

Supporting Information for:

Computational Characterization and Modeling of Buckyball Tweezers: Density Functional Study of Concave-Convex $\pi\cdots\pi$ Interactions

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Table S1. ΔE (kcal/mol) with half counterpoise correction and without counterpoise corrections

Supramolecule	$\frac{1}{2}$ Cp	no Cp	BSSE
C ₆₀ @C ₆₀ H ₂₈	-29.6	-32.7	6.3
C ₆₀ @C ₂₀ H ₁₀	-13.7	-15.1	2.7
C ₆₀ @C ₆₀ H ₃₂ S ₈	-17.8	-22.0	8.4
C ₆₀ @C ₂₀ H ₁₀ S ₄	-9.5	-11.5	3.9

^a M06-2X/DIDZ//M06-L/MIDI!

Table S2. Cartesian Coordinates (Å) of M06-
 L/MIDI! optimized structures

C ₆₀			
C 0	-0.728741	-1.003025	3.333356
C 0	-1.179127	0.383122	3.333356
C 0	0.728741	-1.003025	3.333356
C 0	-1.426546	-1.963472	2.599640
C 0	-2.308200	0.749980	2.599640
C 0	0.000000	1.239808	3.333356
C 0	1.179127	0.383122	3.333356
C 0	1.426546	-1.963472	2.599640
C 0	-0.697806	-2.966498	1.833396
C 0	-2.605673	-1.580351	1.833396
C 0	-2.308200	1.989787	1.833396
C 0	-3.036941	-0.253046	1.833396
C 0	0.000000	2.426985	2.599640
C 0	2.308200	0.749980	2.599640
C 0	0.697806	-2.966498	1.833396
C 0	2.605673	-1.580351	1.833396
C 0	-1.426546	-3.203280	0.593589
C 0	-2.605673	-2.346594	0.593589
C 0	-3.036941	1.753005	0.593589
C 0	-1.179127	2.810107	1.833396
C 0	-3.487327	0.366858	0.593589
C 0	1.179127	2.810107	1.833396
C 0	2.308200	1.989787	1.833396
C 0	3.036941	-0.253046	1.833396
C 0	1.426546	-3.203280	0.593589
C 0	2.605673	-2.346594	0.593589
C 0	-0.728741	-3.430011	-0.593589
C 0	-3.036941	-1.753005	-0.593589
C 0	-2.605673	2.346594	-0.593589
C 0	-0.728741	3.430011	0.593589
C 0	-3.487327	-0.366858	-0.593589
C 0	0.728741	3.430011	0.593589
C 0	3.036941	1.753005	0.593589
C 0	3.487327	0.366858	0.593589
C 0	0.728741	-3.430011	-0.593589
C 0	3.036941	-1.753005	-0.593589
C 0	-1.179127	-2.810107	-1.833396
C 0	-2.308200	-1.989787	-1.833396
C 0	-1.426546	3.203280	-0.593589
C 0	-2.605673	1.580351	-1.833396
C 0	-3.036941	0.253046	-1.833396
C 0	1.426546	3.203280	-0.593589
C 0	2.605673	2.346594	-0.593589
C 0	3.487327	-0.366858	-0.593589
C 0	1.179127	-2.810107	-1.833396
C 0	2.308200	-1.989787	-1.833396
C 0	0.000000	-2.426985	-2.599640
C 0	-2.308200	-0.749980	-2.599640
C 0	-0.697806	2.966498	-1.833396
C 0	-1.426546	1.963472	-2.599640
C 0	0.697806	2.966498	-1.833396
C 0	2.605673	1.580351	-1.833396
C 0	3.036941	0.253046	-1.833396
C 0	2.308200	-0.749980	-2.599640
C 0	0.000000	-1.239808	-3.333356
C 0	-1.179127	-0.383122	-3.333356
C 0	-0.728741	1.003025	-3.333356
C 0	1.426546	1.963472	-2.599640
C 0	1.179127	-0.383122	-3.333356

C 0 0.728741 1.003025 -3.333356

Coroanulene

C 0	-1.321347	3.005932	-0.230674
C 0	-2.450493	2.185559	-0.230674
C 0	0.000000	2.498445	0.082509
C 0	1.321347	3.005932	-0.230674
C 0	2.450493	2.185559	-0.230674
C 0	2.376162	0.772062	0.082509
C 0	3.267130	-0.327791	-0.230674
C 0	2.835834	-1.655182	-0.230674
C 0	1.468549	-2.021284	0.082509
C 0	0.697851	-3.208518	-0.230674
C 0	-0.697851	-3.208518	-0.230674
C 0	-1.468549	-2.021284	0.082509
C 0	-2.835834	-1.655182	-0.230674
C 0	-3.267130	-0.327791	-0.230674
C 0	-2.376162	0.772062	0.082509
C 0	0.000000	1.202204	0.564845
C 0	1.143364	0.371501	0.564845
C 0	0.706638	-0.972603	0.564845
C 0	-0.706638	-0.972603	0.564845
C 0	-1.143364	0.371501	0.564845
H 0	-1.434214	4.042804	-0.558018
H 0	-3.401739	2.613314	-0.558018
H 0	1.434214	4.042804	-0.558018
H 0	3.401739	2.613314	-0.558018
H 0	4.288132	-0.114723	-0.558018
H 0	3.536604	-2.427687	-0.558018
H 0	1.215997	-4.113707	-0.558018
H 0	-1.215997	-4.113707	-0.558018
H 0	-3.536604	-2.427687	-0.558018
H 0	-4.288132	-0.114723	-0.558018

