

Computational and Ion Mobility MS Study of (*all-S*)-cyclohexylhemicucurbit[6]uril Structure and Complexes

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1. DFT Energies (E), Zero Point Energies (ZPE) and BSSE Energies (BSSE) of All Compounds

Compound	E (def2-TZVPD)	BSSE (def2-TZVPD)	ZPE (def2-SV(P))	Total
cycHC[6]	-2982.30164499782	-	1.1810413	-2981.12060369782
Cl@cycHC[6]	-3442.68019646300	0.0010777141	1.1817624	-3441.49735634890
Br@cycHC[6]	-5556.86905528500	0.0014188300	1.1808379	-5555.68679855500
I@cycHC[6]	-3280.28042711600	0.0005094988	1.1801577	-3279.09975991720
HCOO@cycHC[6]	-3171.65021245700	0.0015448740	1.2036020	-3170.44506558300
Cl ⁻	-460.33796023179	-	-	-460.33796023179
Br ⁻	-2574.53164937461	-	-	-2574.53164937461
I ⁻	-297.95399230011	-	-	-297.95399230011
HCOO ⁻	-189.31059744549	-	0.0192414	-189.29135604549
H ⁺ + cycHC[6] (1)	-2982.67169121696	-	1.1928258	-2981.47886541696
H ⁺ + cycHC[6] (4)	-2982.66833787100	-	1.1919558	-2981.47638207100
H ⁺ + cycHC[6] (2)	-2982.66861416693	-	1.1930858	-2981.47552836693
H ⁺ + cycHC[6] (5)	-2982.66649760001	-	1.1918421	-2981.47465550001
H ⁺ + cycHC[6] (3)	-2982.66681999213	-	1.1927009	-2981.47411909213
H ⁺ + cycHC[6] (6)	-2982.65949268619	-	1.1933879	-2981.46610478619
H ₂ O	-76.34502947813	-	0.0200151	-76.32501437813
H ₃ O	-76.62233225726	-	0.0321463	-76.59018595726
HCl + cycHC[6] (1)	-3443.18597389700	0.0005795378	1.1898808	-3441.99551355920
HCl + cycHC[6] (2)	-3443.18550794000	0.0006168957	1.1898899	-3441.99500114430
HBr + cycHC[6] (1)	-5557.36325843400	0.0007153800	1.1886562	-5556.17388685400
HBr + cycHC[6] (2)	-5557.36283781500	0.0007681970	1.1887320	-5556.17333761800
HI + cycHC[6] (1)	-3280.76932976000	0.0003400997	1.1877592	-3279.57910886030
HI + cycHC[6] (2)	-3280.76896058000	0.0003436507	1.1877322	-3279.57872702930
HCOOH + cycHC[6] (1)	-3172.17542574500	0.0004514589	1.2150896	-3170.95988468610
HCOOH + cycHC[6] (2)	-3172.17355176000	0.0004497453	1.2149334	-3170.95816861470
HCl	-460.85591864545	-	0.0063622	-460.84955644545
HBr	-2575.04898717514	-	0.0057377	-2575.04324947514
HI	-298.45401625366	-	0.0050822	-298.44893405366
HCOOH	-189.86404239963	-	0.0326106	-189.83143179963
I + cycHC[6] – opening	-3280.27539822000	0.00011117580	1.1799071	-3279.09537994420
I + cycHC[6] – TS	-3280.26710807600	0.00035325870	1.1796705	-3279.08708431730
HCOO ⁻ + cycHC[6] – opening	-3171.63935117300	0.00079854660	1.2012241	-3170.43732852640
HCOO ⁻ + cycHC[6] – TS	-3171.63509090100	0.00092644280	1.2012249	-3170.43293955820

2. Cartesian coordinates

Empty cycHC[6]

138

C	0.6764555	3.6969259	-1.7781764
C	0.2235408	4.3076557	-3.1032230
C	0.3585566	3.2085934	-4.1861265
C	1.7454226	2.5236694	-4.2182253
C	2.2185563	2.0219844	-2.8322779
C	2.1297639	3.2124839	-1.8801638
N	0.7336817	4.5177695	-0.5648217
C	1.7510963	4.0286242	0.2674826
N	2.4854836	3.0877517	-0.4645562
O	1.9692649	4.3726765	1.4303628
C	3.7782564	2.6136924	0.0015195
C	3.1514131	-0.8060016	4.1842431
C	3.0027292	0.7335347	4.2236218
C	2.6991640	1.3607767	2.8411167
C	4.1302217	-1.3160859	3.0979827
C	3.7143168	-0.6725709	1.7766778
C	3.7765153	0.8577584	1.8827942
N	3.7792368	1.2374748	0.4679145
N	4.4972687	-0.9069134	0.5595404
C	4.7158862	-2.2317356	-0.0051590
C	4.3950105	0.2196843	-0.2697487
O	4.7871213	0.3040961	-1.4349939
C	-0.8776887	3.1322046	4.1842431
C	-2.1366243	2.2336724	4.2236218
C	-2.5280491	1.6571562	2.8411167
C	-0.9253470	4.2349198	3.0979827
C	-1.2746949	3.5529781	1.7766778
C	-2.6310983	2.8416790	1.8827942
N	-2.9613030	2.6541776	0.4679145
N	-1.4632244	4.3482057	0.5595404
C	-0.4252034	5.1999451	-0.0051590
C	-2.3877574	3.6963486	-0.2697487
O	-2.6569156	3.9937206	-1.4349939
C	-3.0582731	0.2497456	-4.2182253
C	-2.9580017	-1.2937776	-4.1861265
C	-3.8423097	-1.9602359	-3.1032230
C	-2.8603680	0.9103339	-2.8322779
C	-3.8469746	0.2381877	-1.8801638
C	-3.5398595	-1.2626353	-1.7781764
N	-4.2793440	-1.6234977	-0.5648217
N	-3.9168132	0.6086160	-0.4645562
C	-4.1526522	1.9652198	0.0015195
C	-4.3644391	-0.4978182	0.2674826
O	-4.7714813	-0.4809048	1.4303628
C	-2.2737244	-2.3262030	4.1842431
C	-0.8661049	-2.9672071	4.2236218
C	-0.1711148	-3.0179329	2.8411167
C	-3.2048746	-2.9188339	3.0979827
C	-2.4396219	-2.8804073	1.7766778
C	-1.1454171	-3.6994374	1.8827942
N	-0.8179337	-3.8916525	0.4679145
N	-3.0340444	-3.4412923	0.5595404

C	-4.2906829	-2.9682095	-0.0051590
C	-2.0072531	-3.9160329	-0.2697487
O	-2.1302057	-4.2978167	-1.4349939
C	1.3128505	-2.7734150	-4.2182253
C	2.5994451	-1.9148158	-4.1861265
C	3.6187689	-2.3474198	-3.1032230
C	0.6418117	-2.9323183	-2.8322779
C	1.7172107	-3.4506716	-1.8801638
C	2.8634040	-2.4342906	-1.7781764
N	3.5456622	-2.8942718	-0.5648217
N	1.4313297	-3.6963678	-0.4645562
C	0.3743958	-4.5789122	0.0015195
C	2.6133428	-3.5308060	0.2674826
O	2.8022165	-3.8917716	1.4303628
H	0.0321875	2.8007969	-1.5813992
H	0.8571749	5.1906910	-3.3499370
H	-0.8336400	4.6422469	-3.0366218
H	0.1294508	3.6380013	-5.1868011
H	-0.4228435	2.4364541	-3.9952446
H	1.7274100	1.6763267	-4.9395128
H	2.5017296	3.2443520	-4.6096472
H	1.5646409	1.1977788	-2.4638461
H	3.2516123	1.6153624	-2.8826983
H	2.7429639	4.0421655	-2.3248835
H	3.4725780	-1.1771723	5.1828433
H	2.1524010	-1.2622704	3.9912886
H	3.9453790	1.1829543	4.6159314
H	2.2048362	1.0137933	4.9470816
H	1.6946596	1.0463730	2.4744807
H	2.6880290	2.4706643	2.8970996
H	5.1804607	-1.0340622	3.3424246
H	4.0711775	-2.4232064	3.0281260
H	2.6472028	-0.9566281	1.5830535
H	4.7716799	1.1356625	2.3236469
H	0.0169577	2.4951692	3.9912886
H	-0.7168279	3.5959269	5.1828433
H	-1.9803888	1.4025475	4.9470816
H	-2.9971580	2.8253213	4.6159314
H	-1.7535154	0.9444318	2.4744807
H	-3.4836725	1.0925692	2.8970996
H	-1.6947062	5.0034416	3.3424246
H	0.0629696	4.7373463	3.0281260
H	-0.4951371	2.7708589	1.5830535
H	-3.3693525	3.5645647	2.3236469
H	-4.0605560	0.5443854	-4.6096472
H	-2.3154465	0.6578176	-4.9395128
H	-3.2153269	-1.7068929	-5.1868011
H	-1.8986094	-1.5844203	-3.9952446
H	-4.9238577	-1.8530103	-3.3499370
H	-3.6034837	-3.0430769	-3.0366218
H	-1.8196274	0.7561294	-2.4638461
H	-3.0247510	2.0082977	-2.8826983
H	-4.8721000	0.3543937	-2.3248835
H	-2.4416551	-1.3725233	-1.5813992
H	-2.1693587	-1.2328988	3.9912886
H	-2.7557501	-2.4187546	5.1828433
H	-0.2244474	-2.4163408	4.9470816
H	-0.9482211	-4.0082756	4.6159314
H	0.7956436	-3.5632335	2.8970996
H	0.0588558	-1.9908047	2.4744807

H	-4.1341471	-2.3141399	3.0281260
H	-3.4857544	-3.9693795	3.3424246
H	-2.1520656	-1.8142308	1.5830535
H	-1.4023274	-4.7002272	2.3236469
H	0.5880365	-2.3341443	-4.9395128
H	1.5588264	-3.7887374	-4.6096472
H	2.3214529	-0.8520339	-3.9952446
H	3.0858761	-1.9311083	-5.1868011
H	4.4371237	-1.5991700	-3.0366218
H	4.0666829	-3.3376807	-3.3499370
H	-0.2268613	-3.6236600	-2.8826983
H	0.2549864	-1.9539082	-2.4638461
H	2.1291361	-4.3965592	-2.3248835
H	2.4094675	-1.4282737	-1.5813992
H	-4.5789832	2.5638322	-0.8329573
H	-4.8855268	1.9076036	0.8356621
H	5.4748650	-2.1228675	-0.8052349
H	5.1120811	-2.8925537	0.7913619
H	0.0691478	-5.2474319	-0.8329573
H	0.7907302	-5.1847921	0.8356621
H	4.0947965	3.2771885	0.8356621
H	4.5098354	2.6835997	-0.8329573
H	-0.8989753	5.8028059	-0.8052349
H	-0.0510156	5.8734690	0.7913619
H	-4.5758897	-3.6799384	-0.8052349
H	-5.0610655	-2.9809153	0.7913619

Cl@cycHC[6]

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Cl	0.0000000	0.0000000	-0.0087105
C	0.6869036	3.5777184	-1.7021690
C	0.1558668	4.0954366	-3.0373050
C	0.3047989	2.9467205	-4.0644429
C	1.7185564	2.3207020	-4.1105141
C	2.2581234	1.9182942	-2.7165729
C	2.1580998	3.1668682	-1.8451125
N	0.7549602	4.4793518	-0.5462681
C	1.8314698	4.0900074	0.2687673
N	2.5901908	3.1646417	-0.4489284
O	2.0789863	4.5162998	1.4011590
C	3.8812883	2.6790223	-0.0010544
C	2.8673481	-0.7563971	4.0647710
C	2.7839509	0.7875116	4.1100263
C	2.6029299	1.4348931	2.7158673
C	3.8896890	-1.3039912	3.0393053
C	3.5952879	-0.6246200	1.7035116
C	3.7349567	0.8965501	1.8461394
N	3.8871243	1.3008970	0.4502088
N	4.4616286	-0.8823108	0.5473795
C	4.6681840	-2.2150447	-0.0005442
C	4.4791841	0.2622805	-0.2682796
O	4.9625109	0.3411880	-1.4020593
C	-0.7786149	2.8613949	4.0647710
C	-2.0739805	2.0172164	4.1100263
C	-2.5441188	1.5367569	2.7158673
C	-0.8155550	4.0205650	3.0393053
C	-1.2567071	3.4259207	1.7035116
C	-2.6439136	2.7862923	1.8461394

