

Supplementary Materials

to accompany

“Inclusion complexes of buckycatcher with C₆₀ and C₇₀”

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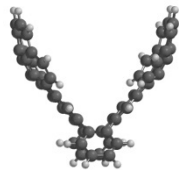
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Computational Details..... 2 –21

NMR Titration Details..... 22 - 23

Computational Results.

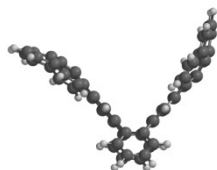
Clip 2a



B97-d/TZVP	E = -2302.2172212 a.u.	Rp = 11.152 Å	
Cartesian Coordinates (in Å):			
C	-2.31165804	1.39031061	-4.74697282
C	-1.49565995	0.70558776	-3.83176705
C	-1.49565995	-0.70558776	-3.83176705
C	-2.31165804	-1.39031061	-4.74697282
C	-3.10789786	-0.69896089	-5.66249384
C	-3.10789786	0.69896089	-5.66249384
C	-0.70836857	-1.48657304	-2.83896803
C	-1.38644437	-2.28477171	-1.91781267
C	-0.72698244	-3.08961987	-0.97300723
C	0.72698244	-3.08961987	-0.97300723
C	1.38644437	-2.28477171	-1.91781267
C	0.70836857	-1.48657304	-2.83896803
C	-1.47352972	-3.85678532	0.03403557
C	-0.71490350	-4.74033611	0.77971840
C	0.71490350	-4.74033611	0.77971840
C	1.47352972	-3.85678532	0.03403557
C	1.14799711	-5.25770919	2.02387272
C	0.00000000	-5.57609044	2.79185170
C	-1.14799711	-5.25770919	2.02387272
C	0.00000000	-5.57482225	4.18224750
C	1.30822106	-5.43607100	4.78665042
C	2.43658971	-5.12310860	4.03383616
C	2.36805794	-4.91794155	2.60259618
C	3.24555046	-4.15773788	1.74699579
C	2.81489923	-3.64839258	0.52126063
C	-1.30822106	-5.43607100	4.78665042
C	-2.43658971	-5.12310860	4.03383616
C	-2.36805794	-4.91794155	2.60259618
C	-3.24555046	-4.15773788	1.74699579
C	-2.81489923	-3.64839258	0.52126063
C	1.49565995	-0.70558776	-3.83176705
C	1.49565995	0.70558776	-3.83176705
C	2.31165804	1.39031061	-4.74697282
C	3.10789786	0.69896089	-5.66249384
C	3.10789786	-0.69896089	-5.66249384
C	2.31165804	-1.39031061	-4.74697282
C	-0.70836857	1.48657304	-2.83896803
C	-1.38644437	2.28477171	-1.91781267
C	-0.72698244	3.08961987	-0.97300723
C	0.72698244	3.08961987	-0.97300723
C	1.38644437	2.28477171	-1.91781267
C	0.70836857	1.48657304	-2.83896803
C	1.47352972	3.85678532	0.03403557
C	0.71490350	4.74033611	0.77971840
C	-0.71490350	4.74033611	0.77971840
C	-1.47352972	3.85678532	0.03403557
C	-1.14799711	5.25770919	2.02387272
C	0.00000000	5.57609044	2.79185170

C	1.14799711	5.25770919	2.02387272
C	2.81489923	3.64839258	0.52126063
C	3.24555046	4.15773788	1.74699579
C	2.36805794	4.91794155	2.60259618
C	2.43658971	5.12310860	4.03383616
C	1.30822106	5.43607100	4.78665042
C	0.00000000	5.57482225	4.18224750
C	-2.81489923	3.64839258	0.52126063
C	-3.24555046	4.15773788	1.74699579
C	-2.36805794	4.91794155	2.60259618
C	-2.43658971	5.12310860	4.03383616
C	-1.30822106	5.43607100	4.78665042
H	4.23778344	-3.88276957	2.10291547
H	3.48887863	-2.99118233	-0.02512046
H	-3.48887863	-2.99118233	-0.02512046
H	-4.23778344	-3.88276957	2.10291547
H	-3.37379924	-4.93393306	4.55619155
H	-1.40304343	-5.48140932	5.87107403
H	1.40304343	-5.48140932	5.87107403
H	3.37379924	-4.93393306	4.55619155
H	3.37379924	4.93393306	4.55619155
H	1.40304343	5.48140932	5.87107403
H	-1.40304343	5.48140932	5.87107403
H	-3.37379924	4.93393306	4.55619155
H	-4.23778344	3.88276957	2.10291547
H	-3.48887863	2.99118233	-0.02512046
H	3.48887863	2.99118233	-0.02512046
H	4.23778344	3.88276957	2.10291547
H	-2.47413577	-2.28244918	-1.93550019
H	2.47413577	-2.28244918	-1.93550019
H	-2.47413577	2.28244918	-1.93550019
H	2.47413577	2.28244918	-1.93550019
H	2.31054368	-2.47854363	-4.73520503
H	3.72437729	-1.24939725	-6.37050969
H	3.72437729	1.24939725	-6.37050969
H	2.31054368	2.47854363	-4.73520503
H	-2.31054368	-2.47854363	-4.73520503
H	-3.72437729	-1.24939725	-6.37050969
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H	-2.31054368	2.47854363	-4.73520503

Clip 2b



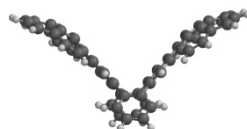
B97-d/TZVP E = -2302.2169368 a.u. Rp = 11.877 Å
Cartesian Coordinates (in Å):

C	1.91104082	-4.31566018	-2.31048022
C	1.21777396	-3.40628856	-1.49525595
C	-0.19333915	-3.41983388	-1.49510732
C	-0.86943815	-4.34286297	-2.30940507
C	-0.16952107	-5.25262883	-3.10481549
C	1.22832807	-5.23869430	-3.10554836
C	-0.98365395	-2.43390124	-0.70832874
C	-1.78634099	-1.51674806	-1.38651631
C	-2.57964762	-0.56219567	0.72705294
C	-2.57964762	-0.56219567	-0.72705294

C	-1.78634099	-1.51674806	1.38651631
C	-0.98365395	-2.43390124	0.70832874
C	-3.43797633	0.36841736	1.47384380
C	-4.01883989	1.36736222	0.71473806
C	-4.01883989	1.36736222	-0.71473806
C	-3.43797633	0.36841736	-1.47384380
C	-5.15235615	2.09526209	-1.14781563
C	-5.85252793	2.54359030	0.00000000
C	-5.15235615	2.09526209	1.14781563
C	-7.22144585	2.78707306	0.00000000
C	-7.84043358	2.75687754	-1.30849452
C	-7.15385529	2.31704110	-2.43697862
C	-5.78087165	1.86387780	-2.36850664
C	-5.06978338	0.96786777	-3.24698169
C	-3.95206121	0.25170729	-2.81644348
C	-7.84043358	2.75687754	1.30849452
C	-7.15385529	2.31704110	2.43697862
C	-5.78087165	1.86387780	2.36850664
C	-5.06978338	0.96786777	3.24698169
C	-3.95206121	0.25170729	2.81644348
C	-0.19333915	-3.41983388	1.49510732
C	1.21777396	-3.40628856	1.49525595
C	1.91104082	-4.31566018	2.31048022
C	1.22832807	-5.23869430	3.10554836
C	-0.16952107	-5.25262883	3.10481549
C	-0.86943815	-4.34286297	2.30940507
C	1.98857865	-2.40523620	-0.70836697
C	2.77563183	-1.47474283	-1.38653445
C	3.56862686	-0.51998250	-0.72696294
C	3.56862686	-0.51998250	0.72696294
C	2.77563183	-1.47474283	1.38653445
C	1.98857865	-2.40523620	0.70836697
C	4.32192177	0.49739349	1.47355078
C	5.19503916	1.25533665	0.71492825
C	5.19503916	1.25533665	-0.71492825
C	4.32192177	0.49739349	-1.47355078
C	5.69459172	2.50683894	-1.14803340
C	6.00200357	3.27932981	0.00000000
C	5.69459172	2.50683894	1.14803340
C	4.10609761	0.98167909	2.81477124
C	4.59793517	2.21447064	3.24542746
C	5.34574448	3.08078639	2.36785381
C	5.52921689	4.51491025	2.43630496
C	5.83147448	5.27208510	1.30800349
C	5.97992549	4.66961367	0.00000000
C	4.10609761	0.98167909	-2.81477124
C	4.59793517	2.21447064	-3.24542746
C	5.34574448	3.08078639	-2.36785381
C	5.52921689	4.51491025	-2.43630496
C	5.83147448	5.27208510	-1.30800349
H	-5.46583243	0.76235226	-4.24084632
H	-3.52571651	-0.48633284	-3.49344971
H	-3.52571651	-0.48633284	3.49344971
H	-5.46583243	0.76235226	4.24084632
H	-7.70113709	2.22316339	3.37434228
H	-8.90001583	2.99176637	1.40386015
H	-8.90001583	2.99176637	-1.40386015
H	-7.70113709	2.22316339	-3.37434228
H	5.33093533	5.03452135	3.37314413
H	5.85949162	6.35712041	1.40242549
H	5.85949162	6.35712041	-1.40242549
H	5.33093533	5.03452135	-3.37314413
H	4.31689339	2.56691400	-4.23717527