C₆₀@ Coroanulene

C 0	-2.452182	-3.735023	1.426253
C 0	-1.714710	-3.299664	2.604690
C 0	-1.617996	-4.681560	0.697687
C 0	-3.252539	-2.827965	0.728692
C 0	-1.807236	-1.975042	3.036017
C 0	-0.424390	-3.977424	2.605713
C 0	-0.364644	-4.831546	1.427164
C 0	-1.617996	-4.681560	-0.697687
C 0	-3.252539	-2.827965	-0.728692
C 0	-3.351187	-1.445372	1.179763
C 0	-0.613246	-1.270304	3.485717
C 0	-2.642238	-1.028338	2.308438
C 0	0.718591	-3.301752	3.036895
C 0	0.834940	-4.974191	0.728952
C 0	-2.452182	-3.735023	-1.426253
C 0	-0.364644	-4.831546	-1.427164
C 0	-3.351187	-1.445372	-1.179763
C 0	-3.409426	-0.590093	0.000000
C 0	-0.711065	0.113965	3.039976
C 0	0.621804	-1.918838	3.486333
C 0	-1.965843	0.263122	2.311671
C 0	1.972366	-3.451592	2.309350
C 0	2.028059	-4.269752	1.179216
C 0	0.834940	-4.974191	-0.728952
C 0	-1.714710	-3.299664	-2.604690
C 0	-0.424390	-3.977424	-2.605713
C 0	-2.642238	-1.028338	-2.308438
C 0	-2.757750	0.643700	0.000000
C 0	0.432343	0.788211	2.606195