N	-3.0701721	2.7158999	0.4502088
N	-1.4667108	4.3050391	0.5473795
C	-0.4158070	5.1502883	-0.0005442
C	-2.4667337	3.7479470	-0.2682796
O	-2.7767329	4.1270665	-1.4020593
C	-2.8690651	0.3279625	-4.1105141
C	-2.7043343	-1.2093967	-4.0644429
C	-3.6246855	-1.9127337	-3.0373050
C	-2.7903532	0.9964451	-2.7165729
C	-3.8216382	0.2855352	-1.8451125
C	-3.4418468	-1.1939832	-1.7021690
N	-4.2567125	-1.5858612	-0.5462681
N	-4.0357555	0.6608502	-0.4489284
C	-4.2607455	2.0217832	-0.0010544
C	-4.4577852	-0.4589043	0.2687673
O	-4.9507235	-0.4576949	1.4011590
C	-2.0887332	-2.1049977	4.0647710
C	-0.7099704	-2.8047280	4.1100263
C	-0.0588111	-2.9716500	2.7158673
C	-3.0741340	-2.7165739	3.0393053
C	-2.3385808	-2.8013006	1.7035116
C	-1.0910432	-3.6828425	1.8461394
N	-0.8169523	-4.0167970	0.4502088
N	-2.9949178	-3.4227284	0.5473795
C	-4.2523770	-2.9352436	-0.0005442
C	-2.0124505	-4.0102275	-0.2682796
O	-2.1857779	-4.4682545	-1.4020593
C	1.1505087	-2.6486645	-4.1105141
C	2.3995354	-1.7373239	-4.0644429
C	3.4688188	-2.1827029	-3.0373050
C	0.5322298	-2.9147393	-2.7165729
C	1.6635384	-3.4524034	-1.8451125
C	2.7549432	-2.3837351	-1.7021690
N	3.5017523	-2.8934906	-0.5462681
N	1.4455647	-3.8254919	-0.4489284
C	0.3794572	-4.7008054	-0.0010544
C	2.6263154	-3.6311031	0.2687673
O	2.8717372	-4.0586049	1.4011590
H	0.1134019	2.6608039	-1.4101201
H	0.7397422	4.9923145	-3.3543733
H	-0.9129419	4.3877439	-2.9475107
H	0.0172856	3.3066122	-5.0788487
H	-0.4251906	2.1518783	-3.7929746
H	1.7085351	1.4337067	-4.7831754
H	2.4285080	3.0501470	-4.5710595
H	1.6465750	1.1095266	-2.2536242
H	3.3047609	1.5502156	-2.7878820
H	2.7059867	3.9962236	-2.3748857
H	3.1003494	-1.1523389	5.0796502
H	1.8654739	-1.1570148	3.7927209
H	3.7167633	1.1920876	4.5728533
H	1.9497785	1.0935389	4.7807119
H	1.6299811	1.1520308	2.2515373
H	2.6317582	2.5439659	2.7873567
H	4.9348603	-1.0756627	3.3574474
H	3.7843605	-2.4070908	2.9503541
H	2.5343405	-0.8345908	1.4117642
H	4.7045915	1.1129559	2.3766820
H	0.0692672	2.1940552	3.7927209
H	-0.5522200	3.2611508	5.0796502

H	-1.9219217	1.1417883	4.7807119
H	-2.8907598	2.6227676	4.5728533
H	-1.8126785	0.8355897	2.2515373
H	-3.5190182	1.0071865	2.7873567
H	-1.5358789	4.8115458	3.3574474
H	0.1924216	4.4808977	2.9503541
H	-0.5443934	2.6120987	1.4117642
H	-3.3161439	3.5178178	2.3766820
H	-3.8557588	0.5780761	-4.5710595
H	-2.0958940	0.7627814	-4.7831754
H	-2.8722530	-1.6383363	-5.0788487
H	-1.6509860	-1.4441650	-3.7929746
H	-4.6933422	-1.8555217	-3.3543733
H	-3.3434268	-2.9845028	-2.9475107
H	-1.7841657	0.8712125	-2.2536242
H	-2.9949065	2.0868991	-2.7878820
H	-4.8138245	0.3453415	-2.3748857
H	-2.3610247	-1.2321930	-1.4101201
H	-1.9347412	-1.0370404	3.7927209
H	-2.5481295	-2.1088119	5.0796502
H	-0.0278568	-2.2353271	4.7807119
H	-0.8260035	-3.8148553	4.5728533
H	0.8872600	-3.5511524	2.7873567
H	0.1826974	-1.9876205	2.2515373
H	-3.9767820	-2.0738069	2.9503541
H	-3.3989814	-3.7358830	3.3574474
H	-1.9899471	-1.7775079	1.4117642
H	-1.3884477	-4.6307737	2.3766820
H	0.3873589	-2.1964882	-4.7831754
H	1.4272508	-3.6282231	-4.5710595
H	2.0761765	-0.7077133	-3.7929746
H	2.8549673	-1.6682759	-5.0788487
H	4.2563686	-1.4032411	-2.9475107
H	3.9536001	-3.1367927	-3.3543733
H	-0.3098544	-3.6371147	-2.7878820
H	0.1375907	-1.9807391	-2.2536242
H	2.1078378	-4.3415650	-2.3748857
H	2.2476228	-1.4286109	-1.4101201
H	-4.6871641	2.6164093	-0.8395324
H	-4.9936133	1.9722550	0.8348086
H	5.4264165	-2.1082937	-0.8034948
H	5.0654614	-2.8719101	0.8006139
H	0.0777051	-5.3674078	-0.8395324
H	0.7887838	-5.3107235	0.8348086
H	4.2048295	3.3384685	0.8348086
H	4.6094590	2.7509985	-0.8395324
H	-0.8873724	5.7535614	-0.8034948
H	-0.0455836	5.8227733	0.8006139
H	-4.5390441	-3.6452677	-0.8034948
H	-5.0198778	-2.9508632	0.8006139

Br@cycHC[6]

139

Br	0.0000000	0.0000000	0.0012423
C	0.6952031	3.5953775	-1.7183239
C	0.1695217	4.1278428	-3.0497954
C	0.3201853	2.9888597	-4.0879063
C	1.7353862	2.3658403	-4.1381508

C	2.2745448	1.9503291	-2.7480452
C	2.1675539	3.1861961	-1.8589322
N	0.7574992	4.4811135	-0.5496463
C	1.8291770	4.0801454	0.2652531
N	2.5916840	3.1646295	-0.4597759
O	2.0706868	4.4920451	1.4043409
C	3.8783569	2.6741316	-0.0047589
C	2.9020425	-0.7466102	4.0903990
C	2.8325980	0.7980406	4.1373357
C	2.6356640	1.4461991	2.7458755
C	3.9094054	-1.3006860	3.0530678
C	3.6023155	-0.6219651	1.7197679
C	3.7486974	0.8995629	1.8562556
N	3.8781622	1.2989613	0.4555235
N	4.4530601	-0.8839378	0.5524302
C	4.6629950	-2.2157589	0.0044168
C	4.4614506	0.2576104	-0.2662010
O	4.9327643	0.3329608	-1.4053350
C	-0.8044379	2.8865476	4.0903990
C	-2.1074225	2.0540815	4.1373357
C	-2.5702772	1.5594525	2.7458755
C	-0.8282756	4.0359875	3.0530678
C	-1.2625202	3.4306793	1.7197679
C	-2.6533930	2.7966857	1.8562556
N	-3.0640145	2.7091063	0.4555235
N	-1.4610175	4.2984321	0.5524302
C	-0.4125940	5.1461516	0.0044168
C	-2.4538224	3.7349244	-0.2662010
O	-2.7547347	4.1054188	-1.4053350
C	-2.9165709	0.3199684	-4.1381508
C	-2.7485211	-1.2171412	-4.0879063
C	-3.6595775	-1.9171113	-3.0497954
C	-2.8263069	0.9946491	-2.7480452
C	-3.8431038	0.2840587	-1.8589322
C	-3.4612898	-1.1956252	-1.7183239
N	-4.2595077	-1.5845432	-0.5496463
N	-4.0364916	0.6621494	-0.4597759
C	-4.2550443	2.0216897	-0.0047589
C	-4.4480981	-0.4559590	0.2652531
O	-4.9255685	-0.4527551	1.4043409
C	-2.0976046	-2.1399375	4.0903990
C	-0.7251756	-2.8521222	4.1373357
C	-0.0653868	-3.0056516	2.7458755
C	-3.0811299	-2.7353014	3.0530678
C	-2.3397953	-2.8087142	1.7197679
C	-1.0953044	-3.6962486	1.8562556
N	-0.8141476	-4.0080676	0.4555235
N	-2.9920427	-3.4144943	0.5524302
C	-4.2504010	-2.9303927	0.0044168
C	-2.0076282	-3.9925348	-0.2662010
O	-2.1780297	-4.4383796	-1.4053350
C	1.1811847	-2.6858087	-4.1381508
C	2.4283357	-1.7717185	-4.0879063
C	3.4900558	-2.2107315	-3.0497954
C	0.5517621	-2.9449781	-2.7480452
C	1.6755498	-3.4702548	-1.8589322
C	2.7660867	-2.3997523	-1.7183239
N	3.5020085	-2.8965703	-0.5496463
N	1.4448076	-3.8267789	-0.4597759
C	0.3766875	-4.6958214	-0.0047589

C	2.6189211	-3.6241864	0.2652531
O	2.8548817	-4.0392899	1.4043409
H	0.1181118	2.6755605	-1.4424116
H	0.7550174	5.0271371	-3.3571615
H	-0.8993574	4.4195195	-2.9596884
H	0.0341594	3.3584379	-5.0992149
H	-0.4105713	2.1906128	-3.8270176
H	1.7280630	1.4846174	-4.8186791
H	2.4434373	3.1016147	-4.5914926
H	1.6662940	1.1305649	-2.3005294
H	3.3225756	1.5868609	-2.8208062
H	2.7170802	4.0236709	-2.3741290
H	3.1439249	-1.1447683	5.1023351
H	1.8934642	-1.1398460	3.8306280
H	3.7757326	1.1938390	4.5869691
H	2.0103814	1.1115714	4.8194517
H	1.6511710	1.1715222	2.3014362
H	2.6730411	2.5550036	2.8147824
H	4.9593588	-1.0781300	3.3597226
H	3.7962758	-2.4032170	2.9659962
H	2.5369030	-0.8310726	1.4431730
H	4.7286676	1.1132799	2.3690126
H	0.0404035	2.2097111	3.8306280
H	-0.5805640	3.2951030	5.1023351
H	-1.9678398	1.1852557	4.8194517
H	-2.9217612	2.6729609	4.5869691
H	-1.8401535	0.8441949	2.3014362
H	-3.5492185	1.0374197	2.8147824
H	-1.5459914	4.8339957	3.3597226
H	0.1831090	4.4892798	2.9659962
H	-0.5487216	2.6125588	1.4431730
H	-3.3284625	3.5385063	2.3690126
H	-3.9077957	0.5652714	-4.5914926
H	-2.1497479	0.7542378	-4.8186791
H	-2.9255722	-1.6496360	-5.0992149
H	-1.6918407	-1.4508716	-3.8270176
H	-4.7311371	-1.8597043	-3.3571615
H	-3.3777375	-2.9886261	-2.9596884
H	-1.8122449	0.8777705	-2.3005294
H	-3.0355497	2.0840045	-2.8208062
H	-4.8431413	0.3412250	-2.3741290
H	-2.3761593	-1.2354924	-1.4424116
H	-1.9338677	-1.0698651	3.8306280
H	-2.5633609	-2.1503346	5.1023351
H	-0.0425416	-2.2968271	4.8194517
H	-0.8539714	-3.8667999	4.5869691
H	0.8761775	-3.5924233	2.8147824
H	0.1889825	-2.0157172	2.3014362
H	-3.9793848	-2.0860628	2.9659962
H	-3.4133674	-3.7558657	3.3597226
H	-1.9881815	-1.7814862	1.4431730
H	-1.4002051	-4.6517862	2.3690126
H	0.4216849	-2.2388552	-4.8186791
H	1.4643585	-3.6668861	-4.5914926
H	2.1024120	-0.7397412	-3.8270176
H	2.8914128	-1.7088019	-5.0992149
H	4.2770949	-1.4308934	-2.9596884
H	3.9761198	-3.1674328	-3.3571615
H	-0.2870260	-3.6708654	-2.8208062
H	0.1459509	-2.0083353	-2.3005294

H	2.1260611	-4.3648959	-2.3741290
H	2.2580475	-1.4400681	-1.4424116
H	-4.6743895	2.6218068	-0.8426659
H	-4.9911262	1.9726661	0.8282526
H	5.4257599	-2.1082492	-0.7939992
H	5.0559342	-2.8723039	0.8078253
H	0.0666435	-5.3590435	-0.8426659
H	0.7871841	-5.3087752	0.8282526
H	4.2039421	3.3361090	0.8282526
H	4.6077460	2.7372367	-0.8426659
H	-0.8870826	5.7529705	-0.7939992
H	-0.0404789	5.8147194	0.8078253
H	-4.5386773	-3.6447213	-0.7939992
H	-5.0154553	-2.9424155	0.8078253

I@cycHC[6]

139

I	0.0000000	0.0000000	-0.0167146
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C	0.2014343	4.1726154	-3.0958743
C	0.3747323	3.0557327	-4.1544440
C	1.8015623	2.4596733	-4.2079875
C	2.3362194	2.0199084	-2.8243107
C	2.2013801	3.2289360	-1.9017415
N	0.7576179	4.4728362	-0.5788475
C	1.8224219	4.0633884	0.2404523
N	2.6044551	3.1715579	-0.4955262
O	2.0460394	4.4533695	1.3908686
C	3.8916173	2.6867959	-0.0313109
C	3.0274637	-0.7351778	4.0983114
C	2.9767300	0.8099788	4.1539099
C	2.7468058	1.4696055	2.7731211
C	4.0026217	-1.2910617	3.0313268
C	3.6595830	-0.6058064	1.7107930
C	3.8227076	0.9146917	1.8414604
N	3.9046562	1.3123192	0.4344461
N	4.4634085	-0.8753279	0.5130868
C	4.6588628	-2.2097816	-0.0341279
C	4.4553216	0.2649445	-0.3063457
O	4.8933679	0.3358961	-1.4588856
C	-0.8770492	2.9894494	4.0983114
C	-2.1898272	2.1729344	4.1539099
C	-2.6461186	1.6440008	2.7731211
C	-0.8832186	4.1119030	3.0313268
C	-1.3051478	3.4721950	1.7107930
C	-2.7035000	2.8532161	1.8414604
N	-3.0888299	2.7253719	0.4344461
N	-1.4736481	4.3030891	0.5130868
C	-0.4157044	5.1395844	-0.0341279
C	-2.4571095	3.7259495	-0.3063457
O	-2.7375785	4.0698328	-1.4588856
C	-3.0309207	0.3303620	-4.2079875
C	-2.8337083	-1.2033386	-4.1544440
C	-3.7143080	-1.9118605	-3.0958743
C	-2.9174017	1.0132712	-2.8243107
C	-3.8970306	0.2919831	-1.9017415
C	-3.4941958	-1.1835970	-1.7715230
N	-4.2523987	-1.5803018	-0.5788475