H	3.45603458	0.42647871	-3.48842974
H	3.45603458	0.42647871	3.48842974
H	4.31689339	2.56691400	4.23717527
H	-1.78048422	-1.53141805	-2.47424281
H	-1.78048422	-1.53141805	2.47424281
H	2.77299288	-1.49195727	-2.47422868
H	2.77299288	-1.49195727	2.47422868
H	-1.95779578	-4.34241744	2.30712149
H	-0.71310168	-5.96705976	3.72001498
H	1.78539959	-5.94188368	3.72159468
H	2.99910125	-4.29318609	2.30987645
H	-1.95779578	-4.34241744	-2.30712149
H	-0.71310168	-5.96705976	-3.72001498
H	1.78539959	-5.94188368	-3.72159468
H	2.99910125	-4.29318609	-2.30987645

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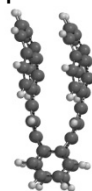


B97-d/TZVP E = -2302.2165423 a.u. Rp = 12.567 Å
Cartesian Coordinates (in Å):

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C	-0.70841061	-3.04555330	-1.49479135
C	-1.39357359	-3.96297248	-2.30778131
C	-0.70267688	-4.88122607	-3.10137772
C	0.69523578	-4.88171475	-3.10160987
C	-1.48802193	-2.05088668	-0.70831658
C	-2.27861607	-1.12349074	-1.38665337
C	-3.05889864	-0.15835039	0.72706801
C	-3.05889864	-0.15835039	-0.72706801
C	-2.27861607	-1.12349074	1.38665337
C	-1.48802193	-2.05088668	0.70831658
C	-3.90319234	0.78499492	1.47390530
C	-4.46851940	1.79265625	0.71471925
C	-4.46851940	1.79265625	-0.71471925
C	-3.90319234	0.78499492	-1.47390530
C	-5.59033426	2.53832800	-1.14784049
C	-6.28332371	2.99768013	0.00000000
C	-5.59033426	2.53832800	1.14784049
C	-7.64816003	3.26275906	0.00000000
C	-8.26745355	3.24242988	-1.30856445
C	-7.58794242	2.79183309	-2.43705481
C	-6.22229321	2.31692250	-2.36854641
C	-5.52517409	1.41003724	-3.24708969
C	-4.41878906	0.67650502	-2.81659195
C	-8.26745355	3.24242988	1.30856445
C	-7.58794242	2.79183309	2.43705481
C	-6.22229321	2.31692250	2.36854641
C	-5.52517409	1.41003724	3.24708969
C	-4.41878906	0.67650502	2.81659195
C	-0.70841061	-3.04555330	1.49479135
C	0.70275129	-3.04632364	1.49474311
C	1.38703258	-3.96419520	2.30794781
C	0.69523578	-4.88171475	3.10160987
C	-0.70267688	-4.88122607	3.10137772
C	-1.39357359	-3.96297248	2.30778131

C	1.48334330	-2.05236944	-0.70831635
C	2.27489354	-1.12582209	-1.38666354
C	3.05617750	-0.16147790	-0.72706461
C	3.05617750	-0.16147790	0.72706461
C	2.27489354	-1.12582209	1.38666354
C	1.48334330	-2.05236944	0.70831635
C	3.90139513	0.78106426	-1.47388460
C	4.46773739	1.78815096	-0.71473068
C	4.46773739	1.78815096	0.71473068
C	3.90139513	0.78106426	1.47388460
C	5.59027702	2.53271456	1.14783348
C	6.28372764	2.99137782	0.00000000
C	5.59027702	2.53271456	-1.14783348
C	4.41684457	0.67208604	-2.81660475
C	5.52392236	1.40458851	-3.24712126
C	6.22195899	2.31073923	-2.36858562
C	7.58808542	2.78437581	-2.43707820
C	8.26803503	3.23428072	-1.30860084
C	7.64882454	3.25514480	0.00000000
C	4.41684457	0.67208604	2.81660475
C	5.52392236	1.40458851	3.24712126
C	6.22195899	2.31073923	2.36858562
C	7.58808542	2.78437581	2.43707820
C	8.26803503	3.23428072	1.30860084
H	-5.92403915	1.21125037	-4.24119247
H	-4.00338102	-0.06745982	-3.49390582
H	-4.00338102	-0.06745982	3.49390582
H	-5.92403915	1.21125037	4.24119247
H	-8.13665960	2.70716398	3.37447847
H	-9.32313070	3.49437752	1.40388002
H	-9.32313070	3.49437752	-1.40388002
H	-8.13665960	2.70716398	-3.37447847
H	8.13658007	2.69919285	-3.37458356
H	9.32395461	3.48521817	-1.40393296
H	9.32395461	3.48521817	1.40393296
H	8.13658007	2.69919285	3.37458356
H	5.92250410	1.20543827	4.24127043
H	4.00070549	-0.07149400	3.49389133
H	4.00070549	-0.07149400	-3.49389133
H	5.92250410	1.20543827	-4.24127043
H	-2.27230420	-1.13760124	-2.47437899
H	-2.27230420	-1.13760124	2.47437899
H	2.26865892	-1.14001334	-2.47438650
H	2.26865892	-1.14001334	2.47438650
H	-2.48186170	-3.95120687	2.30612171
H	-1.25333429	-5.59116905	3.71547964
H	1.24518728	-5.59192774	3.71603409
H	2.47532798	-3.95334171	2.30644835
H	-2.48186170	-3.95120687	-2.30612171
H	-1.25333429	-5.59116905	-3.71547964
H	1.24518728	-5.59192774	-3.71603409
H	2.47532798	-3.95334171	-2.30644835

Clip 2d



B97-d/TZVP E = -2302.2180898 a.u. Rp = 3.966 Å
Cartesian Coordinates (in Å):