C 0	1.816064	-1.214987	3.037711	C 0	-0.729000	3.180294	0.917248
C 0	-2.017833	1.075776	1.178487	C 0	0.729000	3.180294	0.917248
C 0	2.650539	-2.161963	2.308797	C 0	1.382835	2.333448	1.824805
C 0	2.765943	-3.835748	0.000000	C 0	0.706960	1.494805	2.711747
C 0	2.028059	-4.269752	-1.179216	C 0	1.499156	0.704490	3.686307
C 0	-1.807236	-1.975042	-3.036017	C 0	2.341986	1.388043	4.578041
C 0	0.718591	-3.301752	-3.036895	C 0	3.161163	0.698186	5.470089
C 0	-1.965843	0.263122	-2.311671	C 0	3.161163	-0.698186	5.470089
C 0	-2.017833	1.075776	-1.178487	C 0	2.341986	-1.388043	4.578041
C 0	1.723113	0.109996	2.606500	C 0	1.499156	-0.704490	3.686307
C 0	0.372522	1.637853	1.424726	C 0	0.706960	-1.494805	2.711747
C 0	-0.825149	1.778754	0.726909	C 0	1.382835	-2.333448	1.824805
C 0	3.358301	-1.745836	1.179370	C 0	0.729000	-3.180294	0.917248
C 0	3.416676	-2.601519	0.000000	C 0	-0.729000	-3.180294	0.917248
C 0	1.972366	-3.451592	-2.309350	C 0	-1.382835	-2.333448	1.824805
C 0	-0.613246	-1.270304	-3.485717	C 0	-0.706960	-1.494805	2.711747
C 0	0.621804	-1.918838	-3.486333	C 0	-1.499156	-0.704490	3.686307
C 0	-0.711065	0.113965	-3.039976	C 0	-2.341986	-1.388043	4.578041
C 0	-0.825149	1.778754	-0.726909	C 0	-3.161163	-0.698186	5.470089
C 0	2.459113	0.542483	1.425389	C 0	-3.161163	0.698186	5.470089
C 0	1.622377	1.483329	0.696132	C 0	-2.341986	1.388043	4.578041
C 0	3.262162	-0.362877	0.728913	C 0	-1.499156	0.704490	3.686307
C 0	3.358301	-1.745836	-1.179370	C 0	-0.706960	1.494805	2.711747
C 0	2.650539	-2.161963	-2.308797	C 0	-1.482379	4.002062	-0.039328
C 0	1.816064	-1.214987	-3.037711	C 0	-2.844580	3.903212	-0.513544
C 0	0.432343	0.788211	-2.606195	C 0	-3.276996	4.534281	-1.684678
C 0	0.372522	1.637853	-1.424726	C 0	-2.384463	5.321360	-2.504629
C 0	1.622377	1.483329	-0.696132	C 0	-2.455446	5.728151	-3.894251
C 0	3.262162	-0.362877	-0.728913	C 0	-1.323701	6.111042	-4.615572
C 0	1.723113	0.109996	-2.606500	C 0	0.000000	6.131402	-4.023985
C 0	2.459113	0.542483	-1.425389	C 0	1.323701	6.111042	-4.615572
C 0	-3.211291	4.128346	-0.697465	C 0	2.455446	5.728151	-3.894251
C 0	-3.211291	4.128346	0.697465	C 0	2.384463	5.321360	-2.504629
C 0	-2.032168	4.472322	-1.468670	C 0	3.276996	4.534281	-1.684678
C 0	-1.661466	4.155643	-2.834002	C 0	2.844580	3.903212	-0.513544
C 0	-0.335202	4.177852	-3.265662	C 0	1.482379	4.002062	-0.039328
C 0	0.758570	4.517590	-2.375631	C 0	-0.712126	4.897393	-0.743842
C 0	2.175903	4.220085	-2.449135	C 0	-1.143563	5.531908	-1.926062
C 0	2.997147	4.238756	-1.320005	C 0	0.000000	5.922081	-2.657283
C 0	2.485797	4.553242	0.000000	C 0	1.143563	5.531908	-1.926062
C 0	2.997147	4.238756	1.320005	C 0	0.712126	4.897393	-0.743842
C 0	2.175903	4.220085	2.449135	C 0	1.482379	-4.002062	-0.039328
C 0	0.758570	4.517590	2.375631	C 0	2.844580	-3.903212	-0.513544
C 0	-0.335202	4.177852	3.265662	C 0	3.276996	-4.534281	-1.684678
C 0	-1.661466	4.155643	2.834002	C 0	2.384463	-5.321360	-2.504629
C 0	-2.032168	4.472322	1.468670	C 0	2.455446	-5.728151	-3.894251
C 0	-0.993943	4.979247	-0.707379	C 0	1.323701	-6.111042	-4.615572
C 0	0.350517	4.998833	-1.144124	C 0	0.000000	-6.131402	-4.023985
C 0	1.181416	5.011551	0.000000	C 0	-1.323701	-6.111042	-4.615572
C 0	0.350517	4.998833	1.144124	C 0	-2.455446	-5.728151	-3.894251
C 0	-0.993943	4.979247	0.707379	C 0	-2.384463	-5.321360	-2.504629
H 0	-4.105619	3.773880	-1.217009	C 0	-3.276996	-4.534281	-1.684678
H 0	-4.105619	3.773880	1.217009	C 0	-2.844580	-3.903212	-0.513544
H 0	-2.427283	3.800549	-3.528596	C 0	-1.482379	-4.002062	-0.039328
H 0	-0.114081	3.842075	-4.282268	C 0	0.712126	-4.897393	-0.743842
H 0	2.602621	3.876280	-3.395319	C 0	1.143563	-5.531908	-1.926062
H 0	4.035791	3.914997	-1.428448	C 0	0.000000	-5.922081	-2.657283
H 0	4.035791	3.914997	1.428448	C 0	-1.143563	-5.531908	-1.926062
H 0	2.602621	3.876280	3.395319	C 0	-0.712126	-4.897393	-0.743842
H 0	-0.114081	3.842075	4.282268	H 0	-2.475941	2.332681	1.846920
H 0	-2.427283	3.800549	3.528596	H 0	2.475941	2.332681	1.846920
C ₆₀ H ₂₈				H 0	2.341061	2.480446	4.564384
C 0	-1.382835	2.333448	1.824805	H 0	3.800109	1.249698	6.162064
				H 0	3.800109	-1.249698	6.162064