N	-4.0488773	0.6697453	-0.4955262
C	-4.2726421	2.0268415	-0.0313109
C	-4.4302085	-0.4534305	0.2404523
O	-4.8797509	-0.4547626	1.3908686
C	-2.1504145	-2.2542716	4.0983114
C	-0.7869028	-2.9829132	4.1539099
C	-0.1006872	-3.1136063	2.7731211
C	-3.1194031	-2.8208412	3.0313268
C	-2.3544352	-2.8663886	1.7107930
C	-1.1192076	-3.7679078	1.8414604
N	-0.8158264	-4.0376911	0.4344461
N	-2.9897605	-3.4277612	0.5130868
C	-4.2431584	-2.9298028	-0.0341279
C	-1.9982122	-3.9908939	-0.3063457
O	-2.1557894	-4.4057289	-1.4588856
C	1.2293584	-2.7900354	-4.2079875
C	2.4589759	-1.8523941	-4.1544440
C	3.5128738	-2.2607549	-3.0958743
C	0.5811823	-3.0331796	-2.8243107
C	1.6956505	-3.5209191	-1.9017415
C	2.7721230	-2.4342638	-1.7715230
N	3.4947808	-2.8925344	-0.5788475
N	1.4444222	-3.8413032	-0.4955262
C	0.3810248	-4.7136374	-0.0313109
C	2.6077866	-3.6099579	0.2404523
O	2.8337114	-3.9986069	1.3908686
H	0.1520042	2.6851214	-1.5265837
H	0.7766488	5.0857103	-3.3826885
H	-0.8715828	4.4481746	-3.0062419
H	0.0886666	3.4399846	-5.1601893
H	-0.3449808	2.2402070	-3.9131177
H	1.8161321	1.5941762	-4.9083691
H	2.4991250	3.2193349	-4.6378923
H	1.7398269	1.1758027	-2.4074526
H	3.3895866	1.6729402	-2.8964012
H	2.7493444	4.0858476	-2.3854227
H	3.2948299	-1.1387743	5.1014722
H	2.0084468	-1.1198745	3.8656383
H	3.9375101	1.1901444	4.5788234
H	2.1778543	1.1297558	4.8608987
H	1.7431481	1.2104250	2.3644573
H	2.7966667	2.5776959	2.8469109
H	5.0615732	-1.0754580	3.3112303
H	3.8785996	-2.3921427	2.9423154
H	2.5828777	-0.8067441	1.4749972
H	4.8212743	1.1225808	2.3187810
H	-0.0343836	2.2993032	3.8656383
H	-0.6612075	3.4227935	5.1014722
H	-2.0673244	1.3211993	4.8608987
H	-2.9994503	2.8149116	4.5788234
H	-1.9198328	0.9043980	2.3644573
H	-3.6306834	1.1331364	2.8469109
H	-1.5994126	4.9211799	3.3112303
H	0.1323565	4.5550372	2.9423154
H	-0.5927780	2.6402098	1.4749972
H	-3.3828206	3.6140557	2.3187810
H	-4.0375883	0.5546383	-4.6378923
H	-2.2886631	0.7757284	-4.9083691
H	-3.0234474	-1.6432048	-5.1601893
H	-1.7675858	-1.4188656	-3.9131177

H	-4.7926787	-1.8702575	-3.3826885
H	-3.4164408	-2.9789002	-3.0062419
H	-1.8881885	0.9188329	-2.4074526
H	-3.1436021	2.0989980	-2.8964012
H	-4.9131200	0.3380783	-2.3854227
H	-2.4013854	-1.2109212	-1.5265837
H	-1.9740632	-1.1794287	3.8656383
H	-2.6336224	-2.2840192	5.1014722
H	-0.1105300	-2.4509551	4.8608987
H	-0.9380598	-4.0050560	4.5788234
H	0.8340168	-3.7108323	2.8469109
H	0.1766848	-2.1148230	2.3644573
H	-4.0109562	-2.1628945	2.9423154
H	-3.4621605	-3.8457219	3.3112303
H	-1.9900997	-1.8334657	1.4749972
H	-1.4384537	-4.7366364	2.3187810
H	0.4725311	-2.3699046	-4.9083691
H	1.5384633	-3.7739732	-4.6378923
H	2.1125665	-0.8213414	-3.9131177
H	2.9347808	-1.7967799	-5.1601893
H	4.2880236	-1.4692744	-3.0062419
H	4.0160299	-3.2154528	-3.3826885
H	-0.2459846	-3.7719382	-2.8964012
H	0.1483616	-2.0946356	-2.4074526
H	2.1637756	-4.4239259	-2.3854227
H	2.2493812	-1.4742002	-1.5265837
H	-4.7000279	2.6248154	-0.8667395
H	-5.0061406	1.9708441	0.8031694
H	5.4161122	-2.1099131	-0.8389390
H	5.0572221	-2.8633858	0.7689705
H	0.0768571	-5.3827513	-0.8667395
H	0.7962693	-5.3208670	0.8031694
H	4.2098713	3.3500229	0.8031694
H	4.6231708	2.7579358	-0.8667395
H	-0.8808178	5.7454473	-0.8389390
H	-0.0488462	5.8113758	0.7689705
H	-4.5352944	-3.6355342	-0.8389390
H	-5.0083759	-2.9479899	0.7689705

HCOO@cycHC[6]

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C	1.7441001	1.5450594	3.3538622
C	3.0829215	2.2731361	3.4626776
C	4.1128900	1.4584106	2.6423626
C	4.1533595	-0.0441162	3.0069758
C	2.7588074	-0.7161123	2.9903165
C	1.8689853	0.1188260	3.9069698
N	0.5800282	2.0370421	4.1000486
C	-0.2475861	0.9446182	4.4198663
N	0.4615814	-0.2203123	4.1306945
O	-1.3842614	1.0141369	4.8963437
C	-0.0089225	-1.5433943	4.5077763
C	-4.1028044	-2.7534807	1.1585024
C	-4.1693437	-1.8306562	2.3974127
C	-2.7858289	-1.2817246	2.8212366
C	-3.0573753	-3.8884154	1.2831933
C	-1.7321041	-3.2410893	1.6765960
C	-1.8801918	-2.4961117	3.0095774

N	-0.4770989	-2.3558749	3.4050237
N	-0.5643846	-4.0898322	1.9607209
C	-0.0152287	-5.0346449	1.0017104
C	0.2494016	-3.4358727	2.8972939
O	1.3874283	-3.7734947	3.2395596
C	-4.1090279	2.3781264	1.9486357
C	-4.1531195	2.8709890	0.4830084
C	-2.7637875	2.8672612	-0.2014242
C	-3.0448444	3.0884104	2.8208768
C	-1.7159648	3.0097830	2.0697119
C	-1.8442558	3.6904662	0.6989899
N	-0.4373577	3.9265009	0.3653296
N	-0.5300372	3.6819907	2.6129104
C	0.0308855	3.3712879	3.9217789
C	0.2846207	4.1009741	1.5507576
O	1.4235312	4.5668484	1.6459739
C	4.1664663	2.4827278	-1.5688028
C	4.1256186	1.4926932	-2.7571104
C	3.0723513	1.8452770	-3.8371423
C	2.7749411	2.7450050	-0.9427687
C	1.8701447	3.1898080	-2.0904678
C	1.7416745	2.0540473	-3.1160978
N	0.5552594	2.4761120	-3.8699510
N	0.4644660	3.5402020	-1.8760880
C	0.0067921	4.5029347	-0.8916136
C	-0.2615734	3.2554811	-3.0346628
O	-1.4065050	3.6396556	-3.2895414
C	-4.1389063	0.4339480	-3.0970973
C	-4.1803304	-1.0886863	-2.8256728
C	-2.7902996	-1.6931846	-2.5124731
C	-3.0877445	0.8538507	-4.1539450
C	-1.7552982	0.2344059	-3.7362422
C	-1.8771166	-1.2942734	-3.6689946
N	-0.4670793	-1.6899007	-3.7069791
N	-0.5736514	0.3880357	-4.5935555
C	-0.0148586	1.6827836	-4.9518088
C	0.2520803	-0.7396727	-4.4317184
O	1.3961419	-0.8680510	-4.8765992
C	4.1610277	-2.5860597	-1.4648625
C	4.0980868	-3.0138517	0.0204299
C	3.0367415	-4.1022236	0.3136769
C	2.7788755	-2.1994839	-2.0454808
C	1.8562251	-3.3873994	-1.7833639
C	1.7135190	-3.6123612	-0.2718571
N	0.5334339	-4.4881072	-0.2311022
N	0.4513756	-3.3782313	-2.1969855
C	-0.0018329	-3.0570440	-3.5343667
C	-0.2778998	-4.2075508	-1.3387047
O	-1.4157694	-4.6423651	-1.5421015
H	1.4793529	1.4602104	2.2696831
H	3.3907927	2.3417089	4.5330405
H	3.0012120	3.3038135	3.0546460
H	5.1266611	1.9057303	2.7597006
H	3.8475055	1.5551511	1.5648886
H	4.8339780	-0.5768285	2.3055414
H	4.6015593	-0.1609741	4.0242790
H	2.3224210	-0.7208801	1.9648946
H	2.8238960	-1.7700415	3.3365356
H	2.3719572	0.1795030	4.9123533
H	-5.1089297	-3.1871934	0.9555251

H	-3.8354860	-2.1369814	0.2714531
H	-4.6136485	-2.3954504	3.2534670
H	-4.8633272	-0.9840210	2.1924012
H	-2.3564638	-0.6358611	2.0222653
H	-2.8652379	-0.6800527	3.7525782
H	-3.3656677	-4.6278106	2.0609604
H	-2.9588921	-4.4225496	0.3128783
H	-1.4479456	-2.4762571	0.9097301
H	-2.3796534	-3.1854900	3.7486375
H	-3.8793313	1.2889521	1.9486499
H	-5.1138777	2.4889344	2.4166983
H	-4.8586021	2.2367300	-0.0992669
H	-4.5695533	3.9075615	0.4547031
H	-2.3747966	1.8253157	-0.2859605
H	-2.8232375	3.2990426	-1.2241474
H	-3.3175421	4.1566222	2.9937844
H	-2.9643556	2.5818142	3.8069632
H	-1.4798114	1.9301105	1.8919452
H	-2.3323327	4.6937605	0.8521351
H	4.5963595	3.4543025	-1.9143520
H	4.8606029	2.0954737	-0.7892479
H	5.1341542	1.4211137	-3.2243914
H	3.8863020	0.4782430	-2.3658711
H	3.3558946	2.7741674	-4.3868290
H	2.9906624	1.0133506	-4.5697640
H	2.3683094	1.8136369	-0.4818890
H	2.8379996	3.5218399	-0.1492561
H	2.3678242	4.0631075	-2.5960866
H	1.5047332	1.1158644	-2.5539805
H	-3.8968707	0.9585166	-2.1446128
H	-5.1472593	0.7919445	-3.4066197
H	-4.8769788	-1.2951826	-1.9820529
H	-4.6097352	-1.6071490	-3.7176215
H	-2.8533155	-2.7980669	-2.4081129
H	-2.3794320	-1.2855787	-1.5600518
H	-3.0084086	1.9618291	-4.1903500
H	-3.3735331	0.4874190	-5.1683030
H	-1.5121810	0.5978152	-2.7061566
H	-2.3593590	-1.6461544	-4.6237429
H	4.8669932	-1.7315761	-1.5746078
H	4.5885262	-3.4220811	-2.0707857
H	3.8500675	-2.1201629	0.6356227
H	5.1010484	-3.3633891	0.3566614
H	2.9442365	-4.2574483	1.4107058
H	3.3247316	-5.0741800	-0.1546316
H	2.8543886	-1.9709231	-3.1308160
H	2.3697206	-1.3027179	-1.5275715
H	2.3413845	-4.3004258	-2.2308036
H	1.4548629	-2.6230858	0.1866742
H	0.8393089	5.2009207	-0.6529029
H	-0.8371633	5.0628815	-1.3528842
H	0.7876613	-5.5869615	1.5319978
H	-0.8158718	-5.7409339	0.7001486
H	0.8357414	-3.2086041	-4.2508408
H	-0.8356194	-3.7532869	-3.7760933
H	-0.8388306	-1.3983137	5.2341265
H	0.8253629	-2.0967499	4.9923824
H	0.8336172	4.1151053	4.1028591
H	-0.7652254	3.4903016	4.6850147
H	0.7788889	1.4889573	-5.7014403