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C	-6.41907081	0.32232718	2.90159316
C	-5.53970717	1.14435446	2.18672049
C	-4.48307991	0.58610448	1.46170428
C	-4.30233888	-0.81962652	1.45898932
C	-5.18189039	-1.63212380	2.17943941
C	-3.47689250	1.39342173	0.70771661
C	-3.47689250	1.39342173	-0.70771661
C	-2.37070713	1.89722661	-1.38741140
C	-1.19961967	2.31048895	-0.72772428
C	-1.19961967	2.31048895	0.72772428
C	-2.37070713	1.89722661	1.38741140
C	0.04692615	2.53050348	1.47512551
C	1.12567216	2.94393874	0.71496719
C	1.12567216	2.94393874	-0.71496719
C	0.04692615	2.53050348	-1.47512551
C	2.46523042	2.79086868	-1.14662015
C	2.81270453	2.21181829	-2.36375117
C	1.69826440	1.94892211	-3.23839066
C	0.37966836	2.09891214	-2.81130149
C	2.46523042	2.79086868	1.14662015
C	2.81270453	2.21181829	2.36375117
C	1.69826440	1.94892211	3.23839066
C	0.37966836	2.09891214	2.81130149
C	3.29192656	2.70249258	0.00000000
C	4.16925674	1.71433895	-2.43238238
C	4.98291925	1.63793586	-1.30723781
C	4.51687740	2.04582635	0.00000000
C	4.16925674	1.71433895	2.43238238
C	4.98291925	1.63793586	1.30723781
C	-4.48307991	0.58610448	-1.46170428
C	-5.53970717	1.14435446	-2.18672049
C	-6.41907081	0.32232718	-2.90159316
C	-6.24085618	-1.06390033	-2.89764513
C	-5.18189039	-1.63212380	-2.17943941
C	-4.30233888	-0.81962652	-1.45898932
C	-3.11834718	-1.33413418	-0.70699725
C	-3.11834718	-1.33413418	0.70699725
C	-1.91223233	-1.49099357	1.39056075
C	-0.67566351	-1.50621462	0.72776305
C	-0.67566351	-1.50621462	-0.72776305
C	-1.91223233	-1.49099357	-1.39056075
C	0.58716504	-1.40099695	1.47315683
C	1.66665257	-0.99806950	0.71404538
C	1.66665257	-0.99806950	-0.71404538
C	0.58716504	-1.40099695	-1.47315683
C	3.00184798	-1.14223509	-1.14577906
C	3.34873449	-1.70340847	-2.36933991
C	2.23205925	-1.95087307	-3.24790044
C	0.91095854	-1.80810034	-2.81613357
C	3.00184798	-1.14223509	1.14577906
C	3.34873449	-1.70340847	2.36933991
C	2.23205925	-1.95087307	3.24790044
C	0.91095854	-1.80810034	2.81613357
C	3.82722041	-1.22679967	0.00000000
C	4.71187649	-2.18569604	-2.44039081
C	5.52654307	-2.26286737	-1.31247857
C	5.05711939	-1.86929041	0.00000000
C	4.71187649	-2.18569604	2.44039081
C	5.52654307	-2.26286737	1.31247857
H	-2.36860486	1.84987040	-2.47397146
H	-2.36860486	1.84987040	2.47397146
H	-0.41135028	1.77471112	-3.48441165

H	-0.41135028	1.77471112	3.48441165
H	1.87769609	1.51804634	-4.22220943
H	1.87769609	1.51804634	4.22220943
H	4.53190197	1.28213769	-3.36357730
H	4.53190197	1.28213769	3.36357730
H	5.95062786	1.14782874	-1.40004376
H	5.95062786	1.14782874	1.40004376
H	-5.67229067	2.22464351	-2.18797597
H	-5.67229067	2.22464351	2.18797597
H	-7.24161612	0.76536052	-3.45984077
H	-7.24161612	0.76536052	3.45984077
H	0.11357624	-2.10721071	-3.49452279
H	0.11357624	-2.10721071	3.49452279
H	2.40993134	-2.35267701	-4.24491176
H	2.40993134	-2.35267701	4.24491176
H	5.08884129	-2.58991473	-3.37944825
H	5.08884129	-2.58991473	3.37944825
H	6.50877062	-2.72354562	-1.41392174
H	6.50877062	-2.72354562	1.41392174
H	-1.92024659	-1.43268523	-2.47710383
H	-1.92024659	-1.43268523	2.47710383
H	-5.03575516	-2.71071191	-2.17519329
H	-5.03575516	-2.71071191	2.17519329
H	-6.92412075	-1.70389242	-3.45269287
H	-6.92412075	-1.70389242	3.45269287

Complex C60@2

B97-d/TZVP E = -4587.3219883 a.u. Rp = 12.798 Å

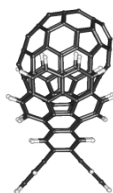
Cartesian Coordinates (in Å):

C	-1.19705112	-6.78248429	2.35733806
C	-0.54183599	-5.86353674	1.51759331
C	0.86877714	-5.82567057	1.51551975
C	1.57530835	-6.70795878	2.35282537
C	0.91318038	-7.62330199	3.17160076
C	-0.48391191	-7.66068296	3.17395987
C	1.65636644	-4.85143802	0.71258456
C	2.53466306	-3.99607419	1.38230751
C	3.44173404	-3.15497768	0.71952324
C	3.43347840	-3.15627326	-0.73434261
C	2.52308649	-4.00274019	-1.38517267
C	1.65254533	-4.85662969	-0.70389877
C	4.33866685	-2.25977428	1.46268916
C	5.29893981	-1.63147919	0.69353296
C	5.28849745	-1.63022409	-0.73419220
C	4.31763559	-2.25848574	-1.48948521
C	5.96639205	-0.46906645	-1.17165663
C	6.39270574	0.24750766	-0.02707703
C	5.98483765	-0.47201511	1.12242424
C	6.58728953	1.62256504	-0.02651167
C	6.52216991	2.23829035	-1.33564482
C	6.10796161	1.53401343	-2.46244049
C	5.71333201	0.14267748	-2.39453033
C	4.84959509	-0.61209596	-3.27015462
C	4.18068986	-1.75590298	-2.83519980
C	6.54676159	2.23413884	1.28569334
C	6.15106671	1.52676026	2.41717370
C	5.75355853	0.13624687	2.35142539
C	4.90510306	-0.62072419	3.23997133
C	4.22670402	-1.76165226	2.81251158
C	0.86571310	-5.84104641	-1.49472383
C	-0.54438716	-5.88234817	-1.49266002
C	-1.20011445	-6.81314515	-2.31874879
C	-0.48685981	-7.70048225	-3.12531442

C	0.91022067	-7.65955460	-3.12749817
C	1.57257682	-6.73206950	-2.32259123
C	-1.38387740	-4.93529874	0.71538831
C	-2.30574161	-4.12797099	1.38643934
C	-3.26027551	-3.34024969	0.72478778
C	-3.25759718	-3.34562083	-0.72918632
C	-2.30370988	-4.14145572	-1.38152079
C	-1.38460169	-4.94383955	-0.70103552
C	-4.19374423	-2.50128573	-1.48319443
C	-5.19496250	-1.92539082	-0.72542320
C	-5.19945096	-1.92195629	0.70223145
C	-4.20205710	-2.49296788	1.46860355
C	-5.94731322	-0.80127853	1.13065456
C	-6.40010694	-0.11009739	-0.01972456
C	-5.93965120	-0.80649769	-1.16394564
C	-4.09234542	-1.99803930	-2.83168952
C	-4.82592114	-0.89494197	-3.26741384
C	-5.72605993	-0.18609697	-2.39018661
C	-6.19636273	1.18118633	-2.46124119
C	-6.64449582	1.86563842	-1.33531292
C	-6.66913664	1.25233479	-0.02360617
C	-4.11043606	-1.98413115	2.81583531
C	-4.84802453	-0.88008772	3.24208403
C	-5.74247476	-0.17547413	2.35567384
C	-6.21393303	1.19185429	2.41759528
C	-6.65302998	1.87152813	1.28535514
H	4.62000664	-0.22505906	-4.26169882
H	3.45469350	-2.20961902	-3.50677668
H	3.51220909	-2.21687142	3.49537998
H	4.69432556	-0.23734674	4.23720302
H	6.04077435	2.06950397	3.35486993
H	6.73054921	3.30332902	1.38169553
H	6.70293892	3.30801682	-1.43139928
H	5.98002372	2.07988699	-3.39606436
H	-6.10314216	1.72961497	-3.39750013
H	-6.88409228	2.92342563	-1.43388599
H	-6.89314925	2.92981266	1.37736599
H	-6.12671465	1.74432777	3.35205891
H	-4.65256863	-0.48054600	4.23598684
H	-3.36791024	-2.39592116	3.49632750
H	-3.34579680	-2.41359900	-3.50550755
H	-4.62325143	-0.49964918	-4.26160501
H	2.53813733	-4.01188964	2.46976786
H	2.51823415	-4.02462365	-2.47254584
H	-2.30437970	-4.14092364	2.47394371
H	-2.30081967	-4.16511905	-2.46886053
H	2.65994015	-6.69147901	-2.32006670
H	1.48177936	-8.34528562	-3.74980546
H	-1.01911751	-8.41865672	-3.74589702
H	-2.28795954	-6.83617949	-2.31329457
H	2.66270620	-6.67021288	2.34680032
H	1.48490256	-8.30236320	3.80101454
H	-1.01634978	-8.36944419	3.80511677
H	-2.28490570	-6.80366055	2.35468970
C	0.66331015	2.47224543	-3.46907102
C	1.42015617	1.32292559	-3.00396243
C	2.57041166	1.81371387	-2.26848602
C	2.52992682	3.26434443	-2.28122351
C	3.00401714	1.13997115	-1.12532844
C	0.75092534	0.17313602	-2.56896973
C	1.34970151	3.67265183	-3.02198754
C	-0.73487266	2.43006841	-3.48162145
C	0.61293558	4.78597150	-2.60443253