H 0	2.341061	-2.480446	4.564384	C 0	0.920324	3.109489	1.422557
H 0	2.475941	-2.332681	1.846920	C 0	-0.151213	2.553969	0.726292
H 0	-2.475941	-2.332681	1.846920	C 0	5.280777	1.961628	1.178786
H 0	-2.341061	-2.480446	4.564384	C 0	5.808001	1.285688	0.000000
H 0	-3.800109	-1.249698	6.162064	C 0	5.081324	-0.227697	-2.309235
H 0	-3.800109	1.249698	6.162064	C 0	1.719163	0.145401	-3.487067
H 0	-2.341061	2.480446	4.564384	C 0	3.107735	0.293126	-3.488645
H 0	-3.550602	3.248698	0.003489	C 0	0.868417	1.241620	-3.039715
H 0	-4.299374	4.348485	-2.023990	C 0	-0.151213	2.553969	-0.726292
H 0	-3.408245	5.657594	-4.425411	C 0	3.262890	3.363236	1.427525
H 0	-1.436903	6.324002	-5.681650	C 0	2.044302	3.679589	0.696561
H 0	1.436903	6.324002	-5.681650	C 0	4.432881	3.057001	0.729556
H 0	3.408245	5.657594	-4.425411	C 0	5.280777	1.961628	-1.178786
H 0	4.299374	4.348485	-2.023990	C 0	4.926738	1.221120	-2.308793
H 0	3.550602	3.248698	0.003489	C 0	3.707263	1.542787	-3.038132
H 0	3.550602	-3.248698	0.003489	C 0	1.442785	2.439068	-2.606572
H 0	4.299374	-4.348485	-2.023990	C 0	0.920324	3.109489	-1.422557
H 0	3.408245	-5.657594	-4.425411	C 0	2.044302	3.679589	-0.696561
H 0	1.436903	-6.324002	-5.681650	C 0	4.432881	3.057001	-0.729556
H 0	-1.436903	-6.324002	-5.681650	C 0	2.892504	2.592196	-2.607421
H 0	-3.408245	-5.657594	-4.425411	C 0	3.262890	3.363236	-1.427525
H 0	-4.299374	-4.348485	-2.023990	C 0	-4.134666	2.071846	-1.381300
H 0	-3.550602	-3.248698	0.003489	C 0	-3.404130	3.075861	-0.728345
				C 0	-3.404130	3.075861	0.728345
				C 0	-4.134666	2.071846	1.381300
				C 0	-4.869709	1.093881	0.706980
				C 0	-5.745992	0.202727	1.506195
				C 0	-6.683812	0.812836	2.357931
				C 0	-7.511269	0.059871	3.187984
				C 0	-7.399540	-1.331844	3.191066
				C 0	-6.463822	-1.948343	2.363837
				C 0	-5.634048	-1.201450	1.507502
				C 0	-4.626077	-1.940516	0.707658
				C 0	-3.736189	-2.779587	1.381906
				C 0	-2.840555	-3.639233	0.727981
				C 0	-2.840555	-3.639233	-0.727981
				C 0	-3.736189	-2.779587	-1.381906
				C 0	-4.626077	-1.940516	-0.707658
				C 0	-5.634048	-1.201450	-1.507502
				C 0	-6.463822	-1.948343	-2.363837
				C 0	-7.399540	-1.331844	-3.191066
				C 0	-7.511269	0.059871	-3.187984
				C 0	-6.683812	0.812836	-2.357931
				C 0	-5.745992	0.202727	-1.506195
				C 0	-4.869709	1.093881	-0.706980
				C 0	-2.610492	4.055256	-1.482051
				C 0	-2.124279	4.014626	-2.843111
				C 0	-1.056682	4.805336	-3.274392
				C 0	-0.365189	5.705042	-2.380159
				C 0	0.964976	6.275190	-2.450030
				C 0	1.626235	6.753961	-1.318866
				C 0	1.026857	6.714115	0.000000
				C 0	1.626235	6.753961	1.318866
				C 0	0.964976	6.275190	2.450030
				C 0	-0.365189	5.705042	2.380159
				C 0	-1.056682	4.805336	3.274392
				C 0	-2.124279	4.014626	2.843111
				C 0	-2.610492	4.055256	1.482051
				C 0	-2.061846	5.056332	-0.713522
				C 0	-0.977301	5.850840	-1.144956
				C 0	-0.304265	6.335072	0.000000
				C 0	-0.977301	5.850840	1.144956
				C 0	-2.061846	5.056332	0.713522
				C 0	-1.886630	-4.462192	1.480660

C 0	-1.410215	-4.335713	2.839779
C 0	-0.223636	-4.932798	3.271875
C 0	0.608491	-5.708640	2.380659
C 0	2.013561	-6.053094	2.450641
C 0	2.745238	-6.415074	1.319296
C 0	2.147627	-6.472791	0.000000
C 0	2.745238	-6.415074	-1.319296
C 0	2.013561	-6.053094	-2.450641
C 0	0.608491	-5.708640	-2.380659
C 0	-0.223636	-4.932798	-3.271875
C 0	-1.410215	-4.335713	-2.839779
C 0	-1.886630	-4.462192	-1.480660
C 0	-1.174026	-5.356318	0.713596
C 0	0.028569	-5.954463	1.145399
C 0	0.771902	-6.321987	0.000000
C 0	0.028569	-5.954463	-1.145399
C 0	-1.174026	-5.356318	-0.713596
H 0	-4.155476	2.066684	-2.474527
H 0	-4.155476	2.066684	2.474527
H 0	-6.760104	1.902454	2.350841
H 0	-8.239479	0.557602	3.830662
H 0	-8.039451	-1.936433	3.835300
H 0	-6.367895	-3.036397	2.361827
H 0	-3.757191	-2.778033	2.475074
H 0	-3.757191	-2.778033	-2.475074
H 0	-6.367895	-3.036397	-2.361827
H 0	-8.039451	-1.936433	-3.835300
H 0	-8.239479	0.557602	-3.830662
H 0	-6.760104	1.902454	-2.350841
H 0	-2.531759	3.279815	-3.541078
H 0	-0.678519	4.658674	-4.289312
H 0	1.512313	6.241491	-3.395986
H 0	2.663909	7.081469	-1.424482
H 0	2.663909	7.081469	1.424482
H 0	1.512313	6.241491	3.395986
H 0	-0.678519	4.658674	4.289312
H 0	-2.531759	3.279815	3.541078
H 0	-1.933288	-3.674655	3.535551
H 0	0.123937	-4.721664	4.286617
H 0	2.545261	-5.938178	3.399094
H 0	3.822121	-6.569281	1.425436
H 0	3.822121	-6.569281	-1.425436
H 0	2.545261	-5.938178	-3.399094
H 0	0.123937	-4.721664	-4.286617
H 0	-1.933288	-3.674655	-3.535551