H	-0.8151939	2.2998443	-5.4082266
C	-0.0338296	0.2095448	-0.1386613
O	-1.1632825	-0.3067518	0.1030053
O	1.1236436	-0.2452515	0.0945717
H	-0.0638210	1.2366907	-0.6330057

Protonated cycHC[6] (I)

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C	1.7772485	1.7289301	3.4193229
C	2.9628962	2.5168520	3.9757216
C	4.2538539	1.8186884	3.4826316
C	4.3016333	0.3077848	3.8000907
C	3.0464306	-0.4593144	3.3138153
C	1.8430494	0.2715935	3.8932253
N	0.4054218	2.1185401	3.8155488
C	-0.4304144	1.0688128	3.9337141
N	0.4496643	-0.2081933	3.5759688
O	-1.5945508	0.9543091	4.2314357
C	-0.0657126	-1.5349687	4.1900736
C	-4.2848601	-3.7968772	1.5876788
C	-4.3946701	-2.8056199	2.7684626
C	-3.1302662	-1.9294898	2.9579426
C	-3.0017998	-4.6631986	1.6159909
C	-1.8198093	-3.7082625	1.7562825
C	-1.9433121	-2.8838985	3.0474339
N	-0.5579766	-2.3817896	3.1674180
N	-0.4482256	-4.2365913	1.8764014
C	0.1570990	-5.1948787	0.9406314
C	0.3190835	-3.3731685	2.6227969
O	1.5321734	-3.3898004	2.8225395
C	-4.3769012	3.3522602	1.8115399
C	-4.3118729	3.8971963	0.3663466
C	-2.9408795	3.6776019	-0.3170323
C	-3.2118171	3.8374613	2.7105956
C	-1.9125600	3.5417765	1.9654350
C	-1.8815280	4.2677454	0.6110727
N	-0.4471841	4.1941649	0.2864399
N	-0.6189157	3.9515890	2.5278558
C	-0.1148269	3.5213510	3.7947496
C	0.2854233	4.1669607	1.4588107
O	1.5045534	4.2891817	1.5881599
C	4.3269226	2.6273289	-1.7818063
C	4.2288944	1.5907608	-2.9256057
C	3.1025304	1.8883041	-3.9457604
C	2.9755182	2.9010235	-1.0770483
C	1.9698445	3.2653470	-2.1680881
C	1.8144750	2.0942469	-3.1507776
N	0.5722974	2.4604619	-3.8370557
N	0.5641192	3.5546518	-1.8527707
C	0.1451326	4.6327326	-0.9775492
C	-0.2135724	3.2344766	-2.9829924
O	-1.3750511	3.5931521	-3.1748018
C	-4.2101152	0.4883500	-3.1183273
C	-4.2717878	-1.0283023	-2.8192410
C	-2.8957107	-1.6450421	-2.4674893
C	-3.1289191	0.8802430	-4.1554887
C	-1.8117154	0.2597989	-3.6928441
C	-1.9396362	-1.2681752	-3.5976582

N	-0.5276940	-1.6667012	-3.5701535
N	-0.6006108	0.3930471	-4.5076506
C	-0.0295148	1.6703827	-4.9051545
C	0.2143500	-0.7261245	-4.3000240
O	1.3722990	-0.8685464	-4.6933287
C	4.3112176	-3.0257360	-1.8210221
C	4.3560909	-3.5252854	-0.3579490
C	3.2332894	-4.5340046	-0.0086464
C	2.9206845	-2.5000208	-2.2520187
C	1.9126828	-3.6048290	-1.9432793
C	1.9098447	-3.9047863	-0.4369087
N	0.6526842	-4.6482661	-0.3015139
N	0.4770075	-3.4231452	-2.1940442
C	-0.0844370	-3.0479966	-3.4857156
C	-0.2409880	-4.2101591	-1.2953675
O	-1.4417108	-4.4793302	-1.3474493
H	1.8481856	1.7649619	2.3052922
H	2.9205322	2.5393557	5.0888921
H	2.9316854	3.5591284	3.5966098
H	5.1368617	2.3236021	3.9297270
H	4.3369021	1.9689256	2.3816002
H	5.2060111	-0.1473434	3.3422821
H	4.4055675	0.1598507	4.9002073
H	2.9914244	-0.4560839	2.2010486
H	3.0682126	-1.5229122	3.6292671
H	1.8942476	0.2616547	5.0062535
H	-5.1796845	-4.4564275	1.5717834
H	-4.3026256	-3.2293530	0.6284950
H	-4.5758091	-3.3729324	3.7112147
H	-5.2818356	-2.1502741	2.6289224
H	-2.9967650	-1.2350184	2.0968393
H	-3.2298792	-1.3032541	3.8712246
H	-3.0222873	-5.3821156	2.4675291
H	-2.9193469	-5.2385641	0.6702258
H	-1.8539816	-3.0060014	0.8861425
H	-2.1285381	-3.5904295	3.8957302
H	-4.3576887	2.2375516	1.7829973
H	-5.3469470	3.6323558	2.2773727
H	-5.1129437	3.4270461	-0.2448042
H	-4.5345613	4.9896849	0.3760211
H	-2.7427785	2.5920420	-0.4741856
H	-2.9126457	4.1470544	-1.3218226
H	-3.2920875	4.9295046	2.9137681
H	-3.2471172	3.3076549	3.6876330
H	-1.8837359	2.4409933	1.7502234
H	-2.1440572	5.3429304	0.7878220
H	4.7101472	3.5905101	-2.1922310
H	5.0815844	2.2930933	-1.0352195
H	5.2052990	1.5245119	-3.4539173
H	4.0447525	0.5810583	-2.4887304
H	3.3329827	2.8018174	-4.5401900
H	2.9936056	1.0338089	-4.6468112
H	2.6217949	1.9940501	-0.5311186
H	3.0762952	3.7120055	-0.3244309
H	2.3919663	4.1380880	-2.7333774
H	1.6362939	1.1642233	-2.5492188
H	-3.9988776	1.0377260	-2.1700295
H	-5.2061198	0.8430525	-3.4632284
H	-4.9938720	-1.2190304	-1.9941575
H	-4.6795173	-1.5601652	-3.7103712

H	-2.9693712	-2.7467871	-2.3449929
H	-2.5137586	-1.2379515	-1.5023653
H	-3.0423125	1.9861774	-4.2110111
H	-3.3930072	0.4996597	-5.1685728
H	-1.5997736	0.6478421	-2.6612100
H	-2.3922178	-1.6384361	-4.5555742
H	5.0762028	-2.2316379	-1.9689164
H	4.6018666	-3.8598642	-2.5015818
H	4.2648219	-2.6495976	0.3277773
H	5.3481207	-3.9810949	-0.1455748
H	3.2406847	-4.7399995	1.0834842
H	3.3860153	-5.5001518	-0.5418209
H	2.9094677	-2.2239239	-3.3273079
H	2.6505197	-1.5778028	-1.6858720
H	2.2501613	-4.5295636	-2.4823026
H	1.8139732	-2.9249522	0.0999427
H	1.0269091	5.2641387	-0.7384431
H	-0.6158671	5.2422049	-1.5102804
H	0.9964049	-5.6871722	1.4697182
H	-0.6156596	-5.9515219	0.7034456
H	0.6929820	-3.2066142	-4.2636661
H	-0.9515108	-3.7143962	-3.6834235
H	-0.8638191	-1.2502246	4.9032092
H	0.8123976	-1.9788381	4.7041735
H	0.7306452	4.1710061	4.0921404
H	-0.9156029	3.5800187	4.5581328
H	0.7471858	1.4594529	-5.6662057
H	-0.8279865	2.2906660	-5.3576996
H	0.3546100	-0.3478386	2.5468771

Protonated cycHC[6] (II)

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C	1.8116150	1.7410582	3.6033475
C	2.9949688	2.6006162	4.0280492
C	4.2601212	1.9030772	3.4632683
C	4.3674991	0.4035172	3.8265238
C	3.0896281	-0.4131971	3.5001093
C	1.9383441	0.3226573	4.1754738
N	0.4199596	2.0957140	4.0054420
C	-0.2526791	0.9413400	4.1175873
N	0.5268676	-0.1579789	4.0728914
O	-1.5654964	0.9504926	4.2796649
C	0.0895238	-1.5320323	4.4172139
C	-4.2694113	-3.4870513	1.7779139
C	-4.3215092	-2.6055101	3.0458097
C	-3.0241957	-1.7811108	3.2652821
C	-3.0108046	-4.3831378	1.6932231
C	-1.7989030	-3.4726740	1.8683852
C	-1.8455287	-2.7511478	3.2258331
N	-0.4592362	-2.2654172	3.3129435
N	-0.4438275	-4.0396875	1.9079034
C	0.0952773	-5.0102973	0.9489934
C	0.3729535	-3.2361444	2.6771130
O	1.5876174	-3.3140669	2.8377843
C	-4.3751959	2.9722912	1.6836072
C	-4.2880122	3.4887912	0.2288002
C	-2.8832937	3.3329959	-0.4007312
C	-3.2657233	3.5324861	2.6096967

C	-1.9277082	3.2793978	1.9161222
C	-1.8936429	3.9946989	0.5554515
N	-0.4512251	4.0144134	0.2759347
N	-0.6736886	3.7536066	2.5100360
C	-0.2039624	3.4400373	3.8227680
C	0.2462619	4.0414173	1.4718399
O	1.4442209	4.2668126	1.6395473
C	4.3133198	2.5246790	-1.7350328
C	4.2364211	1.5288468	-2.9160961
C	3.1445888	1.8737661	-3.9591583
C	2.9446473	2.7917641	-1.0614582
C	1.9796744	3.2063426	-2.1707682
C	1.8364980	2.0710734	-3.1958015
N	0.6185253	2.4777816	-3.9055672
N	0.5702737	3.5054948	-1.8889847
C	0.1347120	4.5289841	-0.9631869
C	-0.1807586	3.2337104	-3.0471944
O	-1.3339251	3.6112287	-3.2570208
C	-4.2470380	0.6001690	-3.3991323
C	-4.3386242	-0.9123690	-3.0870116
C	-2.9863983	-1.5400824	-2.6681203
C	-3.1162413	0.9688614	-4.3907999
C	-1.8276318	0.3371558	-3.8667166
C	-1.9785970	-1.1881424	-3.7606663
N	-0.5735681	-1.6015860	-3.6706124
N	-0.5838958	0.4474286	-4.6343809
C	0.0292231	1.7150444	-5.0008978
C	0.2060916	-0.6822495	-4.3863774
O	1.3735010	-0.8463511	-4.7407624
C	4.2811440	-3.0891329	-1.9355647
C	4.3300197	-3.5406926	-0.4573361
C	3.1673246	-4.4821093	-0.0553308
C	2.9096695	-2.5108844	-2.3600966
C	1.8552889	-3.5540094	-1.9970321
C	1.8677244	-3.8038366	-0.4814297
N	0.5807747	-4.4838432	-0.3034698
N	0.4236451	-3.3125668	-2.2295139
C	-0.1431221	-2.9821389	-3.5318569
C	-0.3113578	-4.0329891	-1.2891897
O	-1.5254868	-4.2458599	-1.3082012
H	1.8150871	1.6833615	2.4884963
H	3.0412960	2.6792782	5.1382418
H	2.9057410	3.6196635	3.5985132
H	5.1653670	2.4392096	3.8210193
H	4.2524641	2.0152109	2.3546935
H	5.2339754	-0.0476730	3.2966029
H	4.5860145	0.3011486	4.9150759
H	2.9151238	-0.4682131	2.4025920
H	3.1849507	-1.4587087	3.8596918
H	2.1613525	0.3947368	5.2699991
H	-5.1841088	-4.1171987	1.7355889
H	-4.3016456	-2.8353248	0.8743400
H	-4.4793713	-3.2516291	3.9396325
H	-5.1948142	-1.9192169	2.9979298
H	-2.9155556	-1.0027433	2.4742808
H	-3.1108581	-1.2772506	4.2643858
H	-3.0248425	-5.1704011	2.4822514
H	-2.9713414	-4.8784550	0.7005300
H	-1.8435076	-2.6990111	1.0597039
H	-2.0129097	-3.5209455	4.0237807