C	2.93104019	3.98505989	-1.15109519
C	3.41951893	1.88565973	0.04424416
C	2.31290756	-0.04997921	-0.67658403
C	3.38580796	3.28115949	0.03353679
C	2.16608088	5.14067139	-0.71795451
C	1.02873635	5.53386529	-1.43083006
C	-0.83895727	4.74223871	-2.61750965
C	-1.50000158	3.58706631	-3.04798368
C	-1.42958972	1.23720713	-3.02984494
C	-0.70079471	0.12932438	-2.58209598
C	1.20740890	-0.52784143	-1.38299523
C	2.98266916	1.15706337	1.21677214
C	2.29952642	-0.03958154	0.77227513
C	-1.13558984	-0.59857808	-1.40416302
C	0.04303279	-1.01237272	-0.66599530
C	-2.66749383	3.10869624	-2.32900684
C	-2.62049531	1.65808299	-2.31588231
C	-1.31985524	5.46298442	-1.45206864
C	-0.16581543	5.95236463	-0.71840803
C	2.15286041	5.15191243	0.73517392
C	2.90920325	4.00251188	1.19917880
C	2.48763349	3.29814622	2.33234032
C	2.52780567	1.84727561	2.34162038
C	1.18111880	-0.50768798	1.46504110
C	0.02993604	-1.00226515	0.73319752
C	-3.03322065	0.95892578	-1.18037564
C	-2.28010505	-0.18753743	-0.71828150
C	-2.44484538	5.00276677	-0.75992948
C	-3.13123381	3.80331865	-1.20620187
C	-0.17891833	5.96313993	0.68028494
C	1.00200512	5.55454101	1.42075848
C	1.36386624	1.36716118	3.06263657
C	0.70261283	0.21108629	2.63199472
C	-1.16182217	-0.57752890	1.44348217
C	-2.29366335	-0.17710274	0.73063368
C	-3.51391707	1.67755719	-0.01903378
C	-3.56435945	3.07266849	-0.02959753
C	-2.45823180	5.01338579	0.69323184
C	-1.34661889	5.48448680	1.39963613
C	0.56463339	4.82416266	2.59737931
C	1.29339986	3.71692550	3.04448233
C	-0.88724635	4.78056517	2.58420771
C	0.59866875	2.52329539	3.49615878
C	-0.74897097	0.16745545	2.61860472
C	-3.05485921	0.97622590	1.16151858
C	-3.15281559	3.82063126	1.14401920
C	-2.70996852	3.14249831	2.28491906
C	-1.55640556	3.63153104	3.01887107
C	-0.79950548	2.48140954	3.48332736
C	-1.48578247	1.28191228	3.03625100
C	-2.66300775	1.69198328	2.29408228

Complex 5a



B97-d/TZVP E = -4968.2652872 a.u. Rp = 12.777 Å
Cartesian Coordinates (in Å):

C	5.06797524	2.29936385	-2.08110191
C	5.89897484	1.17307146	-2.09318976
C	6.52371734	0.72403427	-0.86283944
C	6.52298902	-0.72680450	-0.86336685
C	4.82422217	3.00948035	-0.84308331
C	6.29135276	1.41952156	0.32994032
C	3.82179516	2.29178550	-2.81832071
C	5.51176916	-0.00025391	-2.85399954
C	5.89789027	-1.17446402	-2.09399943
C	4.30966839	0.00055758	-3.57145104
C	6.29011693	-1.42294291	0.32897281
C	5.42470772	2.57891710	0.33895272
C	6.04330495	0.69484063	1.55837520
C	5.06591606	-2.30004878	-2.08272685
C	6.04268024	-0.69882915	1.55788732
C	5.42243943	-2.58156480	0.33712048
C	3.44832217	3.45034855	-0.82960580
C	3.44988130	1.16508719	-3.55024381
C	2.82895255	3.00645603	-2.04921429
C	4.66725174	2.57712839	1.57044432
C	5.04939546	1.41310607	2.32396359
C	5.04810979	-1.41672651	2.32293081
C	4.66493768	-2.57988475	1.56857265
C	4.82158603	-3.01082984	-0.84519530
C	2.70895392	3.53703254	0.38071126
C	3.34127529	3.08846007	1.62819035
C	4.11489123	0.73371052	3.15446026
C	4.11426399	-0.73708517	3.15391512
C	3.33853737	-3.09005761	1.62599817
C	3.44526480	-3.45051077	-0.83202815
C	1.29743241	3.43959955	0.26310748
C	1.45628772	2.63991265	-2.08630639
C	2.51079522	2.57621272	2.66402205
C	2.89265937	1.41354883	3.41790352
C	2.89143447	-1.41605179	3.41687270
C	2.50851935	-2.57780057	2.66217162
C	2.70579418	-3.53723914	0.37821857
C	0.47621507	2.99837080	1.36291378
C	0.68026831	2.99610084	-0.95227396
C	1.07080918	2.57550069	2.54650265
C	1.68679031	0.69590182	3.76914407
C	1.68618267	-0.69763588	3.76869291
C	1.06855188	-2.57584146	2.54471320
C	1.29437200	-3.43841716	0.26065200
C	3.44875717	-1.16320657	-3.55093615
C	3.81970105	-2.29077144	-2.81984491
C	2.07403888	0.72077706	-3.53734415
C	2.82623686	-3.00516973	-2.05131774
C	1.06126875	1.45650863	-2.86129493
C	-0.66398842	2.29137013	0.83100892
C	-0.52458179	2.28389863	-0.60577871
C	0.54934101	1.42069400	3.24361876
C	0.54804539	-1.42107867	3.24264168
C	0.47356131	-2.99721728	1.36075992
C	0.67755844	-2.99355415	-0.95440564
C	2.07336548	-0.71768277	-3.53775270
C	1.45390244	-2.63728192	-2.08814605
C	-0.08290894	0.72105199	-2.44133621
C	-1.17309582	1.17226915	1.49464872
C	-0.90371109	1.16363667	-1.33779056
C	-0.55193239	0.72570549	2.72677805
C	-0.55261549	-0.72475925	2.72626074
C	-0.66605016	-2.28888993	0.82939921

C	-0.52671052	-2.28057480	-0.60744776
C	1.05992553	-1.45297180	-2.86232717
C	-0.08361305	-0.71677179	-2.44188719
C	-1.56544918	0.00170157	0.73502846
C	-1.43501618	0.00209330	-0.65904002
C	-1.17423771	-1.16979831	1.49380312
C	-0.90486484	-1.15945883	-1.33867218
C	-7.40282719	1.38705903	1.93015402
C	-6.43174906	0.70562386	1.17413928
C	-6.43169916	-0.70519539	1.17414003
C	-7.40275226	-1.38668799	1.93010957
C	-8.36853495	-0.69871005	2.66530912
C	-8.36854539	0.69898155	2.66534829
C	-5.41310213	-1.51929680	0.45760552
C	-4.63963081	-2.41637306	1.19827021
C	-3.76921098	-3.34625432	0.60970038
C	-3.65259791	-3.34732804	-0.83951400
C	-4.41678917	-2.41707422	-1.56061829
C	-5.29898154	-1.51959482	-0.95426824
C	-2.95693866	-4.25760533	1.42700325
C	-2.29489905	-5.23998494	0.71681149
C	-2.18285711	-5.24315227	-0.70653413
C	-2.72335425	-4.26251856	-1.51561186
C	-1.01136268	-5.95754614	-1.04754748
C	-0.39541059	-6.38900992	0.15230329
C	-1.18900026	-5.94920422	1.23961635
C	0.97082709	-6.61482652	0.25949369
C	1.68544147	-6.58301855	-0.99923794
C	1.08011363	-6.16437233	-2.18021740
C	-0.30058099	-5.73208286	-2.22175342
C	-0.96196950	-4.85841411	-3.16063317
C	-2.11638769	-4.15390053	-2.82007590
C	1.48320537	-6.57021747	1.61327170
C	0.70222080	-6.14405426	2.68364968
C	-0.66956541	-5.71632990	2.50843723
C	-1.47037063	-4.83949666	3.32828362
C	-2.56009673	-4.14107688	2.80945524
C	-6.18868895	-0.70522471	-1.82559182
C	-6.18871027	0.70572034	-1.82568751
C	-7.02482020	1.38698780	-2.72890173
C	-7.85837343	0.69895754	-3.61121594
C	-7.85834760	-0.69864423	-3.61118479
C	-7.02479039	-1.38654286	-2.72878356
C	-5.41326416	1.51980330	0.45755526
C	-4.63983861	2.41692463	1.19824812
C	-3.76918675	3.34660343	0.60971790
C	-3.65271120	3.34788783	-0.83950039
C	-4.41687746	2.41759136	-1.56060983
C	-5.29914943	1.52015400	-0.95430570
C	-2.72349367	4.26305124	-1.51555493
C	-2.18267268	5.24349468	-0.70643704
C	-2.29462293	5.24020773	0.71693380
C	-2.95682526	4.25784536	1.42703012
C	-1.18831948	5.94886912	1.23975344
C	-0.39462729	6.38839689	0.15241625
C	-1.01086572	5.95737367	-1.04748000
C	-2.11652987	4.15418557	-2.82002585
C	-0.96188010	4.85826802	-3.16061178
C	-0.30024170	5.73169669	-2.22174698
C	1.08064619	6.16338327	-2.18029293
C	1.68631879	6.58125160	-0.99924975
C	0.97177546	6.61324897	0.25952133
C	-2.56006900	4.14111534	2.80948951