C₂₀H₁₀S₄

C 0	-3.563636	0.697579	-1.609290
C 0	-2.405650	1.388722	-1.257239
C 0	-1.237276	0.711263	-0.873770
C 0	-1.237276	-0.711263	-0.873770
C 0	-2.405650	-1.388722	-1.257239
C 0	-3.563636	-0.697579	-1.609290
C 0	0.000000	-1.405859	-0.500351
C 0	0.000000	1.405859	-0.500351
C 0	1.237276	0.711263	-0.873770
C 0	1.237276	-0.711263	-0.873770
C 0	0.000000	-2.580645	0.209254
C 0	0.000000	2.580645	0.209254
S 0	1.483406	3.394510	0.784132
S 0	-1.483406	3.394510	0.784132
C 0	0.671351	4.473440	1.911301
C 0	-0.671351	4.473440	1.911301
S 0	1.483406	-3.394510	0.784132

S 0	-1.483406	-3.394510	0.784132
C 0	0.671351	-4.473440	1.911301
C 0	-0.671351	-4.473440	1.911301
C 0	2.405650	-1.388722	-1.257239
C 0	3.563636	-0.697579	-1.609290
C 0	2.405650	1.388722	-1.257239
C 0	3.563636	0.697579	-1.609290
H 0	-4.455004	1.251018	-1.908072
H 0	-2.394709	2.476942	-1.326498
H 0	-2.394709	-2.476942	-1.326498
H 0	-4.455004	-1.251018	-1.908072
H 0	1.304549	5.101982	2.535745
H 0	-1.304549	5.101982	2.535745
H 0	1.304549	-5.101982	2.535745
H 0	-1.304549	-5.101982	2.535745
H 0	2.394709	-2.476942	-1.326498
H 0	4.455004	-1.251018	-1.908072
H 0	2.394709	2.476942	-1.326498
H 0	4.455004	1.251018	-1.908072

C₆₀@C₂₀H₁₀S₄

C 0	-3.935781	4.454322	0.697230
C 0	-2.725683	4.451451	1.384606
C 0	-1.490628	4.401461	0.714531
C 0	-1.490628	4.401461	-0.714531
C 0	-2.725683	4.451451	-1.384606
C 0	-3.935781	4.454322	-0.697230
C 0	-0.208088	4.365295	-1.426686
C 0	-0.208088	4.365295	1.426686
C 0	0.916674	4.981802	0.711662
C 0	0.916674	4.981802	-0.711662
C 0	-0.047534	3.767322	-2.662213
C 0	-0.047534	3.767322	2.662213
S 0	1.546241	3.521733	3.431496
S 0	-1.356140	2.980934	3.586479
C 0	0.983815	2.515864	4.753046
C 0	-0.334421	2.271555	4.824674
S 0	1.546241	3.521733	-3.431496
S 0	-1.356140	2.980934	-3.586479
C 0	0.983815	2.515864	-4.753046
C 0	-0.334421	2.271555	-4.824674
C 0	1.962269	5.640933	-1.384570
C 0	3.003232	6.256738	-0.698042
C 0	1.962269	5.640933	1.384570
C 0	3.003232	6.256738	0.698042
H 0	-4.873984	4.491092	1.252585
H 0	-2.742457	4.541720	2.469442
H 0	-2.742457	4.541720	-2.469442
H 0	-4.873984	4.491092	-1.252585
H 0	1.737750	2.148092	5.448120
H 0	-0.831323	1.669495	5.585022
H 0	1.737750	2.148092	-5.448120
H 0	-0.831323	1.669495	-5.585022
H 0	1.932841	5.715748	-2.471151
H 0	3.794280	6.763417	-1.252227
H 0	1.932841	5.715748	2.471151
H 0	3.794280	6.763417	1.252227
C 0	1.304408	-5.405333	-0.728173
C 0	-0.078126	-5.510587	-1.178916
C 0	1.304408	-5.405333	0.728173
C 0	2.206521	-4.598586	-1.425824
C 0	-0.498898	-4.805480	-2.307917
C 0	-0.933584	-5.574468	0.000000
C 0	-0.078126	-5.510587	1.178916