H	-4.3000827	1.8587329	1.6781766
H	-5.3734805	3.2127329	2.1105926
H	-5.0405759	2.9620396	-0.3976432
H	-4.5711991	4.5668791	0.2065765
H	-2.6195213	2.2573133	-0.5292328
H	-2.8402877	3.7890820	-1.4118608
H	-3.4036624	4.6244688	2.7793894
H	-3.3148950	3.0334326	3.6025378
H	-1.8445703	2.1783368	1.7163404
H	-2.2314693	5.0524094	0.7122705
H	4.7203875	3.4960742	-2.1008693
H	5.0407101	2.1540369	-0.9786271
H	5.2272963	1.4674474	-3.4173439
H	4.0268700	0.5080397	-2.5190052
H	3.4036716	2.8024280	-4.5176831
H	3.0469355	1.0427598	-4.6895026
H	2.5636039	1.8724695	-0.5574976
H	3.0339391	3.5782036	-0.2808448
H	2.4302305	4.0914565	-2.6928119
H	1.6281239	1.1252969	-2.6305939
H	-4.0717482	1.1574187	-2.4483951
H	-5.2227522	0.9615907	-3.7919073
H	-5.0988861	-1.0861954	-2.2928463
H	-4.7129420	-1.4495350	-3.9896666
H	-3.0789840	-2.6388085	-2.5342681
H	-2.6402895	-1.1274694	-1.6922252
H	-3.0138760	2.0732341	-4.4520941
H	-3.3407683	0.5828345	-5.4114963
H	-1.6532572	0.7330915	-2.8313320
H	-2.3955724	-1.5630394	-4.7329616
H	5.0797641	-2.3379132	-2.1234722
H	4.5191243	-3.9586213	-2.5925322
H	4.2929525	-2.6397360	0.1992127
H	5.3029340	-4.0369386	-0.2466812
H	3.1845098	-4.6510073	1.0431222
H	3.2644432	-5.4713460	-0.5584019
H	2.8918590	-2.2692747	-3.4431922
H	2.6952195	-1.5590971	-1.8204044
H	2.1371867	-4.5121950	-2.5094339
H	1.8251022	-2.8062659	0.0269987
H	1.0034593	5.1616349	-0.6834375
H	-0.6336165	5.1528985	-1.4693969
H	0.9282310	-5.5380171	1.4541073
H	-0.7123124	-5.7355822	0.7291593
H	0.6298438	-3.1834624	-4.3043373
H	-1.0198994	-3.6432928	-3.7005075
H	-0.6410603	-1.4886409	5.2584612
H	1.0057128	-2.0471706	4.7777565
H	0.5834835	4.1663181	4.1033424
H	-1.0393548	3.5118144	4.5471325
H	0.8235362	1.4947864	-5.7406822
H	-0.7407493	2.3582913	-5.4704446
H	-1.9703908	0.0448222	4.2273748

Protonated cycHC[6] (III)

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C	1.8067613	1.7215666	3.6536657
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C	3.1615728	2.4083617	3.7644113
C	4.1255344	1.6435985	2.8216540
C	4.1271628	0.1144643	3.0401972
C	2.7124798	-0.5126401	3.0166952
C	1.8778546	0.2435055	4.0511101
N	0.6548474	2.2280250	4.4765106
C	-0.2949033	0.9728243	4.6000814
N	0.4552896	-0.0952086	4.2582698
O	-1.4376706	1.1020009	4.9708193
C	-0.0374887	-1.4857550	4.4614867
C	-4.1963986	-2.9563491	1.2896322
C	-4.2642868	-1.9591019	2.4690656
C	-2.9023873	-1.2959643	2.7956578
C	-3.0695055	-4.0091363	1.4234237
C	-1.7727513	-3.2480731	1.6914578
C	-1.8923948	-2.4250639	2.9821200
N	-0.4743200	-2.1473771	3.2684098
N	-0.5213116	-3.9784039	1.9334365
C	0.0232369	-5.0003411	1.0355901
C	0.2863587	-3.2517423	2.7881350
O	1.4482627	-3.4923461	3.1147821
C	-4.2505783	2.6273313	2.0068800
C	-4.2397065	3.1269870	0.5431405
C	-2.8547311	3.0194492	-0.1409539
C	-3.1246946	3.2280975	2.8887037
C	-1.8119258	3.0161466	2.1367302
C	-1.8640171	3.7319475	0.7755890
N	-0.4348367	3.8452960	0.4362086
N	-0.5383597	3.5310150	2.6716000
C	-0.0933992	3.5413494	3.9934705
C	0.3056324	3.9353526	1.5941385
O	1.4735238	4.2921323	1.7328434
C	4.3315853	2.6974022	-1.8016898
C	4.2684298	1.7086348	-2.9895403
C	3.1125558	1.9923343	-3.9804279
C	2.9789626	2.8659999	-1.0662305
C	1.9383013	3.2244896	-2.1255064
C	1.8294887	2.0937874	-3.1592343
N	0.5568426	2.4256782	-3.8109761
N	0.5246023	3.4161030	-1.7758941
C	0.0598496	4.4027714	-0.8296615
C	-0.2547636	3.1111788	-2.9113777
O	-1.4374936	3.4165308	-3.0648737
C	-4.2740536	0.3346200	-3.4514611
C	-4.3084940	-1.1869411	-3.1746600
C	-2.9433226	-1.7650835	-2.7275203
C	-3.1323027	0.7716060	-4.4020640
C	-1.8339191	0.1849514	-3.8517071
C	-1.9184416	-1.3472255	-3.7795967
N	-0.4985364	-1.6965592	-3.6492718
N	-0.5733774	0.3651151	-4.5781457
C	-0.0137476	1.6620369	-4.9174298
C	0.2620650	-0.7288980	-4.3156742
O	1.4512732	-0.8249357	-4.6213615
C	4.2901309	-2.8664335	-1.5725500
C	4.2625423	-3.3291208	-0.0967091
C	3.1385980	-4.3470475	0.2189657
C	2.9164157	-2.3796568	-2.0948284
C	1.9136043	-3.4957888	-1.8106384
C	1.8295061	-3.7529086	-0.2980669

N	0.5824438	-4.5157689	-0.2090587
N	0.4925717	-3.3568955	-2.1511829
C	-0.0008946	-3.0522742	-3.4884371
C	-0.2589311	-4.1354350	-1.2697638
O	-1.4443625	-4.4430357	-1.3948479
H	1.4443042	1.7810508	2.6053496
H	3.5287587	2.3717362	4.8170544
H	3.0852701	3.4678889	3.4450000
H	5.1531629	2.0477233	2.9467600
H	3.8271051	1.8697278	1.7726296
H	4.7558850	-0.3724888	2.2641268
H	4.6093850	-0.1231941	4.0173847
H	2.2455639	-0.4079931	2.0103415
H	2.7440194	-1.5992213	3.2434461
H	2.3952892	0.1464028	5.0391584
H	-5.1767089	-3.4695160	1.1808218
H	-4.0361414	-2.3923079	0.3413365
H	-4.6241798	-2.4901855	3.3811153
H	-5.0214247	-1.1731581	2.2543708
H	-2.5749478	-0.6312852	1.9627406
H	-2.9886349	-0.6679034	3.7098448
H	-3.2784555	-4.7141062	2.2600824
H	-2.9853306	-4.5925164	0.4823653
H	-1.6149701	-2.5382421	0.8400787
H	-2.2834377	-3.0993031	3.7893950
H	-4.1424373	1.5178173	2.0145537
H	-5.2368469	2.8441316	2.4721019
H	-4.9931673	2.5608821	-0.0465351
H	-4.5674805	4.1923889	0.5159468
H	-2.5524597	1.9543961	-0.2717839
H	-2.8676956	3.4700487	-1.1552795
H	-3.2937299	4.3157939	3.0616393
H	-3.1131018	2.7213496	3.8775428
H	-1.6957173	1.9197583	1.9440882
H	-2.2534792	4.7698276	0.9440203
H	4.6568278	3.6972180	-2.1725829
H	5.1140215	2.3696889	-1.0815060
H	5.2387203	1.7173053	-3.5327676
H	4.1430625	0.6725947	-2.5965751
H	3.2866680	2.9409891	-4.5379910
H	3.0377028	1.1628029	-4.7151064
H	2.6832549	1.9173226	-0.5591988
H	3.0522425	3.6504609	-0.2813094
H	2.3000767	4.1463712	-2.6531027
H	1.7104929	1.1290466	-2.6016025
H	-4.1498474	0.8778703	-2.4847584
H	-5.2528245	0.6631055	-3.8651021
H	-5.0824893	-1.4111098	-2.4072241
H	-4.6325055	-1.7194463	-4.0993437
H	-2.9925229	-2.8690544	-2.6183692
H	-2.6455074	-1.3584072	-1.7331081
H	-3.0770603	1.8805438	-4.4386582
H	-3.3107745	0.3982430	-5.4365155
H	-1.7084492	0.5667791	-2.8044884
H	-2.2846642	-1.7221847	-4.7719465
H	5.0481400	-2.0616761	-1.6989571
H	4.6335312	-3.7117730	-2.2135225
H	4.1207903	-2.4374610	0.5598603
H	5.2488741	-3.7619427	0.1806286
H	3.0871264	-4.5259971	1.3144815

H	3.3354560	-5.3233633	-0.2803457
H	2.9610879	-2.1346351	-3.1767293
H	2.5973406	-1.4473411	-1.5726724
H	2.3030683	-4.4284290	-2.2982519
H	1.6858122	-2.7590175	0.2053739
H	0.8893417	5.0982120	-0.5825596
H	-0.7769388	4.9677256	-1.2947179
H	0.8104360	-5.5385402	1.5993122
H	-0.7939084	-5.7044673	0.7841859
H	0.8308575	-3.2010358	-4.2100818
H	-0.8244090	-3.7622437	-3.7165655
H	-0.8638970	-1.4192932	5.2014324
H	0.8133983	-2.0573662	4.8907595
H	0.6659373	4.3360045	4.1394931
H	-0.9311349	3.6319233	4.7134291
H	0.7844495	1.4958543	-5.6671943
H	-0.8131508	2.2826031	-5.3676381
H	0.9775516	2.4342869	5.4449472

Protonated cycHC[6] (IV)

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C	1.8178353	1.6337699	3.4281443
C	3.1277097	2.3728402	3.6728839
C	4.2207173	1.5844903	2.9038079
C	4.2430994	0.0696232	3.2144418
C	2.8595047	-0.6171057	3.0813074
C	1.9051929	0.1931464	3.9501740
N	0.5491896	2.0980293	4.0629372
C	-0.1963926	0.9924605	4.2763591
N	0.4625501	-0.1581201	4.0853676
O	-1.4559102	0.9764372	4.6863564
C	-0.0578483	-1.5150830	4.4011651
C	-4.2290673	-3.1839248	1.3136639
C	-4.3237515	-2.1942573	2.4969014
C	-2.9841705	-1.4829997	2.8165353
C	-3.0663447	-4.1967176	1.4410477
C	-1.7945911	-3.3925955	1.7017480
C	-1.9286608	-2.5726814	2.9942029
N	-0.5164914	-2.2458847	3.2570532
N	-0.5196990	-4.0838708	1.9331294
C	0.0519308	-5.0799853	1.0229976
C	0.2746437	-3.3265335	2.7754639
O	1.4461479	-3.5273178	3.0904220
C	-4.2294117	2.7793176	2.0307773
C	-4.2321246	3.2445706	0.5553588
C	-2.8471956	3.1517883	-0.1285703
C	-3.1187646	3.4447963	2.8818975
C	-1.7910742	3.2456229	2.1471680
C	-1.8654832	3.9113174	0.7608220
N	-0.4420888	4.0195230	0.4185751
N	-0.5532336	3.8237985	2.6723407
C	0.0258065	3.4836346	3.9368926
C	0.3052008	4.1304374	1.5763530
O	1.4898018	4.4336616	1.6854016
C	4.3081707	2.7405825	-1.7688842
C	4.2401323	1.7264171	-2.9348300
C	3.0913784	1.9993199	-3.9370599
C	2.9544069	2.9405221	-1.0436647

C	1.9222410	3.2846124	-2.1159582
C	1.8058994	2.1313850	-3.1235907
N	0.5382763	2.4592281	-3.7867050
N	0.5090057	3.5014819	-1.7776752
C	0.0543459	4.5263453	-0.8653922
C	-0.2698346	3.1725881	-2.9055768
O	-1.4511871	3.4809288	-3.0688575
C	-4.2622130	0.3597922	-3.3217383
C	-4.2927910	-1.1611063	-3.0402405
C	-2.9192631	-1.7400417	-2.6206100
C	-3.1399205	0.7934270	-4.2967534
C	-1.8308701	0.2069732	-3.7714507
C	-1.9160798	-1.3249450	-3.6946889
N	-0.4952964	-1.6777678	-3.5937406
N	-0.5851057	0.3839444	-4.5226205
C	-0.0330393	1.6794807	-4.8804668
C	0.2539940	-0.7109674	-4.2757169
O	1.4363444	-0.8100481	-4.6049097
C	4.2940627	-2.8678596	-1.5618451
C	4.2762778	-3.3594672	-0.0952252
C	3.1597690	-4.3899658	0.2060810
C	2.9149959	-2.3789970	-2.0679175
C	1.9206171	-3.5068531	-1.8009238
C	1.8451176	-3.7938231	-0.2935858
N	0.6023852	-4.5662707	-0.2141415
N	0.4970862	-3.3696244	-2.1318784
C	-0.0030734	-3.0388165	-3.4596603
C	-0.2458610	-4.1695098	-1.2628011
O	-1.4310691	-4.4797323	-1.3875278
H	1.6343506	1.6049015	2.3265176
H	3.3523216	2.4092393	4.7630952
H	3.0697191	3.4106572	3.2839623
H	5.2150268	2.0278137	3.1269275
H	4.0529163	1.7349413	1.8123947
H	4.9685632	-0.4379774	2.5426035
H	4.6216665	-0.0913030	4.2509385
H	2.5088492	-0.6096963	2.0243283
H	2.9017259	-1.6797726	3.3973283
H	2.3150351	0.2106200	4.9915017
H	-5.1922422	-3.7294217	1.2092688
H	-4.0933413	-2.6122843	0.3661237
H	-4.6562634	-2.7423831	3.4093566
H	-5.1100926	-1.4349887	2.2915148
H	-2.6889077	-0.7996837	1.9865722
H	-3.0937976	-0.8671564	3.7362425
H	-3.2469595	-4.9095281	2.2777435
H	-2.9668939	-4.7751126	0.4985456
H	-1.6671386	-2.6769990	0.8499283
H	-2.2863501	-3.2593510	3.8059418
H	-4.0834753	1.6741343	2.0651740
H	-5.2209933	2.9776722	2.4926750
H	-4.9748503	2.6459472	-0.0152298
H	-4.5865104	4.3003559	0.5059153
H	-2.5209067	2.0911545	-0.2335633
H	-2.8740191	3.5741544	-1.1547838
H	-3.3115930	4.5310988	3.0285687
H	-3.1254549	2.9953209	3.9088630
H	-1.6456630	2.1438304	1.9771975
H	-2.2698072	4.9481743	0.8990047
H	4.6464087	3.7281832	-2.1603817