C	-1.46994597	4.83887788	3.32828060
C	-0.66884844	5.71552491	2.50850096
C	0.70325213	6.14213626	2.68356052
C	1.48445470	6.56764025	1.61310560
H	-0.49452211	-4.65119484	-4.12204019
H	-2.49757409	-3.42346957	-3.53080365
H	-3.04852812	-3.40829515	3.44863134
H	-1.15740450	-4.62511667	4.34901029
H	1.17531918	-6.03336827	3.65833201
H	2.53722607	-6.77805717	1.79170491
H	2.75414559	-6.79110843	-1.01131275
H	1.69862775	-6.06129033	-3.07045038
H	1.69910712	6.06009438	-3.07053950
H	2.75515604	6.78864211	-1.01132691
H	2.53880160	6.77412731	1.79128346
H	1.17630534	6.03075868	3.65815555
H	-1.15699754	4.62430526	4.34897406
H	-3.04877949	3.40852960	3.44852522
H	-2.49798014	3.42386231	-3.53074179
H	-0.49467880	4.65101420	-4.12213549
H	-4.74557626	-2.41475495	2.28076588
H	-4.34825009	-2.41602943	-2.64608584
H	-4.74578607	2.41525372	2.28075286
H	-4.34814581	2.41640118	-2.64605832
H	-7.01680686	-2.47454834	-2.72375389
H	-8.50349987	-1.25092834	-4.29157316
H	-8.50354436	1.25115748	-4.29165732
H	-7.01688631	2.47502594	-2.72393185
H	-7.39376967	-2.47475553	1.92672947
H	-9.11566516	-1.25081347	3.23202192
H	-9.11570303	1.25103930	3.23207489
H	-7.39394496	2.47512523	1.92680562

Complex 5b



B97-d/TZVP E = -4968.2636069 a.u. Rp = 12.936 Å
Cartesian Coordinates (in Å):

C	-0.10781880	0.97213108	-3.21727958
C	-1.21658377	0.56016424	-3.96683662
C	-1.60606545	-0.83787885	-3.96741791
C	-3.05611231	-0.89980546	-3.96799581
C	0.65010364	0.01133024	-2.44125693
C	-0.87042029	-1.76232215	-3.21687823
C	-0.17483466	2.18523992	-2.43423388
C	-2.42611638	1.36142648	-3.96715163
C	-3.56286502	0.45940653	-3.96775979
C	-2.47717727	2.54247415	-3.21712483
C	-3.71077366	-1.88615205	-3.21929949
C	0.27185059	-1.32865763	-2.43948761
C	-1.55443287	-2.76896301	-2.43596133
C	-4.70364950	0.77724639	-3.21974474
C	-2.94476283	-2.83530034	-2.44063531
C	-4.88527646	-1.55093347	-2.44217657
C	1.06632329	0.64189367	-1.20764345
C	-1.33314390	2.95519242	-2.43574521
C	0.55300326	1.98241819	-1.20441129
C	0.29411633	-2.07660796	-1.20435385

C	-0.83059707	-2.96525534	-1.20379370
C	-3.65303149	-3.09845992	-1.20815628
C	-4.85208388	-2.30494433	-1.20895454
C	-5.37162429	-0.24481259	-2.44208222
C	1.19298611	-0.09810670	0.00000000
C	0.78781226	-1.50971043	0.00000000
C	-1.49412360	-3.31477774	0.00000000
C	-2.96060313	-3.38359060	0.00000000
C	-5.38776660	-1.77934819	0.00000000
C	-5.83952228	0.34709243	-1.20894189
C	1.06632329	0.64189367	1.20764345
C	0.16294800	2.62299453	0.00000000
C	0.29411633	-2.07660796	1.20435385
C	-0.83059707	-2.96525534	1.20379370
C	-3.65303149	-3.09845992	1.20815628
C	-4.85208388	-2.30494433	1.20895454
C	-5.89999088	-0.40081285	0.00000000
C	0.65010364	0.01133024	2.44125693
C	0.55300326	1.98241819	1.20441129
C	0.27185059	-1.32865763	2.43948761
C	-1.55443287	-2.76896301	2.43596133
C	-2.94476283	-2.83530034	2.44063531
C	-4.88527646	-1.55093347	2.44217657
C	-5.83952228	0.34709243	1.20894189
C	-3.65660274	2.86379503	-2.44085073
C	-4.74846628	1.99799634	-2.44246228
C	-1.80286672	3.54408474	-1.20473355
C	-5.45436091	1.73254453	-1.20900272
C	-1.06021136	3.43587667	0.00000000
C	-0.10781880	0.97213108	3.21727958
C	-0.17483466	2.18523992	2.43423388
C	-0.87042029	-1.76232215	3.21687823
C	-3.71077366	-1.88615205	3.21929949
C	-5.37162429	-0.24481259	2.44208222
C	-5.45436091	1.73254453	1.20900272
C	-3.23828899	3.49132855	-1.20795017
C	-5.12070802	2.40486528	0.00000000
C	-1.80286672	3.54408474	1.20473355
C	-1.21658377	0.56016424	3.96683662
C	-1.33314390	2.95519242	2.43574521
C	-1.60606545	-0.83787885	3.96741791
C	-3.05611231	-0.89980546	3.96799581
C	-4.70364950	0.77724639	3.21974474
C	-4.74846628	1.99799634	2.44246228
C	-3.96933186	3.31952121	0.00000000
C	-3.23828899	3.49132855	1.20795017
C	-2.42611638	1.36142648	3.96715163
C	-2.47717727	2.54247415	3.21712483
C	-3.56286502	0.45940653	3.96775979
C	-3.65660274	2.86379503	2.44085073
C	6.90570687	-1.79603453	2.33940689
C	6.04083719	-1.06338601	1.50569884
C	6.12246354	0.34506609	1.50601979
C	7.06625335	0.97211755	2.34017719
C	7.92605173	0.23321429	3.15311790
C	7.84520480	-1.16204218	3.15271259
C	5.21867846	1.21718207	0.70841335
C	4.45562120	2.17276874	1.38379919
C	3.71001944	3.16414605	0.72780887
C	3.71001944	3.16414605	-0.72780887
C	4.45562120	2.17276874	-1.38379919
C	5.21867846	1.21718207	-0.70841335
C	2.92506029	4.15311218	1.47954890

