143	2.704856
C	0.482829	3.320712	1.061019
C	-3.718437	1.175881	-0.161474
C	-3.258647	-0.897839	0.784960
C	-2.218082	3.041568	0.372459
C	-1.860563	-2.872726	0.793799
C	3.258647	0.897839	0.784960
C	1.860563	2.872726	0.793799
C	2.328224	-1.111981	1.901710
C	-0.002831	3.902927	-0.153719
C	-3.893312	0.161987	-1.182955
C	-3.212491	2.422560	-0.483899
C	-3.582218	-1.120442	-0.597669
C	-1.347501	3.805500	-0.481950
C	-0.482829	-3.320712	1.061019
C	-2.150966	-3.078843	-0.578821
C	3.271937	-0.523373	1.041301
C	3.582218	1.120442	-0.597669
C	1.729584	-2.401635	1.546128
C	1.015791	3.755047	-1.173247
C	2.150966	3.078843	-0.578821
C	-3.537681	0.435150	-2.495323
C	-2.901007	2.736547	-1.867809
C	-2.929967	-2.139666	-1.334871

C	0.002831	-3.902927	-0.153719
C	0.357639	-2.641368	1.946702
C	-1.015791	-3.755047	-1.173247
C	3.718437	-1.175881	-0.161474
C	3.893312	-0.161987	-1.182955
C	2.929967	2.139666	-1.334871
C	0.651198	3.497160	-2.481534
C	-3.041425	1.750397	-2.847618
C	-2.807634	-0.556793	-3.255329
C	-2.522022	-1.843354	-2.716608
C	-0.651198	-3.497160	-2.481534
C	3.212491	-2.422560	-0.483899
C	3.537681	-0.435150	-2.495323
C	2.522022	1.843354	-2.716608
C	-1.737270	3.592850	-1.866551
C	-0.752150	3.425700	-2.841363
C	-2.001552	1.559314	-3.835406
C	-1.856348	0.136816	-4.079185
C	-1.378938	-2.502634	-3.249607
C	0.752150	-3.425700	-2.841363
C	1.347501	-3.805500	-0.481950
C	2.218082	-3.041568	0.372459
C	2.901007	-2.736547	-1.867809
C	3.041425	-1.750397	-2.847618
C	2.807634	0.556793	-3.255329
C	1.378938	2.502634	-3.249607
C	-0.880059	2.379183	-3.830292
C	-0.594425	-0.433170	-4.389939
C	-0.433633	-1.811828	-4.072444
C	1.737270	-3.592850	-1.866551
C	0.880059	-2.379183	-3.830292
C	2.001552	-1.559314	-3.835406
C	1.856348	-0.136816	-4.079185
C	0.433633	1.811828	-4.072444
C	0.594425	0.433170	-4.389939
Cl	-1.281108	0.979680	5.240809
Cl	0.897823	3.047824	4.346396
Cl	1.281108	-0.979680	5.240809
Cl	-0.897823	-3.047824	4.346396

3. Optimized coordinates of C_2-$^{\#11188}C_{72}Cl_4$ in the toluene solution:

Table S4. Coordinates of optimized structure of C_2-$^{\#11188}C_{72}Cl_4$ in the toluene solution at the B3LYP/6-311++G(3*df*, 3*pd*)//B3LYP/6-31G(*d*, *p*) level.