C O 2.206521 -4.598586 1.425824
C O 3.147475 -3.758138 -0.697622
C O 1.766900 -3.864053 -2.604606
C O -1.792990 -4.134964 -2.309271
C O 0.443116 -3.965207 -3.036126
C O -2.171624 -4.930640 0.000000
C O -0.498898 -4.805480 2.307917
C O 3.147475 -3.758138 0.697622
C O 1.766900 -3.864053 2.604606
C O 3.291451 -2.503959 -1.428087
C O 2.437757 -2.569211 -2.605156
C O -1.651389 -2.880895 -3.037796
C O -2.610465 -4.195169 -1.178984
C O -0.269820 -2.776167 -3.485811
C O -2.610465 -4.195169 1.178984
C O -1.792990 -4.134964 2.309271
C O 0.443116 -3.965207 3.036126
C O 3.291451 -2.503959 1.428087
C O 2.437757 -2.569211 2.605156
C O 3.426419 -1.302258 -0.729130
C O 1.753751 -1.429623 -3.035498
C O -2.334125 -1.740306 -2.605775
C O -3.322194 -3.006283 -0.728769
C O 0.370771 -1.536256 -3.482586
C O -3.322194 -3.006283 0.728769
C O -1.651389 -2.880895 3.037796
C O -0.269820 -2.776167 3.485811
C O 3.426419 -1.302258 0.729130
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C O 2.717093 -0.112705 -1.179235
C O 1.895124 -0.175917 -2.306800
C O -3.187523 -1.805227 -1.427119
C O -1.667484 -0.444094 -2.606794
C O -0.340772 -0.350186 -3.029334
C O -3.187523 -1.805227 1.427119
C O -2.334125 -1.740306 2.605775
C O 0.370771 -1.536256 3.482586
C O 2.717093 -0.112705 1.179235
C O 1.895124 -0.175917 2.306800
C O 2.278056 0.623779 0.000000
C O 0.601175 0.490133 -2.301952
C O -3.047504 -0.549773 -0.698328
C O -2.108265 0.290966 -1.426684
C O -3.047504 -0.549773 0.698328
C O -1.667484 -0.444094 2.606794
C O -0.340772 -0.350186 3.029334
C O 0.601175 0.490133 2.301952
C O 1.037387 1.260684 0.000000
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C O -2.108265 0.290966 1.426684
C O 0.179679 1.188972 1.173907
C O -1.204180 1.091847 0.726667

C₆₀H₃₂S₈

C O 3.553741 -1.394466 2.358943
C O 3.553747 1.394482 2.358924
C O 4.424743 0.705493 1.500730
C O 5.391179 1.501132 0.704244
C O 6.280872 2.347076 1.387417
C O 7.169558 3.169764 0.698193
C O 7.169558 3.169764 -0.698193
C O 6.280872 2.347076 -1.387417
C O 5.391179 1.501132 -0.704244

C O 4.424743 0.705493 -1.500730
C O 3.553747 1.394482 -2.358924
C O 3.553741 -1.394466 -2.358943
C O 4.424738 -0.705491 -1.500737
C O 5.391146 -1.501157 -0.704245
C O 6.280819 -2.347126 -1.387416
C O 7.169478 -3.169842 -0.698193
C O 7.169478 -3.169842 0.698193
C O 6.280819 -2.347126 1.387416
C O 5.391146 -1.501157 0.704245
C O 4.424738 -0.705491 1.500737
C O 2.686685 -0.701484 3.202082
S O 1.594670 -1.488224 4.341559
C O 2.686686 0.701507 3.202068
C O 0.787010 0.000028 4.904589
S O 1.594663 1.488271 4.341532
C O -0.380198 0.000029 5.623864
C O -1.073689 -1.236645 6.005755
C O -1.073711 1.236699 6.005722
C O -0.395059 -2.399340 6.403125
C O -2.495747 -1.237030 6.003253
C O -2.495769 1.237044 6.003246
C O -0.395106 2.399414 6.403077
C O -1.085585 -3.555820 6.761131
C O -3.172831 -2.404086 6.391807
C O -3.190148 -0.000002 5.627722
C O -3.172879 2.404087 6.391797
C O -1.085656 3.555878 6.761080
C O -2.480764 -3.558223 6.754234
C O -4.366441 -0.000014 4.921072
C O -2.480836 3.558244 6.754205
S O -5.182018 1.483322 4.349662
S O -5.181982 -1.483381 4.349680
C O -6.269524 0.671320 3.231362
C O -6.269507 -0.671422 3.231373
C O 2.686685 -0.701484 -3.202082
S O 1.594670 -1.488224 -4.341559
C O 2.686686 0.701507 -3.202068
C O 0.787010 0.000028 -4.904589
S O 1.594663 1.488271 -4.341532
C O -0.380198 0.000029 -5.623864
C O -1.073689 -1.236645 -6.005755
C O -1.073711 1.236699 -6.005722
C O -2.495747 -1.237030 -6.003253
C O -0.395059 -2.399340 -6.403125
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C O -3.172831 -2.404086 -6.391807
C O -3.190148 -0.000002 -5.627722
C O -1.085585 -3.555820 -6.761131
C O -3.172879 2.404087 -6.391797
C O -1.085656 3.555878 -6.761080
C O -2.480764 -3.558223 -6.754234
C O -4.366441 -0.000014 -4.921072
C O -2.480836 3.558244 -6.754205
S O -5.182018 1.483322 -4.349662
S O -5.181982 -1.483381 -4.349680
C O -6.269524 0.671320 -3.231362
C O -6.269507 -0.671422 -3.231373
H O 3.556094 -2.485614 2.365941
H O 3.556139 2.485631 2.365960
H O 6.268069 2.345736 2.479783
H O 7.858635 3.811518 1.249927
H O 7.858635 3.811518 -1.249927