C	2.39597164	5.17208365	0.71316580
C	2.39597164	5.17208365	-0.71316580
C	2.92506029	4.15311218	-1.47954890
C	1.31510289	5.97185277	-1.14615986
C	0.64187080	6.45566387	0.00000000
C	1.31510289	5.97185277	1.14615986
C	-0.70357855	6.80011635	0.00000000
C	-1.31136033	6.82425074	-1.31439107
C	-0.64503868	6.35873108	-2.44656282
C	0.69450315	5.81377382	-2.37982472
C	1.37566404	4.90527922	-3.26985567
C	2.43718833	4.10925224	-2.83661911
C	-1.31136033	6.82425074	1.31439107
C	-0.64503868	6.35873108	2.44656282
C	0.69450315	5.81377382	2.37982472
C	1.37566404	4.90527922	3.26985567
C	2.43718833	4.10925224	2.83661911
C	6.12246354	0.34506609	-1.50601979
C	6.04083719	-1.06338601	-1.50569884
C	6.90570687	-1.79603453	-2.33940689
C	7.84520480	-1.16204218	-3.15271259
C	7.92605173	0.23321429	-3.15311790
C	7.06625335	0.97211755	-2.34017719
C	5.04147517	-1.82425591	0.70843700
C	4.17151913	-2.68356989	1.38393595
C	3.31296095	-3.57829123	0.72728601
C	3.31296095	-3.57829123	-0.72728601
C	4.17151913	-2.68356989	-1.38393595
C	5.04147517	-1.82425591	-0.70843700
C	2.40407610	-4.45524164	-1.47787004
C	1.75156130	-5.40255934	-0.71382632
C	1.75156130	-5.40255934	0.71382632
C	2.40407610	-4.45524164	1.47787004
C	0.57815418	-6.05993979	1.14701113
C	-0.15064668	-6.45653706	0.00000000
C	0.57815418	-6.05993979	-1.14701113
C	1.91731357	-4.33365482	-2.83061445
C	0.76170346	-4.98432977	-3.26336797
C	-0.02237763	-5.80907271	-2.37620974
C	-1.42354491	-6.16582790	-2.44250520
C	-2.14239143	-6.54130620	-1.31101719
C	-1.53106269	-6.60924580	0.00000000
C	1.91731357	-4.33365482	2.83061445
C	0.76170346	-4.98432977	3.26336797
C	-0.02237763	-5.80907271	2.37620974
C	-1.42354491	-6.16582790	2.44250520
C	-2.14239143	-6.54130620	1.31101719
H	0.98822457	4.74441198	-4.27449004
H	2.82463078	3.35979862	-3.52388738
H	2.82463078	3.35979862	3.52388738
H	0.98822457	4.74441198	4.27449004
H	-1.19454305	6.31196301	3.38564845
H	-2.35403703	7.12194754	1.41556147
H	-2.35403703	7.12194754	-1.41556147
H	-1.19454305	6.31196301	-3.38564845
H	-1.96346759	-6.03668769	-3.37907240
H	-3.21666968	-6.69178093	-1.40715986
H	-3.21666968	-6.69178093	1.40715986
H	-1.96346759	-6.03668769	3.37907240
H	0.39006180	-4.76624715	4.26315989
H	2.39353638	-3.63284792	3.51302759
H	2.39353638	-3.63284792	-3.51302759
H	0.39006180	-4.76624715	-4.26315989

H	4.47498141	2.17041498	2.47122669
H	4.47498141	2.17041498	-2.47122669
H	4.19101455	-2.68369728	2.47137160
H	4.19101455	-2.68369728	-2.47137160
H	7.12160205	2.05874398	-2.33571188
H	8.65439980	0.74410823	-3.77974819
H	8.50950791	-1.75406635	-3.77909453
H	6.83476091	-2.88178047	-2.33438053
H	7.12160205	2.05874398	2.33571188
H	8.65439980	0.74410823	3.77974819
H	8.50950791	-1.75406635	3.77909453
H	6.83476091	-2.88178047	2.33438053

Complex 5c



B97-d/TZVP E = -4968.2576818 a.u. Rp = 13.496 Å

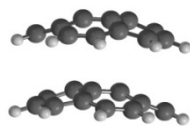
Cartesian Coordinates (in Å):

C	0.57719530	1.41260349	3.20966236
C	1.52957617	0.71536970	3.95340794
C	1.52341728	-0.72993399	3.95278030
C	2.89812010	-1.18585626	3.96075656
C	-0.40966062	0.69680662	2.43743626
C	0.56534991	-1.41818467	3.20852920
C	0.96313082	2.57233822	2.43862832
C	2.90834840	1.15899686	3.96106572
C	3.75619807	-0.01716596	3.96474958
C	3.27934042	2.28567333	3.21938256
C	3.25916887	-2.31580260	3.21924696
C	-0.41541659	-0.69367716	2.43698313
C	0.94062341	-2.58149910	2.43801192
C	4.94177554	-0.02241586	3.21939933
C	2.26197530	-3.02218407	2.44150203
C	4.47981288	-2.31203140	2.44172906
C	-0.64549333	1.41693343	1.20789974
C	2.28846728	3.00091312	2.44177690
C	0.20426813	2.57766514	1.20847235
C	-0.65792380	-1.41181580	1.20773964
C	0.18139487	-2.58022583	1.20826884
C	2.87125346	-3.46599697	1.20827994
C	4.24124564	-3.02792521	1.20854561
C	5.30512139	-1.18828847	2.44235511
C	-0.97096884	0.73981891	0.00000000
C	-0.97752486	-0.73186485	0.00000000
C	0.72707542	-3.09635659	0.00000000
C	2.12500277	-3.55575480	0.00000000
C	4.89941243	-2.66744630	0.00000000
C	5.91523627	-0.74577536	1.20873695
C	-0.64549333	1.41693343	-1.20789974
C	0.75449827	3.08875686	0.00000000
C	-0.65792380	-1.41181580	-1.20773964
C	0.18139487	-2.58022583	-1.20826884
C	2.87125346	-3.46599697	-1.20827994
C	4.24124564	-3.02792521	-1.20854561
C	5.76932895	-1.48168053	0.00000000
C	-0.40966062	0.69680662	-2.43743626
C	0.20426813	2.57766514	-1.20847235
C	-0.41541659	-0.69367716	-2.43698313

C	0.94062341	-2.58149910	-2.43801192
C	2.26197530	-3.02218407	-2.44150203
C	4.47981288	-2.31203140	-2.44172906
C	5.91523627	-0.74577536	-1.20873695
C	4.49983898	2.27104449	2.44175703
C	5.31528705	1.14018198	2.44231634
C	2.90165291	3.43917289	1.20837050
C	5.92147887	0.69230566	1.20870813
C	2.15639371	3.53564498	0.00000000
C	0.57719530	1.41260349	-3.20966236
C	0.96313082	2.57233822	-2.43862832
C	0.56534991	-1.41818467	-3.20852920
C	3.25916887	-2.31580260	-3.21924696
C	5.30512139	-1.18828847	-2.44235511
C	5.92147887	0.69230566	-1.20870813
C	4.26761240	2.98899299	1.20857391
C	5.78202789	1.42944850	0.00000000
C	2.90165291	3.43917289	-1.20837050
C	1.52957617	0.71536970	-3.95340794
C	2.28846728	3.00091312	-2.44177690
C	1.52341728	-0.72993399	-3.95278030
C	2.89812010	-1.18585626	-3.96075656
C	4.94177554	-0.02241586	-3.21939933
C	5.31528705	1.14018198	-2.44231634
C	4.92256137	2.62278876	0.00000000
C	4.26761240	2.98899299	-1.20857391
C	2.90834840	1.15899686	-3.96106572
C	3.27934042	2.28567333	-3.21938256
C	3.75619807	-0.01716596	-3.96474958
C	4.49983898	2.27104449	-2.44175703
C	-7.01793526	-2.37728744	1.38614650
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C	-6.12012591	-1.53409251	-0.70549270
C	-7.01793526	-2.37728744	-1.38614650
C	-7.91089615	-3.19956318	-0.69879261
C	-7.91089615	-3.19956318	0.69879261
C	-5.17785030	-0.72507011	-1.52494216
C	-4.36310761	-1.38976568	-2.44588892
C	-3.58623860	-0.72151453	-3.40367410
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C	-4.38580987	1.37882607	-2.43207640
C	-5.19248222	0.69146053	-1.52133143
C	-2.77995584	-1.45863485	-4.38745582
C	-2.27829826	-0.68396421	-5.41450897
C	-2.28301127	0.74246168	-5.40109696
C	-2.79157438	1.49415240	-4.36080444
C	-1.22676695	1.18724256	-6.22627270
C	-0.56838807	0.04798403	-6.74806679
C	-1.21969845	-1.10560660	-6.24901765
C	0.76549781	0.05610751	-7.13269927
C	1.37244130	1.37142255	-7.15434080
C	0.72312375	2.49439362	-6.64612635
C	-0.59779416	2.41625096	-6.05930820
C	-1.23911789	3.28483581	-5.10153284
C	-2.28619584	2.84276337	-4.29021637
C	1.38053185	-1.25455913	-7.18122242
C	0.73814235	-2.39159678	-6.69582606
C	-0.58313594	-2.33375989	-6.10739626
C	-1.21814452	-3.22513820	-5.16663408
C	-2.26621218	-2.80533066	-4.34473493
C	-6.15717387	1.47619172	-0.70500458
C	-6.15717387	1.47619172	0.70500458
C	-7.07613186	2.29522026	1.38658909