Atoms	Coordinates		
	X	Y	Z
C	-0.482841	0.632482	3.649780
C	-1.562027	0.204091	2.703955
C	0.344632	1.839058	3.053076
C	0.482841	-0.632482	3.649780
C	-2.328472	1.111753	1.900420
C	-1.555575	-1.149514	2.482662
C	1.555575	1.149514	2.482662
C	-0.358368	2.643270	1.945464
C	-3.271543	0.522223	1.039804
C	-1.729919	2.401157	1.544758
C	-2.362057	-1.740465	1.464675
C	-0.344632	-1.839058	3.053076
C	2.362057	1.740465	1.464675
C	1.562027	-0.204091	2.703955
C	0.482841	3.322030	1.059635
C	-3.718265	1.174684	-0.162543
C	-3.257715	-0.898635	0.783688
C	-2.218473	3.040668	0.371333
C	-1.860743	-2.874955	0.793099
C	3.257715	0.898635	0.783688
C	1.860743	2.874955	0.793099
C	2.328472	-1.111753	1.900420
C	-0.003526	3.903816	-0.155133
C	-3.892758	0.161234	-1.183963
C	-3.212501	2.421347	-0.484979
C	-3.581224	-1.120904	-0.598676
C	-1.348071	3.804394	-0.483067
C	-0.482841	-3.322030	1.059635
C	-2.149902	-3.079288	-0.579912
C	3.271543	-0.522223	1.039804
C	3.581224	1.120904	-0.598676
C	1.729919	-2.401157	1.544758
C	1.014656	3.754883	-1.174452
C	2.149902	3.079288	-0.579912
C	-3.536900	0.434320	-2.496128
C	-2.900619	2.734822	-1.868507
C	-2.928677	-2.140005	-1.335718

C	0.003526	-3.903816	-0.155133
C	0.358368	-2.643270	1.945464
C	-1.014656	-3.754883	-1.174452
C	3.718265	-1.174684	-0.162543
C	3.892758	-0.161234	-1.183963
C	2.928677	2.140005	-1.335718
C	0.650408	3.497220	-2.482547
C	-3.042853	1.749997	-2.849560
C	-2.807222	-0.557522	-3.256197
C	-2.521255	-1.843778	-2.717436
C	-0.650408	-3.497220	-2.482547
C	3.212501	-2.421347	-0.484979
C	3.536900	-0.434320	-2.496128
C	2.521255	1.843778	-2.717436
C	-1.738436	3.592680	-1.867557
C	-0.752771	3.425174	-2.842078
C	-2.002320	1.559076	-3.836575
C	-1.856305	0.136617	-4.079686
C	-1.378163	-2.502971	-3.250458
C	0.752771	-3.425174	-2.842078
C	1.348071	-3.804394	-0.483067
C	2.218473	-3.040668	0.371333
C	2.900619	-2.734822	-1.868507
C	3.042853	-1.749997	-2.849560
C	2.807222	0.557522	-3.256197
C	1.378163	2.502971	-3.250458
C	-0.880882	2.379230	-3.831217
C	-0.594168	-0.433077	-4.389472
C	-0.432966	-1.811652	-4.072417
C	1.738436	-3.592680	-1.867557
C	0.880882	-2.379230	-3.831217
C	2.002320	-1.559076	-3.836575
C	1.856305	-0.136617	-4.079686
C	0.432966	1.811652	-4.072417
C	0.594168	0.433077	-4.389472
Cl	-1.279336	0.978375	5.246433
Cl	0.899696	3.048100	4.355660
Cl	1.279336	-0.978375	5.246433
Cl	-0.899696	-3.048100	4.355660

5. The details of calculations:

The two C_{72} isomers and the chlorinated derivative $C_{72}Cl_4$ have been optimized at the B3LYP/6-311++G(3*df*, 3*pd*)//B3LYP/6-31G(*d*, *p*) level by using the Gaussian 09 program, with eight-cores CPU (Intel Xeon X5450, 3.0GHz) and 6000MB memory. The total CPU times are listed below. The potential pitfall of the optimization process is that the hybrid density functional method (B3LYP) is difficult to describe the weak interaction. But according to our calculations, the little effects on the systems of the present work can be reasonably neglected. Due to the symmetries possessed by the fullerene molecules, there may be some possible problems that should be paid attention to in the convergence process.

Table S5. The total CPU times (hour) for the optimization and single point calculations of the two C_{72} isomers and the corresponding chloride $C_{72}Cl_4$.

Molecule	CPU time (h)
D_{6d}-$^{\#11190}C_{72}$	68.8
C_{2v}-$^{\#11188}C_{72}$	122.7
C_2-$^{\#11188}C_{72}Cl_4$	257.5