H O 6.268069 2.345736 -2.479783
H O 3.556139 2.485631 -2.365960
H O 3.556094 -2.485614 -2.365941
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H O 7.858538 -3.811614 -1.249930
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H O 6.268021 -2.345781 2.479782
H O 0.692914 -2.384612 6.475485
H O 0.692868 2.384711 6.475430
H O -0.532118 -4.443955 7.069313
H O -4.261208 -2.394689 6.458104
H O -4.261254 2.394658 6.458110
H O -0.532207 4.444028 7.069253
H O -3.033845 -4.448477 7.057053
H O -3.033933 4.448486 7.057030
H O -6.901896 1.305182 2.611573
H O -6.901866 -1.305300 2.611587
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H O -0.532207 4.444028 -7.069253
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H O -3.033933 4.448486 -7.057030
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H O -6.901866 -1.305300 -2.611587

C₆₀@C₆₀H₃₂S₈

C O 0.333465 2.778558 4.603273
C O 2.562835 1.100492 4.590591
C O 1.471571 0.789827 5.416209
C O 1.624297 -0.336174 6.369708
C O 2.709670 -0.293560 7.262530
C O 2.950597 -1.329724 8.161979
C O 2.109735 -2.444762 8.171098
C O 1.042483 -2.508238 7.277977
C O 0.779562 -1.462440 6.375801
C O -0.342171 -1.638438 5.421573
C O -0.333465 -2.778558 4.603273
C O -2.562835 -1.100492 4.590591
C O -1.471571 -0.789827 5.416209
C O -1.624297 0.336174 6.369708
C O -2.709670 0.293560 7.262530
C O -2.950597 1.329724 8.161979
C O -2.109735 2.444762 8.171098
C O -1.042483 2.508238 7.277977
C O -0.779562 1.462440 6.375801
C O 0.342171 1.638438 5.421573
C O 1.431428 3.088945 3.801126
C O 1.533745 4.536127 2.810332
S O 2.553992 2.247365 3.797788
C O 3.110704 4.166329 2.063167
S O 3.903388 2.741625 2.787971
C O 3.639742 4.872879 1.006003
C O 2.949539 6.013071 0.387830
C O 4.938166 4.543729 0.400014
C O 2.151264 6.902154 1.127428
C O 3.142415 6.263940 -1.001652
C O 5.136769 4.803718 -0.985958
C O 6.016577 4.044970 1.151556
C O 1.510802 7.983920 0.529045
C O 2.513895 7.382762 -1.576665
C O 4.040479 5.390077 -1.762732

C O 6.400364 4.544929 -1.546195
C O 7.248303 3.762044 0.567301
C O 1.690496 8.223576 -0.833295
C O 3.865631 5.134345 -3.108033
C O 7.440870 4.012206 -0.791336
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S O 2.495020 5.757162 -4.063024
C O 3.801124 3.888640 -5.423496
C O 2.715262 4.677786 -5.431443
C O -2.553992 -2.247365 3.797788
S O -3.903388 -2.741625 2.787971
C O -1.431428 -3.088945 3.801126
C O -3.110704 -4.166329 2.063167
S O -1.533745 -4.536127 2.810332
C O -3.639742 -4.872879 1.006003
C O -4.938166 -4.543729 0.400014
C O -2.949539 -6.013071 0.387830
C O -5.136769 -4.803718 -0.985958
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C O -3.142415 -6.263940 -1.001652
C O -2.151264 -6.902154 1.127428
C O -6.400364 -4.544929 -1.546195
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C O -2.513895 -7.382762 -1.576665
C O -1.510802 -7.983920 0.529045
C O -7.440870 -4.012206 -0.791336
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H O -0.535685 3.438072 4.607573
H O 3.437889 0.448967 4.588234
H O 3.363548 0.580933 7.247047
H O 3.792309 -1.267349 8.853561
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H O 2.722268 7.638733 -2.614873
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C 0	2.892631	1.511132	-0.373393
C 0	0.436010	2.671884	0.508949
C 0	0.305752	3.545429	-1.796635
C 0	1.076598	3.173381	-2.975232
C 0	2.887915	1.508283	-3.223581
C 0	3.467529	0.387616	-1.101668
C 0	2.214535	0.980079	0.798949
C 0	-1.012416	2.511317	0.510232
C 0	1.012416	1.542746	1.229212
C 0	-1.082886	3.393569	-1.798057
C 0	0.433434	2.665494	-4.105019
C 0	3.468783	0.386348	-2.497243
C 0	2.216541	0.980881	-4.403039
C 0	3.149196	-0.835140	-0.373251
C 0	2.374095	-0.467958	0.803717
C 0	-1.328472	1.287994	1.236292
C 0	-1.756178	2.863137	-0.619825
C 0	-0.074430	0.694310	1.683978
C 0	-1.756267	2.861136	-2.977087
C 0	-1.013979	2.507108	-4.106275
C 0	1.013978	1.548189	-4.835592
C 0	3.151402	-0.835255	-3.225317
C 0	2.375637	-0.467446	-4.402644
C 0	2.846330	-2.007577	-1.069913
C 0	1.328472	-1.287994	1.236292
C 0	-2.374095	0.467958	0.803717
C 0	-2.846330	2.007577	-1.069913
C 0	0.074430	-0.694310	1.683978
C 0	-2.846730	2.007182	-2.527697
C 0	-1.330735	1.286875	-4.835245
C 0	-0.077058	0.693726	-5.285510
C 0	2.846730	-2.007182	-2.527697
C 0	1.330735	-1.286875	-4.835245
C 0	1.756178	-2.863137	-0.619825
C 0	1.012416	-2.511317	0.510232
C 0	-3.149196	0.835140	-0.373251
C 0	-2.214535	-0.980079	0.798949
C 0	-1.012416	-1.542746	1.229212
C 0	-3.151402	0.835255	-3.225317
C 0	-2.375637	0.467446	-4.402644
C 0	0.077058	-0.693726	-5.285510
C 0	1.756267	-2.861136	-2.977087
C 0	1.013979	-2.507108	-4.106275
C 0	1.082886	-3.393569	-1.798057
C 0	-0.436010	-2.671884	0.508949
C 0	-3.467529	-0.387616	-1.101668
C 0	-2.892631	-1.511132	-0.373393
C 0	-3.468783	-0.386348	-2.497243
C 0	-2.216541	-0.980881	-4.403039
C 0	-1.013978	-1.548189	-4.835592
C 0	-0.433434	-2.665494	-4.105019
C 0	-0.305752	-3.545429	-1.796635
C 0	-1.081564	-3.180833	-0.618284
C 0	-2.334602	-2.587122	-1.069711
C 0	-2.887915	-1.508283	-3.223581
C 0	-1.076598	-3.173381	-2.975232
C 0	-2.325137	-2.576792	-2.523311