C	-7.99050720	3.09342876	0.69883936
C	-7.99050720	3.09342876	-0.69883936
C	-7.07613186	2.29522026	-1.38658909
C	-5.17785030	-0.72507011	1.52494216
C	-4.36310761	-1.38976568	2.44588892
C	-3.58623860	-0.72151453	3.40367410
C	-3.59438859	0.73310546	3.39294709
C	-4.38580987	1.37882607	2.43207640
C	-5.19248222	0.69146053	1.52133143
C	-2.79157438	1.49415240	4.36080444
C	-2.28301127	0.74246168	5.40109696
C	-2.27829826	-0.68396421	5.41450897
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C	-0.56838807	0.04798403	6.74806679
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C	-2.28619584	2.84276337	4.29021637
C	-1.23911789	3.28483581	5.10153284
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C	0.76549781	0.05610751	7.13269927
C	-2.26621218	-2.80533066	4.34473493
C	-1.21814452	-3.22513820	5.16663408
C	-0.58313594	-2.33375989	6.10739626
C	0.73814235	-2.39159678	6.69582606
C	1.38053185	-1.25455913	7.18122242
H	-0.83403138	4.27994472	-4.92401873
H	-2.64820499	3.51289365	-3.51289465
H	-2.62254343	-3.49306260	-3.58034486
H	-0.80715384	-4.22124181	-5.00955636
H	1.29624156	-3.32649408	-6.66589095
H	2.41398078	-1.34747453	-7.51215834
H	2.40524642	1.47731570	-7.48334724
H	1.27533175	3.43197205	-6.59722947
H	1.27533175	3.43197205	6.59722947
H	2.40524642	1.47731570	7.48334724
H	2.41398078	-1.34747453	7.51215834
H	1.29624156	-3.32649408	6.66589095
H	-0.80715384	-4.22124181	5.00955636
H	-2.62254343	-3.49306260	3.58034486
H	-2.64820499	3.51289365	3.51289465
H	-0.83403138	4.27994472	4.92401873
H	-4.37587012	-2.47734670	-2.45283752
H	-4.41722929	2.46606700	-2.42897203
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Complex 3

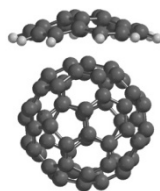


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6	0	0.000000	-2.481538	1.925833
6	0	2.360083	-0.766838	1.925833
6	0	0.695343	3.176310	1.548399
6	0	-0.695343	3.176310	1.548399
6	0	-2.805978	1.642845	1.548399
6	0	-3.235723	0.320223	1.548399
6	0	-2.429533	-2.160976	1.548399
6	0	-1.304444	-2.978402	1.548399
6	0	1.304444	-2.978402	1.548399
6	0	2.429533	-2.160976	1.548399
6	0	3.235723	0.320223	1.548399
6	0	2.805978	1.642845	1.548399
1	0	1.213819	4.043884	1.142788
1	0	-1.213819	4.043884	1.142788
1	0	-3.470872	2.404039	1.142788
1	0	-4.221053	0.095218	1.142788
1	0	-3.358935	-2.558106	1.142788
1	0	-1.394935	-3.985036	1.142788
1	0	1.394935	-3.985036	1.142788
1	0	3.358935	-2.558106	1.142788
1	0	4.221053	0.095218	1.142788
1	0	3.470872	2.404039	1.142788
6	0	0.708816	0.975601	-1.154998
6	0	-0.708816	0.975601	-1.154998
6	0	-1.146888	-0.372646	-1.154998
6	0	0.000000	-1.205909	-1.154998
6	0	1.146888	-0.372646	-1.154998
6	0	1.456846	2.005176	-1.715122
6	0	-1.456846	2.005176	-1.715122
6	0	-2.357226	-0.765909	-1.715122
6	0	0.000000	-2.478534	-1.715122
6	0	2.357226	-0.765909	-1.715122
6	0	0.695803	3.174873	-2.092092
6	0	-0.695803	3.174873	-2.092092
6	0	-2.804468	1.642838	-2.092092
6	0	-3.234499	0.319341	-2.092092
6	0	-2.429060	-2.159543	-2.092092
6	0	-1.303227	-2.977509	-2.092092
6	0	1.303227	-2.977509	-2.092092
6	0	2.429060	-2.159543	-2.092092
6	0	3.234499	0.319341	-2.092092
6	0	2.804468	1.642838	-2.092092
1	0	1.216578	4.048071	-2.484285

1	0	-1.216578	4.048071	-2.484285
1	0	-3.474001	2.407957	-2.484285
1	0	-4.225887	0.093888	-2.484285
1	0	-3.363629	-2.559871	-2.484285
1	0	-1.395164	-3.990045	-2.484285
1	0	1.395164	-3.990045	-2.484285
1	0	3.363629	-2.559871	-2.484285
1	0	4.225887	0.093888	-2.484285
1	0	3.474001	2.407957	-2.484285

Complex 4



B97-d/TZVP E = -3052.8363674 a.u.

Stoichiometry C80H10
Framework group CS[SG(C6),X(C74H10)]
Deg. of freedom 135
Full point group CS NOp 2
Largest Abelian subgroup CS NOp 2
Largest concise Abelian subgroup CS NOp 2

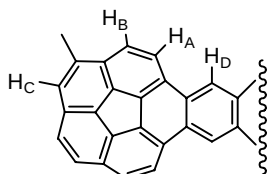
Standard orientation:

6	0	-2.444761	-3.766299	1.425808
6	0	-1.710413	-3.330495	2.600535
6	0	-1.611077	-4.707896	0.699328
6	0	-3.247783	-2.858705	0.726440
6	0	-1.805811	-2.003381	3.033251
6	0	-0.423143	-4.003422	2.600568
6	0	-0.361815	-4.854533	1.425401
6	0	-1.611077	-4.707896	-0.699328
6	0	-3.247783	-2.858705	-0.726440
6	0	-3.348246	-1.481215	1.175933
6	0	-0.617134	-1.298827	3.481463
6	0	-2.639775	-1.061224	2.307291
6	0	0.721064	-3.324827	3.032811
6	0	0.841214	-4.996279	0.726198
6	0	-2.444761	-3.766299	-1.425808
6	0	-0.361815	-4.854533	-1.425401
6	0	-3.348246	-1.481215	-1.175933
6	0	-3.408567	-0.629744	0.000000
6	0	-0.716521	0.079497	3.034521
6	0	0.622368	-1.947245	3.481995
6	0	-1.966723	0.226465	2.308434
6	0	1.970916	-3.472123	2.307123
6	0	2.029388	-4.291964	1.175249
6	0	0.841214	-4.996279	-0.726198
6	0	-1.710413	-3.330495	-2.600535
6	0	-0.423143	-4.003422	-2.600568
6	0	-2.639775	-1.061224	-2.307291
6	0	-2.756996	0.607420	0.000000
6	0	0.427660	0.755510	2.599016
6	0	1.811242	-1.243409	3.034418
6	0	-2.020807	1.040392	1.173580