H	5.0836041	2.4207786	-1.0376785
H	5.2126184	1.7130406	-3.4741039
H	4.1027618	0.7005142	-2.5195723
H	3.2770678	2.9342652	-4.5136580
H	3.0112571	1.1552448	-4.6543991
H	2.6463838	2.0074409	-0.5150180
H	3.0315761	3.7415723	-0.2765974
H	2.2962594	4.1897136	-2.6637796
H	1.6754932	1.1808167	-2.5440284
H	-4.1172750	0.9053025	-2.3588798
H	-5.2490126	0.6884508	-3.7157300
H	-5.0514788	-1.3826606	-2.2566940
H	-4.6366690	-1.6951665	-3.9567206
H	-2.9663792	-2.8441046	-2.5095077
H	-2.6000972	-1.3315508	-1.6334740
H	-3.0839580	1.9021112	-4.3379550
H	-3.3401326	0.4168784	-5.3259965
H	-1.6840001	0.5910217	-2.7273832
H	-2.3043894	-1.7008008	-4.6783129
H	5.0464732	-2.0560684	-1.6756140
H	4.6391595	-3.6982209	-2.2211715
H	4.1329277	-2.4821303	0.5795897
H	5.2663558	-3.7922123	0.1685128
H	3.1147367	-4.5887392	1.2984025
H	3.3597969	-5.3558334	-0.3120269
H	2.9531271	-2.1131533	-3.1452823
H	2.5932660	-1.4591945	-1.5255542
H	2.3128886	-4.4271979	-2.3092642
H	1.6980170	-2.8109970	0.2295294
H	0.8922872	5.2201959	-0.6433479
H	-0.7750770	5.0839850	-1.3518542
H	0.8518623	-5.6060220	1.5800435
H	-0.7472758	-5.8011739	0.7627339
H	0.8229236	-3.1769977	-4.1900009
H	-0.8308505	-3.7417797	-3.6948917
H	-0.8727999	-1.3969877	5.1455316
H	0.7915205	-2.0657240	4.8594387
H	0.8900665	4.1555750	4.1093912
H	-0.7022876	3.6526852	4.7608389
H	0.7619975	1.5052714	-5.6318151
H	-0.8367368	2.2916867	-5.3345609
H	-1.8850697	1.8669222	4.6230841

Protonated cycHC[6] (V)

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C	2.1029569	0.8125226	3.6862058
C	3.2101714	1.6649049	4.2948892
C	4.1685089	0.6803574	5.0116414
C	3.4377315	-0.2373303	6.0148178
C	2.2451853	-1.0071403	5.3967584
C	1.3197458	0.0166356	4.7329359
N	1.0072141	1.4371145	2.8529773
C	-0.1321314	0.3753176	2.8952859
N	0.1647684	-0.4415481	3.9345981
O	-1.0589039	0.4138059	2.1213807
C	-0.6724441	-1.6127059	4.2659043
C	-4.1227298	-4.4516005	1.1886007
C	-4.5105483	-3.5090424	2.3515236

C	-3.4281854	-2.4465215	2.6725643
C	-2.7255895	-5.0997646	1.3462081
C	-1.7354209	-3.9669205	1.6025801
C	-2.1160050	-3.1992278	2.8772240
N	-0.8589983	-2.4819509	3.1395717
N	-0.3160847	-4.2609072	1.8614506
C	0.5305622	-5.0677374	0.9810339
C	0.2129388	-3.2816118	2.6864286
O	1.3944493	-3.1078532	2.9944963
C	-3.8962029	4.3636799	2.1363532
C	-3.8358912	5.1639076	0.8146437
C	-2.7543473	4.6588233	-0.1722304
C	-2.5195430	4.2292058	2.8361068
C	-1.5511042	3.6720373	1.7987430
C	-1.4339783	4.6275799	0.5944525
N	-0.1954550	4.1341414	-0.0437362
N	-0.1199083	3.4991210	2.1182873
C	0.4907740	2.8652265	3.2248533
C	0.6073280	3.5722124	0.9092277
O	1.7621117	3.1268178	0.8003339
C	4.3324442	3.1051639	-3.3012217
C	4.0492273	1.9930524	-4.3372272
C	2.6496077	2.0927091	-4.9907464
C	3.2209985	3.2485145	-2.2321297
C	1.9012658	3.4164185	-2.9814062
C	1.6276261	2.1864888	-3.8605030
N	0.2031298	2.3731272	-4.1658174
N	0.6196002	3.5260408	-2.2658409
C	0.3242169	4.5926563	-1.3393924
C	-0.4013192	3.0758619	-3.1296186
O	-1.6022630	3.2988414	-2.9775389
C	-4.2805526	0.1127579	-2.5928515
C	-4.1796690	-1.3972790	-2.2727283
C	-2.7226000	-1.9078088	-2.1565676
C	-3.4286964	0.5523582	-3.8094608
C	-2.0109946	0.0377875	-3.5746113
C	-2.0043666	-1.4917410	-3.4391121
N	-0.5826896	-1.7786456	-3.6398899
N	-0.9680802	0.2348568	-4.5873773
C	-0.5664590	1.5396552	-5.0823155
C	-0.0335370	-0.8048178	-4.4787552
O	1.0722888	-0.8514169	-5.0196518
C	4.0645803	-1.7926735	-1.5399372
C	4.1335028	-2.2459553	-0.0626608
C	3.3487787	-3.5496813	0.2282997
C	2.6226378	-1.7218124	-2.0980489
C	1.9745729	-3.0784228	-1.8288640
C	1.9367058	-3.3553642	-0.3187240
N	0.9531829	-4.4402908	-0.2547672
N	0.5805752	-3.3374288	-2.1908033
C	0.0141133	-3.0930787	-3.5063297
C	0.0464455	-4.2858095	-1.3207560
O	-1.0239158	-4.8796228	-1.4518305
H	2.5630584	0.0705898	2.9947842
H	2.7989522	2.3923634	5.0311352
H	3.7483577	2.2398056	3.5102706
H	4.9628386	1.2559101	5.5330594
H	4.6843365	0.0589746	4.2438935
H	4.1564775	-0.9674814	6.4449760
H	3.0717165	0.3757256	6.8717708

H	2.5680608	-1.7551429	4.6412189
H	1.7121097	-1.5633511	6.1981990
H	0.9473632	0.7117498	5.5278217
H	-4.8941210	-5.2450095	1.0812639
H	-4.1355372	-3.8775370	0.2331782
H	-4.6935909	-4.1154017	3.2693879
H	-5.4731145	-3.0021900	2.1200110
H	-3.3181837	-1.7128148	1.8431522
H	-3.7235179	-1.8750981	3.5819679
H	-2.7129706	-5.8224238	2.1948117
H	-2.4570273	-5.6424424	0.4158525
H	-1.8022419	-3.2578383	0.7392642
H	-2.2736178	-3.9504090	3.6953536
H	-4.2871379	3.3407497	1.9284664
H	-4.6215051	4.8392626	2.8317148
H	-4.8309582	5.1358524	0.3201281
H	-3.6375615	6.2365764	1.0469549
H	-2.9908293	3.6468213	-0.5656974
H	-2.6994484	5.3301365	-1.0549284
H	-2.1628288	5.2167551	3.2078406
H	-2.6113080	3.5529916	3.7165975
H	-1.9467225	2.6957597	1.4302749
H	-1.2366475	5.6588683	0.9880364
H	4.4422603	4.0797885	-3.8325223
H	5.3091635	2.9153990	-2.8032483
H	4.8332855	2.0083964	-5.1259753
H	4.1326628	0.9996786	-3.8378371
H	2.5793067	2.9921463	-5.6447475
H	2.4587399	1.1914093	-5.6102800
H	3.1719006	2.3528209	-1.5742960
H	3.4336739	4.1182052	-1.5725724
H	2.0059828	4.3038616	-3.6609291
H	1.7459895	1.2744193	-3.2216957
H	-3.9443360	0.6969318	-1.7039340
H	-5.3450122	0.3886226	-2.7610043
H	-4.7339307	-1.6178451	-1.3329821
H	-4.6941165	-1.9761106	-3.0748708
H	-2.6980645	-3.0112539	-2.0189001
H	-2.2131631	-1.4531327	-1.2749561
H	-3.4348160	1.6602858	-3.8898616
H	-3.8369950	0.1302100	-4.7560132
H	-1.6558770	0.4649441	-2.6010774
H	-2.5781633	-1.9244968	-4.3016515
H	4.5627393	-0.8038406	-1.6519334
H	4.6527126	-2.5039807	-2.1652829
H	3.7164689	-1.4368326	0.5849273
H	5.1958832	-2.3705095	0.2428335
H	3.3254262	-3.7402335	1.3226776
H	3.8328379	-4.4228463	-0.2655113
H	2.6272150	-1.4835699	-3.1840740
H	2.0394981	-0.9182382	-1.5904230
H	2.6178618	-3.8603779	-2.3134944
H	1.5056140	-2.4459594	0.1771667
H	1.2581157	5.1723228	-1.1763907
H	-0.4546744	5.2692740	-1.7533998
H	1.4310988	-5.3491409	1.5623808
H	-0.0330089	-5.9842979	0.7172035
H	0.8108513	-3.1724143	-4.2781756
H	-0.7535012	-3.8781665	-3.6799706
H	-1.6736292	-1.2692576	4.6042751

H	-0.1590943	-2.1113623	5.1184273
H	1.4112038	3.4019692	3.5316037
H	-0.2095790	2.7833582	4.0783329
H	0.0443588	1.3794201	-5.9925296
H	-1.4802792	2.1049330	-5.3541289
H	1.3598160	1.6107676	1.8707131

Protonated cycHC[6] (VI)

139

C	1.7122677	0.8407438	3.7883623
C	2.9592511	1.6905158	3.5357766
C	4.1498100	0.7212375	3.3512973
C	4.3391072	-0.2407047	4.5438440
C	3.0556121	-1.0386586	4.8916095
C	1.9377498	-0.0166321	5.0397650
N	0.4361604	1.5178392	4.1197734
C	-0.3434874	0.8064528	4.9569775
N	0.5261013	-0.4416962	5.4209638
O	-1.4486963	0.9673691	5.4162451
C	-0.0379260	-1.8403424	5.0331837
C	-4.1001240	-2.5486462	1.5316699
C	-4.2040380	-1.8273074	2.8938853
C	-2.8672615	-1.1996921	3.3633923
C	-2.9418420	-3.5710003	1.4587574
C	-1.6680259	-2.8390845	1.8786218
C	-1.8130320	-2.2993977	3.3089803
N	-0.3926044	-2.0423627	3.6734484
N	-0.3983555	-3.5704788	1.9792378
C	0.0990163	-4.5815776	1.0323226
C	0.3871704	-3.0390552	2.9664138
O	1.5370411	-3.3447660	3.2719430
C	-4.2584380	2.5369572	1.8351537
C	-4.2657836	3.1470249	0.4136937
C	-2.9266763	2.9748929	-0.3439073
C	-3.0479320	2.9723188	2.7006653
C	-1.7881694	2.7120346	1.8750953
C	-1.8341894	3.5247814	0.5693470
N	-0.4177739	3.5261513	0.1698175
N	-0.4652243	3.0804040	2.3847558
C	0.0368534	2.9054553	3.7008381
C	0.3701091	3.4541272	1.3089930
O	1.5739206	3.6928526	1.4002754
C	4.3582638	2.8180951	-2.3802216
C	4.2607971	1.8789257	-3.6052141
C	3.0333867	2.1557847	-4.5080372
C	3.0512539	2.8920654	-1.5534528
C	1.9302129	3.2535897	-2.5263425
C	1.8021367	2.1697610	-3.6066438
N	0.4803303	2.4800790	-4.1676678
N	0.5328952	3.3591806	-2.0840943
C	0.0741439	4.2262086	-1.0235486
C	-0.2997762	3.0851096	-3.1819589
O	-1.5017704	3.3456859	-3.2514359
C	-4.3822317	0.3916619	-3.7313552
C	-4.3954174	-1.1172056	-3.3914147
C	-3.0202670	-1.6582652	-2.9279715
C	-3.2527835	0.8014923	-4.7081679
C	-1.9440008	0.2551207	-4.1428163