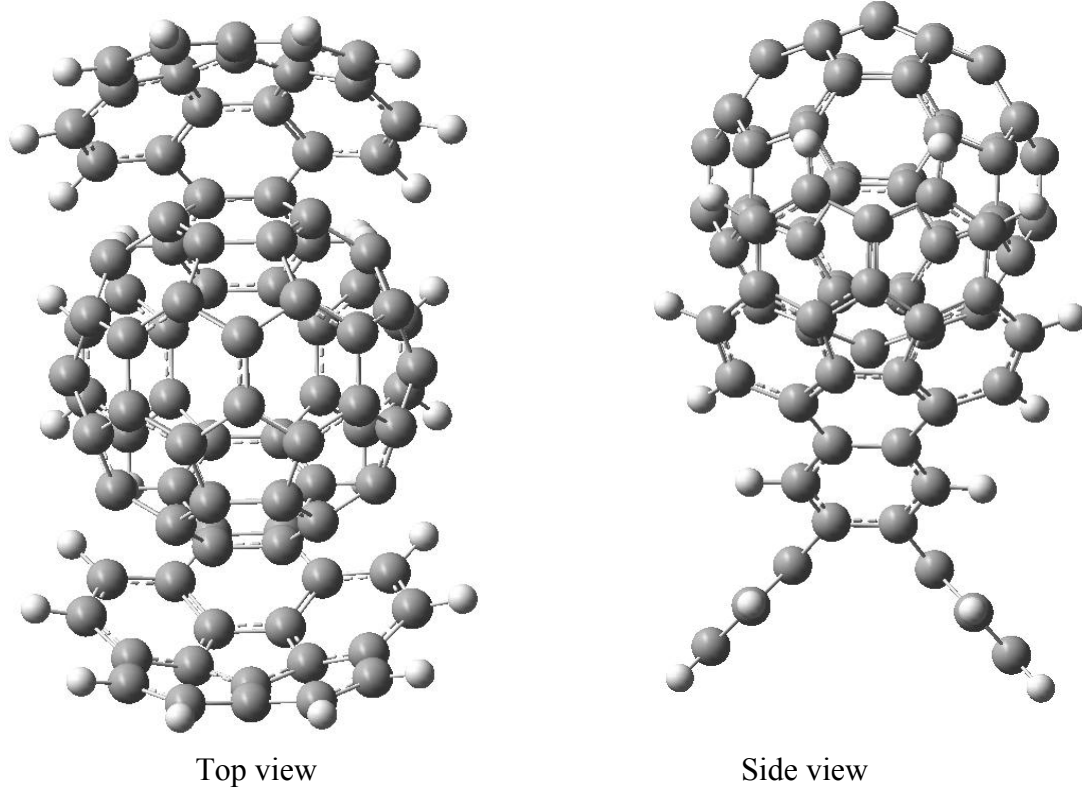


Figure S1. Different views of the structure of $C_{60}@C_{60}H_{28}$