6	0	2.644937	-2.185518	2.307593
6	0	2.763756	-3.856946	0.000000
6	0	2.029388	-4.291964	-1.175249
6	0	-1.805811	-2.003381	-3.033251
6	0	0.721064	-3.324827	-3.032811
6	0	-1.966723	0.226465	-2.308434
6	0	-2.020807	1.040392	-1.173580
6	0	1.715304	0.083475	2.601206
6	0	0.366293	1.600163	1.421368
6	0	-0.833281	1.740073	0.723474
6	0	3.352604	-1.766203	1.175619
6	0	3.413016	-2.618075	0.000000
6	0	1.970916	-3.472123	-2.307123
6	0	-0.617134	-1.298827	-3.481463
6	0	0.622368	-1.947245	-3.481995
6	0	-0.716521	0.079497	-3.034521
6	0	-0.833281	1.740073	-0.723474
6	0	2.448159	0.516753	1.424468
6	0	1.611705	1.452243	0.697427
6	0	3.254341	-0.388355	0.726614
6	0	3.352604	-1.766203	-1.175619
6	0	2.644937	-2.185518	-2.307593
6	0	1.811242	-1.243409	-3.034418
6	0	0.427660	0.755510	-2.599016
6	0	0.366293	1.600163	-1.421368
6	0	1.611705	1.452243	-0.697427
6	0	3.254341	-0.388355	-0.726614
6	0	1.715304	0.083475	-2.601206
6	0	2.448159	0.516753	-1.424468
6	0	-3.190327	4.201437	-0.696267
6	0	-3.190327	4.201437	0.696267
6	0	-2.020319	4.576361	-1.462875
6	0	-1.652041	4.222026	-2.817708
6	0	-0.327632	4.235329	-3.247424
6	0	0.760211	4.606628	-2.366213
6	0	2.164992	4.262489	-2.436590
6	0	2.983946	4.273489	-1.309507
6	0	2.480431	4.630101	0.000000
6	0	2.983946	4.273489	1.309507
6	0	2.164992	4.262489	2.436590
6	0	0.760211	4.606628	2.366213
6	0	-0.327632	4.235329	3.247424
6	0	-1.652041	4.222026	2.817708
6	0	-2.020319	4.576361	1.462875
6	0	-0.988391	5.121117	-0.708434
6	0	0.358404	5.136510	-1.146204
6	0	1.190940	5.145560	0.000000
6	0	0.358404	5.136510	1.146204
6	0	-0.988391	5.121117	0.708434
1	0	-4.064418	3.808790	-1.213776
1	0	-4.064418	3.808790	1.213776
1	0	-2.411950	3.831899	-3.493419
1	0	-0.102200	3.854192	-4.242467
1	0	2.575584	3.881224	-3.370722
1	0	4.002762	3.900740	-1.406634
1	0	4.002762	3.900740	1.406634
1	0	2.575584	3.881224	3.370722
1	0	-0.102200	3.854192	4.242467
1	0	-2.411950	3.831899	3.493419

NMR Determination of the Association Constant between C₇₀ and **2**.

600 µL of 4.75*10⁻⁴ M solution of buckycatcher in toluene-*d*₈ was titrated with 20, 40, 60, 80, 100, 130, 170, 230, 300, 400, 500 and 1300 µL of 1.035*10⁻³ M solution of C₇₀ in toluene-*d*₈ and the ¹H NMR spectrum was recorded after each addition. Three of the four symmetry independent protons of the corannulene subunits (A, B and C) and one symmetry independent hydrogen atom (D) of the clips benzene rings exhibited measurable chemical shift changes upon titration.



The titration induced chemical shift changes (Hz) of these protons are shown below:

Add [µL]	[Clip] [mol/L]	[C ₇₀] [mol/L]	ΔδA [Hz]	ΔδB [Hz]	ΔδC [Hz]	ΔδD [Hz]
0	0.0004750	0.00000000	0.0	0.0	0.0	0.0
20	0.0004597	0.00003339	4.4	3.5	-1.5	1.9
40	0.0004453	0.00006469	8.4	6.7	-2.8	3.6
60	0.0004318	0.00009409	12.4	9.5	-4.0	5.3
80	0.0004191	0.00012176	16.5	12.6	-5.3	7.1
100	0.0004071	0.00014786	20.3	15.6	-6.6	8.7
130	0.0003904	0.00018432	25.4	19.4	-8.0	10.7
170	0.0003701	0.00022851	31.2	23.7	-10.2	13.1
230	0.0003434	0.00028681	37.5	28.9	-12.2	16.3
300	0.0003167	0.00034500	45.0	33.9	-14.2	19.0
400	0.0002850	0.00041400	51.0	38.6	-16.4	21.6
500	0.0002591	0.00047045	54.5	41.5	-17.1	23.5
1300	0.0001500	0.00070816	66.1	49.6	-21.1	28.2

K_a was evaluated from these changes by an application of a nonlinear curve-fitting using the equation shown below:

$$\Delta\delta = (L(1 + K_a * X + K_a * Y) - (L^2 * (1 + K_a * X + K_a * Y)^2 - 4 K_a^2 X Y L^2)^{1/2}) / 2 K_a Y$$

where X = [C₇₀]_{total};

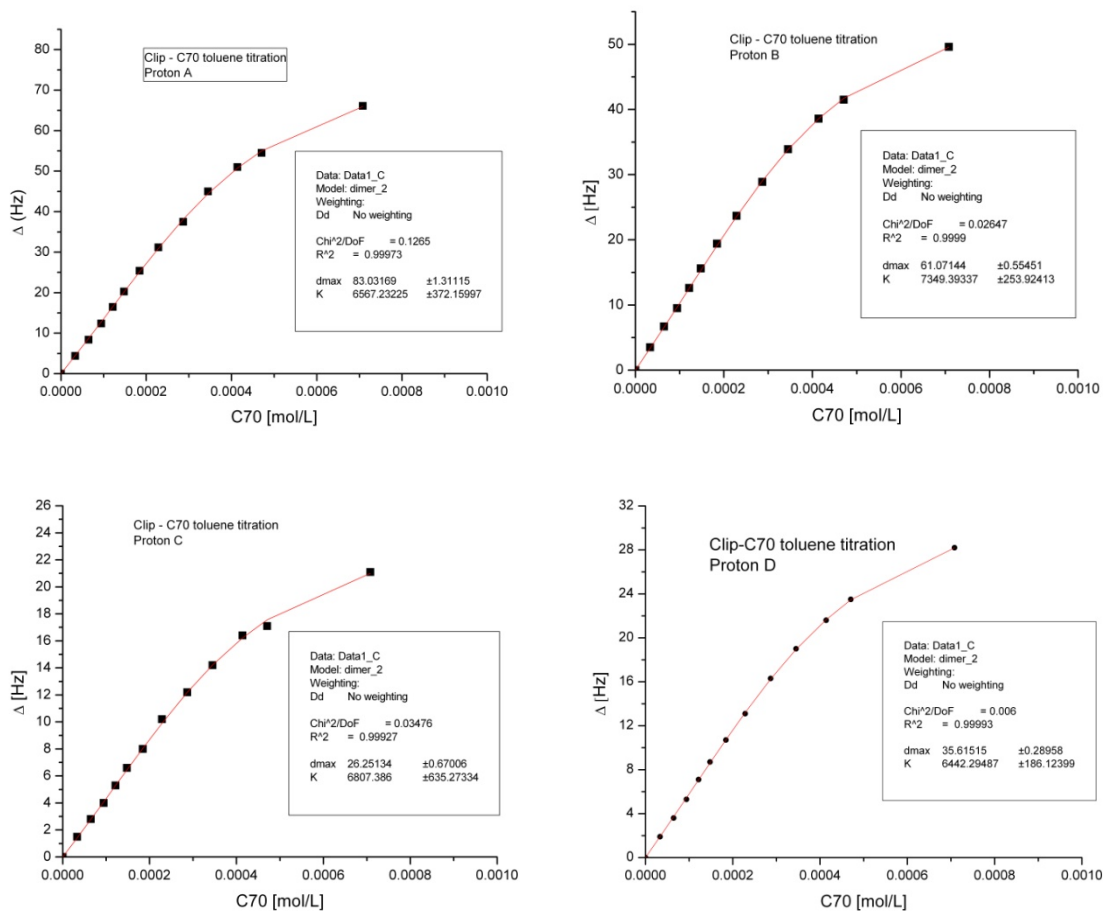
Y = [**2**]_{total};

L = Δδ_{max}; that is Δδ at 100% complexation

K_a = [C₇₀@**2**] / ([C₇₀] * [**2**])

K_a and L were optimized as parameters in the curve fitting. The nonlinear curve-fitting tools of

Origin[®] (v.7.5) package were employed for this purpose and the results are shown below.



The K_a values are $6.6 \pm 0.4 \cdot 10^3 \text{ M}^{-1}$, $7.3 \pm 0.3 \cdot 10^3 \text{ M}^{-1}$, $6.8 \pm 0.6 \cdot 10^3 \text{ M}^{-1}$ and $6.4 \pm 0.2 \cdot 10^3 \text{ M}^{-1}$ as calculated for four protons of the pincers in **2**. The average value of $6.8 \pm 0.4 \cdot 10^3 \text{ M}^{-1}$ is therefore used as the experimental estimation of K_a .