C	-2.0070989	-1.2731379	-4.0040514
N	-0.5807168	-1.5910477	-3.8662787
N	-0.6900325	0.4233314	-4.8877126
C	-0.1389195	1.7217429	-5.2492546
C	0.1601654	-0.6469377	-4.5877234
O	1.3472174	-0.7464460	-4.9012950
C	4.2344755	-2.3732292	-1.7149661
C	4.2351117	-2.7387911	-0.2117283
C	3.1635305	-3.7887824	0.1748407
C	2.8371686	-1.9886212	-2.2594523
C	1.8896324	-3.1293278	-1.8945217
C	1.8250811	-3.2872780	-0.3665666
N	0.6113384	-4.0914343	-0.2194779
N	0.4623796	-3.0836293	-2.2377562
C	-0.0450237	-2.9090753	-3.5971743
C	-0.2532036	-3.8185788	-1.2976507
O	-1.4264089	-4.1818646	-1.3836789
H	1.5415160	0.1857256	2.9031680
H	3.1418758	2.3605844	4.4079075
H	2.8160495	2.3376495	2.6437159
H	5.0791661	1.3095186	3.1935668
H	3.9944213	0.1301068	2.4186100
H	5.1601864	-0.9575783	4.3300713
H	4.6597210	0.3425990	5.4386577
H	2.8089486	-1.7803128	4.1024601
H	3.2053812	-1.6028574	5.8395926
H	2.2103793	0.6902208	5.8563324
H	-5.0617008	-3.0580997	1.3050721
H	-3.9542823	-1.7925253	0.7254026
H	-4.5453201	-2.5522964	3.6690723
H	-4.9860297	-1.0379404	2.8466500
H	-2.5698031	-0.3575626	2.6967734
H	-2.9777089	-0.7836764	4.3878809
H	-3.1297250	-4.4309905	2.1424599
H	-2.8347965	-3.9656597	0.4256202
H	-1.5268514	-1.9732574	1.1827651
H	-2.1700311	-3.1458037	3.9518872
H	-4.2464657	1.4247834	1.7509758
H	-5.2030319	2.7956798	2.3621219
H	-5.0928359	2.6970212	-0.1778750
H	-4.4970437	4.2353614	0.4843875
H	-2.7270022	1.9013268	-0.5682482
H	-2.9436499	3.4999983	-1.3211063
H	-3.1158527	4.0539515	2.9588134
H	-3.0376190	2.4009133	3.6550123
H	-1.7756606	1.6245120	1.6003997
H	-2.1175746	4.5783415	0.8322274
H	4.6159280	3.8463652	-2.7267063
H	5.1992065	2.4963740	-1.7264156
H	5.1932484	1.9518022	-4.2069148
H	4.2013979	0.8230956	-3.2514932
H	3.1351170	3.1331799	-5.0331378
H	2.9461579	1.3562868	-5.2744275
H	2.8292905	1.9121014	-1.0709928
H	3.1431750	3.6387898	-0.7358316
H	2.2167098	4.2156478	-3.0286816
H	1.7542814	1.1786617	-3.0889466
H	-4.2569085	0.9762774	-2.7898134
H	-5.3682414	0.6900599	-4.1506924
H	-5.1626390	-1.3193844	-2.6111723

H	-4.7163975	-1.6922989	-4.2915577
H	-3.0570959	-2.7572548	-2.7729571
H	-2.7231247	-1.2066767	-1.9530462
H	-3.2122598	1.9086263	-4.7888821
H	-3.4338495	0.3849354	-5.7257002
H	-1.8177686	0.6829853	-3.1156634
H	-2.3722440	-1.6987518	-4.9762431
H	4.9512111	-1.5422125	-1.8974761
H	4.6179779	-3.2411595	-2.3005509
H	4.0531293	-1.8134262	0.3863847
H	5.2422665	-3.1046967	0.0861895
H	3.1278799	-3.9114718	1.2792975
H	3.4040636	-4.7817833	-0.2691378
H	2.8647968	-1.8162577	-3.3560331
H	2.4773010	-1.0395478	-1.7990535
H	2.3216253	-4.0734308	-2.3197554
H	1.6406615	-2.2691236	0.0719708
H	0.9138702	4.8817221	-0.7109204
H	-0.7628247	4.8488538	-1.4079437
H	0.8946684	-5.1371252	1.5679088
H	-0.7395961	-5.2669942	0.7977910
H	0.7916962	-3.0935305	-4.3050049
H	-0.8439087	-3.6635581	-3.7581245
H	-0.9236843	-1.9464737	5.6953245
H	0.7664907	-2.5459555	5.3351355
H	0.9479891	3.5308580	3.7931548
H	-0.7182747	3.2199725	4.4501121
H	0.6264152	1.5575640	-6.0326923
H	-0.9580086	2.3393734	-5.6666790
H	0.4401099	-0.4333800	6.4538751

Non-dissociated HCl complex with cycHC[6] (a)

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Cl	-4.3157522	-5.8293712	-2.4137319
C	0.6987813	3.7764608	-1.8111441
C	0.2369464	4.3672863	-3.1420930
C	0.3928932	3.2614210	-4.2147813
C	1.7923466	2.6021060	-4.2390386
C	2.2739609	2.1221925	-2.8480340
C	2.1612921	3.3188823	-1.9061001
N	0.7375305	4.6095949	-0.6057359
C	1.7623991	4.1483066	0.2330193
N	2.5150339	3.2136953	-0.4879434
O	1.9721907	4.5084935	1.3926602
C	3.8110611	2.7615775	-0.0105389
C	3.2238637	-0.5725324	4.2499279
C	3.0659228	0.9665871	4.2559594
C	2.7508742	1.5603853	2.8615665
C	4.2018700	-1.0994693	3.1706590
C	3.7783460	-0.4861095	1.8371346
C	3.8288518	1.0465528	1.9099332
N	3.8229163	1.3954516	0.4868369
N	4.5593714	-0.7402099	0.6226352
C	4.7923129	-2.0730051	0.0863147
C	4.4442848	0.3675493	-0.2310342
O	4.8311240	0.4291630	-1.3990371
C	-0.8472776	3.2660749	4.1754416
C	-2.0836051	2.3380306	4.2284890

C	-2.4533091	1.7235684	2.8564899
C	-0.9168076	4.3444483	3.0661765
C	-1.2454469	3.6281369	1.7575221
C	-2.5839731	2.8856293	1.8744740
N	-2.9059231	2.6608020	0.4632168
N	-1.4510924	4.3943753	0.5250595
C	-0.4387438	5.2674026	-0.0526685
C	-2.3581634	3.7054528	-0.2925809
O	-2.6351415	3.9755826	-1.4622312
C	-3.0505085	0.2117656	-4.2059931
C	-2.9902242	-1.3340239	-4.1754868
C	-3.8748732	-1.9735246	-3.0772809
C	-2.8196883	0.8691444	-2.8236242
C	-3.7993554	0.2121683	-1.8534414
C	-3.5135814	-1.2939971	-1.7568730
N	-4.2183569	-1.6424707	-0.5187874
N	-3.8432413	0.5900826	-0.4386186
C	-4.0908236	1.9505624	0.0139924
C	-4.2842153	-0.5085702	0.3064878
O	-4.6704473	-0.4835932	1.4762351
C	-2.2364164	-2.2342089	4.2410149
C	-0.8046871	-2.8190776	4.2939308
C	-0.1033654	-2.8662486	2.9133367
C	-3.1429063	-2.8771496	3.1616526
C	-2.3718177	-2.8306256	1.8442904
C	-1.0518809	-3.6016677	1.9703369
N	-0.7188216	-3.8232992	0.5576508
N	-2.9430131	-3.4247973	0.6246270
C	-4.2188521	-2.9773734	0.0534654
C	-1.9022200	-3.8964211	-0.1630240
O	-1.9847640	-4.3315056	-1.3308361
C	1.4421006	-2.7646055	-4.1468588
C	2.7099927	-1.8786844	-4.1164478
C	3.7240655	-2.2704074	-3.0129105
C	0.7557037	-2.9086778	-2.7666253
C	1.8282816	-3.3822447	-1.7877353
C	2.9535008	-2.3412655	-1.6961445
N	3.6296708	-2.7589152	-0.4635323
N	1.5294916	-3.5967300	-0.3682487
C	0.4961574	-4.4942734	0.1100727
C	2.7023826	-3.3908984	0.3731917
O	2.8816685	-3.7215116	1.5465035
H	0.0711180	2.8692955	-1.6076955
H	0.8554558	5.2593948	-3.3957296
H	-0.8259103	4.6836905	-3.0800557
H	0.1568004	3.6771144	-5.2195779
H	-0.3740644	2.4769577	-4.0167024
H	1.7909729	1.7474007	-4.9518865
H	2.5351895	3.3331249	-4.6366716
H	1.6364147	1.2883888	-2.4724863
H	3.3142620	1.7350448	-2.8943689
H	2.7590464	4.1563760	-2.3569051
H	3.5515787	-0.9201085	5.2546694
H	2.2264048	-1.0393625	4.0721477
H	4.0080728	1.4299375	4.6328156
H	2.2710201	1.2583727	4.9783436
H	1.7487205	1.2265730	2.5068336
H	2.7288158	2.6709019	2.8926824
H	5.2510242	-0.8065756	3.4061442
H	4.1501299	-2.2081662	3.1240633

H	2.7127724	-0.7814966	1.6526876
H	4.8232717	1.3424530	2.3405523
H	0.0632548	2.6473031	3.9996820
H	-0.7027724	3.7542630	5.1648954
H	-1.9107322	1.5270928	4.9706617
H	-2.9608509	2.9159631	4.6041304
H	-1.6574464	1.0255201	2.5074647
H	-3.3942079	1.1353781	2.9194417
H	-1.7045118	5.0992333	3.2927150
H	0.0600656	4.8685042	2.9892893
H	-0.4464300	2.8626001	1.5810157
H	-3.3418733	3.5985422	2.2992911
H	-4.0500503	0.5308791	-4.5846673
H	-2.3073497	0.6016165	-4.9370604
H	-3.2781960	-1.7400260	-5.1703111
H	-1.9355148	-1.6538774	-4.0035333
H	-4.9560913	-1.8174273	-3.2956984
H	-3.7038070	-3.0693989	-3.0379179
H	-1.7749992	0.7007798	-2.4723726
H	-2.9710318	1.9691198	-2.8712934
H	-4.8294818	0.3419759	-2.2816051
H	-2.4114627	-1.4234346	-1.5958766
H	-2.1743792	-1.1408306	4.0329291
H	-2.7180809	-2.3313998	5.2392792
H	-0.1867054	-2.2312573	5.0084856
H	-0.8460366	-3.8555988	4.7043624
H	0.8823175	-3.3748982	2.9790884
H	0.0874599	-1.8374453	2.5290226
H	-4.0905488	-2.3045006	3.0793706
H	-3.3876963	-3.9327775	3.4211051
H	-2.1237567	-1.7590571	1.6327372
H	-1.2709152	-4.6028421	2.4299201
H	0.7170202	-2.3566344	-4.8858205
H	1.7145631	-3.7823567	-4.5128244
H	2.4087231	-0.8181896	-3.9492970
H	3.2088011	-1.9047905	-5.1105881
H	4.5287606	-1.5067367	-2.9523313
H	4.1922825	-3.2577526	-3.2323807
H	-0.0947170	-3.6224063	-2.8189440
H	0.3404626	-1.9321285	-2.4257362
H	2.2643389	-4.3301307	-2.2017641
H	2.4782938	-1.3394119	-1.5285635
H	-4.5299673	2.5321249	-0.8254848
H	-4.8173593	1.8942625	0.8541112
H	5.5513942	-1.9730873	-0.7149204
H	5.1936916	-2.7137226	0.8963650
H	0.2102909	-5.1918948	-0.7058451
H	0.9170776	-5.0667338	0.9653871
H	4.1227835	3.4450380	0.8093097
H	4.5422566	2.8188264	-0.8461488
H	-0.9305354	5.8451178	-0.8604331
H	-0.0835431	5.9628219	0.7337459
H	-4.5167786	-3.7105522	-0.7220455
H	-4.9732784	-2.9882112	0.8647659
H	-3.2317198	-5.1582353	-1.9151119

Non-dissociated HCl complex with cycHC[6] (b)

Cl	-0.7325922	-6.4105856	-2.9147717
C	0.6489035	3.7796839	-1.8102064
C	0.1934102	4.3668966	-3.1449626
C	0.3628246	3.2609627	-4.2156651
C	1.7659088	2.6092437	-4.2294363
C	2.2396933	2.1322142	-2.8349022
C	2.1140435	3.3284620	-1.8942405
N	0.6759795	4.6144665	-0.6055940
C	1.6961936	4.1569892	0.2415310
N	2.4577546	3.2253586	-0.4733771
O	1.8952250	4.5184903	1.4026304
C	3.7518721	2.7773438	0.0140825
C	3.1546132	-0.5730641	4.2592786
C	2.9909267	0.9654856	4.2698706
C	2.6805336	1.5629423	2.8759763
C	4.1392361	-1.0932718	3.1828291
C	3.7203201	-0.4768066	1.8493034
C	3.7648847	1.0557838	1.9279714
N	3.7656352	1.4096425	0.5063490
N	4.5096140	-0.7240157	0.6390878
C	4.7459821	-2.0554880	0.0985555
C	4.3974151	0.3867343	-0.2107621
O	4.7941536	0.4560372	-1.3748876
C	-0.9319752	3.2933420	4.1723204
C	-2.1687923	2.3660980	4.2257610
C	-2.5330594	1.7436054	2.8558929
C	-0.9970559	4.3652045	3.0566448
C	-1.3202868	3.6411079	1.7509844
C	-2.6595123	2.8995887	1.8662000
N	-2.9742978	2.6659079	0.4545502
N	-1.5195888	4.3995790	0.5128276
C	-0.5052797	5.2716749	-0.0634927
C	-2.4222387	3.7061804	-0.3049579
O	-2.6942577	3.9690544	-1.4775513
C	-3.0805187	0.1797162	-4.1963040
C	-2.9751460	-1.3627352	-4.1431356
C	-3.8476523	-2.0149295	-3.0417748
C	-2.8732546	0.8613220	-2.8220828
C	-3.8463116	0.1971457	-1.8503745
C	-3.5296926	-1.3005162	-1.7292613
N	-4.2516146	-1.6463093	-0.5003334
N	-3.9074229	0.5905714	-0.4397964
C	-4.1570403	1.9539553	0.0029256
C	-4.3366018	-0.5052646	0.3146851
O	-4.7298189	-0.4758086	1.4818916
C	-2.1735644	-2.1934810	4.2346018
C	-0.7589570	-2.8196198	4.2709165
C	-0.0816979	-2.9052990	2.8801069
C	-3.1152346	-2.8224799	3.1778436
C	-2.3639575	-2.8168998	1.8480850
C	-1.0661395	-3.6268857	1.9633861
N	-0.7608632	-3.8872626	0.5484648
N	-2.9667499	-3.4161789	0.6510775
C	-4.2410637	-2.9756410	0.0861999
C	-1.9524933	-3.9228694	-0.1553017
O	-2.1306394	-4.3327440	-1.3210459
C	1.4019247	-2.7183707	-4.1382322
C	2.6736970	-1.8391794	-4.1032553
C	3.6841611	-2.2409686	-3.0004218
C	0.7143402	-2.8739130	-2.7599353

C	1.7858717	-3.3577926	-1.7855493
C	2.9102500	-2.3169727	-1.6857224
N	3.5853284	-2.7398591	-0.4551261
N	1.4867164	-3.5867122	-0.3654768
C	0.4756758	-4.5205412	0.0956814
C	2.6628388	-3.3865695	0.3745193
O	2.8496411	-3.7320004	1.5426803
H	0.0239738	2.8697792	-1.6098822
H	0.8091841	5.2619105	-3.3950674
H	-0.8714357	4.6781443	-3.0907247
H	0.1312677	3.6746898	-5.2223546
H	-0.4010556	2.4721863	-4.0222979
H	1.7743138	1.7543248	-4.9419117
H	2.5076850	3.3441319	-4.6218827
H	1.6038578	1.2950780	-2.4640058
H	3.2821779	1.7501908	-2.8734593
H	2.7114191	4.1686745	-2.3405487
H	3.4787779	-0.9227981	5.2644314
H	2.1595802	-1.0426274	4.0754706
H	3.9295906	1.4308918	4.6528165
H	2.1915498	1.2519025	4.9894943
H	1.6811243	1.2272118	2.5153693
H	2.6548828	2.6733265	2.9109339
H	5.1863214	-0.7978648	3.4241548
H	4.0915384	-2.2019968	3.1321047
H	2.6568240	-0.7756944	1.6577186
H	4.7560117	1.3531067	2.3652666
H	-0.0208385	2.6734263	4.0037077
H	-0.7912626	3.7871571	5.1595209
H	-1.9992004	1.5593307	4.9732109
H	-3.0473631	2.9465352	4.5944030
H	-1.7358175	1.0436330	2.5143156
H	-3.4740925	1.1557596	2.9189732
H	-1.7856911	5.1212508	3.2756381
H	-0.0197856	4.8884523	2.9803286
H	-0.5206117	2.8743925	1.5828611
H	-3.4193861	3.6151678	2.2828113
H	-4.0868400	0.4657902	-4.5838399
H	-2.3448606	0.5792749	-4.9295336
H	-3.2420299	-1.7917367	-5.1342842
H	-1.9130708	-1.6481278	-3.9587468
H	-4.9318708	-1.9088768	-3.2762930
H	-3.6128163	-3.0978932	-2.9692639
H	-1.8277680	0.7199057	-2.4617470
H	-3.0461380	1.9571214	-2.8861155
H	-4.8759767	0.2994658	-2.2872252
H	-2.4282618	-1.4019877	-1.5453144
H	-2.0830791	-1.1047790	4.0126868
H	-2.6413593	-2.2649156	5.2416113
H	-0.1120890	-2.2412218	4.9673064
H	-0.8235546	-3.8490325	4.6958077
H	0.8916310	-3.4372544	2.9375849
H	0.1310768	-1.8874462	2.4786056
H	-4.0481811	-2.2250219	3.1012102
H	-3.3858186	-3.8671986	3.4552200
H	-2.0882556	-1.7554431	1.6166354
H	-1.3090204	-4.6124021	2.4435989
H	0.6778041	-2.3009947	-4.8730483
H	1.6637088	-3.7361934	-4.5096661
H	2.3788953	-0.7773770	-3.9319010

H	3.1736813	-1.8642087	-5.0969500
H	4.4922371	-1.4812607	-2.9343071
H	4.1476636	-3.2293748	-3.2243720
H	-0.1198170	-3.6019521	-2.8348915
H	0.2912300	-1.9040941	-2.4091662
H	2.2139275	-4.3034579	-2.2082200
H	2.4357638	-1.3152038	-1.5140394
H	-4.5909664	2.5301945	-0.8428350
H	-4.8887338	1.9031143	0.8388936
H	5.5066478	-1.9507941	-0.7005331
H	5.1467682	-2.6982587	0.9072768
H	0.2310137	-5.2301404	-0.7219949
H	0.9072696	-5.0855827	0.9501207
H	4.0526614	3.4597832	0.8388014
H	4.4901150	2.8414333	-0.8149440
H	-0.9933844	5.8439073	-0.8773429
H	-0.1572693	5.9721147	0.7216537
H	-4.5225549	-3.7127583	-0.6911581
H	-4.9985265	-2.9832698	0.8951091
H	-1.3935891	-5.4732751	-2.1635611

Non-dissociated HBr complex with cycHC[6] (a)

140

Br	-4.3160817	-6.1459118	-2.3458413
C	0.7016186	3.7793297	-1.8106771
C	0.2419070	4.3712580	-3.1419092
C	0.3968164	3.2653799	-4.2147738
C	1.7950768	2.6034866	-4.2380840
C	2.2747681	2.1224484	-2.8467972
C	2.1633952	3.3191356	-1.9046704
N	0.7409653	4.6120364	-0.6049548
C	1.7645627	4.1489239	0.2344877
N	2.5161671	3.2132126	-0.4863292
O	1.9740950	4.5084046	1.3942623
C	3.8113203	2.7589453	-0.0084748
C	3.2140076	-0.5773518	4.2485887
C	3.0587621	0.9620145	4.2556189
C	2.7458325	1.5571614	2.8613736
C	4.1922824	-1.1052011	3.1700249
C	3.7715570	-0.4901188	1.8364605
C	3.8241167	1.0424114	1.9106189
N	3.8207821	1.3924004	0.4878050
N	4.5544591	-0.7441762	0.6231487
C	4.7876445	-2.0767853	0.0865501
C	4.4422538	0.3643627	-0.2297420
O	4.8312790	0.4265753	-1.3970642
C	-0.8500952	3.2771971	4.1772137
C	-2.0895338	2.3534140	4.2306399
C	-2.4598085	1.7378583	2.8592800
C	-0.9150409	4.3540662	3.0662970
C	-1.2459313	3.6374859	1.7584146
C	-2.5867385	2.8990818	1.8757289
N	-2.9086803	2.6737624	0.4644370
N	-1.4487948	4.4030286	0.5251073
C	-0.4340301	5.2729955	-0.0529656
C	-2.3575804	3.7162281	-0.2920472
O	-2.6336380	3.9862111	-1.4620280
C	-3.0631686	0.2243753	-4.2073620

C	-2.9815366	-1.3201395	-4.1716612
C	-3.8543072	-1.9692762	-3.0691835
C	-2.8349033	0.8882607	-2.8278441
C	-3.8060459	0.2250659	-1.8534992
C	-3.5060368	-1.2778232	-1.7519302
N	-4.2125833	-1.6280150	-0.5154205
N	-3.8495030	0.6057050	-0.4390858
C	-4.0949229	1.9661672	0.0145393
C	-4.2828351	-0.4936031	0.3090395
O	-4.6667125	-0.4696806	1.4794441
C	-2.2284543	-2.2407407	4.2413759
C	-0.8000002	-2.8336180	4.2911431
C	-0.0999976	-2.8801225	2.9099057
C	-3.1393603	-2.8759568	3.1611883
C	-2.3691925	-2.8301560	1.8433427
C	-1.0527461	-3.6078537	1.9652658
N	-0.7223648	-3.8265761	0.5510850
N	-2.9440741	-3.4180480	0.6224420
C	-4.2179284	-2.9632024	0.0545086
C	-1.9060405	-3.8886296	-0.1687865
O	-1.9939049	-4.3132580	-1.3413052
C	1.4482920	-2.7646390	-4.1555923
C	2.7150934	-1.8774615	-4.1206298
C	3.7264779	-2.2699053	-3.0149354
C	0.7579277	-2.9102952	-2.7775176
C	1.8278950	-3.3838607	-1.7957805
C	2.9524479	-2.3425343	-1.7003118
N	3.6258076	-2.7614596	-0.4666286
N	1.5251852	-3.5991083	-0.3770281
C	0.4908860	-4.4973734	0.0979459
C	2.6968130	-3.3945812	0.3672652
O	2.8737162	-3.7271444	1.5402431
H	0.0721514	2.8732275	-1.6079396
H	0.8621670	5.2623375	-3.3948856
H	-0.8204606	4.6895410	-3.0807044
H	0.1623105	3.6817695	-5.2196616
H	-0.3717507	2.4822452	-4.0175619
H	1.7927416	1.7489123	-4.9511013
H	2.5395130	3.3332538	-4.6350409
H	1.6355636	1.2895872	-2.4719082
H	3.3145199	1.7336514	-2.8924025
H	2.7628578	4.1557011	-2.3549668
H	3.5399673	-0.9262656	5.2534199
H	2.2159270	-1.0422539	4.0693274
H	4.0014181	1.4234636	4.6334953
H	2.2638178	1.2546746	4.9775815
H	1.7435718	1.2249656	2.5054372
H	2.7253635	2.6676840	2.8931837
H	5.2416565	-0.8143830	3.4069905
H	4.1387105	-2.2137582	3.1226021
H	2.7058996	-0.7839326	1.6499952
H	4.8184180	1.3364248	2.3427741
H	0.0585281	2.6551329	4.0032581
H	-0.7048421	3.7664506	5.1660176
H	-1.9201822	1.5431489	4.9743503
H	-2.9652305	2.9349631	4.6043095
H	-1.6654932	1.0372445	2.5119254
H	-3.4021320	1.1520727	2.9224810
H	-1.6999089	5.1122155	3.2914470
H	0.0638334	4.8742588	2.9890342

H	-0.4492358	2.8693122	1.5828590
H	-3.3426209	3.6147833	2.2994006
H	-4.0682930	0.5292616	-4.5830209
H	-2.3279927	0.6213004	-4.9426445
H	-3.2656899	-1.7340186	-5.1643347
H	-1.9220300	-1.6240077	-4.0007811
H	-4.9384522	-1.8377421	-3.2888106
H	-3.6534693	-3.0602264	-3.0218414
H	-1.7877944	0.7305952	-2.4788795
H	-2.9958312	1.9866535	-2.8782764
H	-4.8384738	0.3436381	-2.2794384
H	-2.4032372	-1.3952614	-1.5859557
H	-2.1606607	-1.1470904	4.0363380
H	-2.7097231	-2.3381209	5.2397896
H	-0.1781843	-2.2514699	5.0069676
H	-0.8466757	-3.8711716	4.6983227
H	0.8832652	-3.3935113	2.9731435
H	0.0955686	-1.8510811	2.5286726
H	-4.0840053	-2.2980336	3.0811790
H	-3.3896956	-3.9308442	3.4181656
H	-2.1164490	-1.7591321	1.6340852
H	-1.2759827	-4.6096917	2.4210491
H	0.7249842	-2.3568915	-4.8964373
H	1.7228498	-3.7818617	-4.5214429
H	2.4123371	-0.8174664	-3.9527769
H	3.2166234	-1.9017162	-5.1134481
H	4.5306540	-1.5059533	-2.9512703
H	4.1956939	-3.2568124	-3.2343476
H	-0.0918994	-3.6244912	-2.8330412
H	0.3410829	-1.9342252	-2.4370387
H	2.2656131	-4.3313444	-2.2090002
H	2.4764633	-1.3409874	-1.5327551
H	-4.5330652	2.5488483	-0.8246055
H	-4.8216174	1.9107726	0.8545385
H	5.5487889	-1.9770545	-0.7127555
H	5.1864772	-2.7183711	0.8971355
H	0.2026989	-5.1900301	-0.7213044
H	0.9110505	-5.0755249	0.9497673
H	4.1233835	3.4414066	0.8120743
H	4.5432147	2.8158248	-0.8435298
H	-0.9240196	5.8512339	-0.8614557
H	-0.0775605	5.9682700	0.7329849
H	-4.5216692	-3.6926843	-0.7223589
H	-4.9716034	-2.9726538	0.8665153
H	-3.1853924	-5.2685447	-1.8568250

Non-dissociated HBr complex with cycHC[6] (b)

140

Br	-0.8773918	-6.7221365	-2.8767686
C	0.6494229	3.7924237	-1.8087104
C	0.1952403	4.3839671	-3.1419729
C	0.3632536	3.2806406	-4.2155477
C	1.7654832	2.6269566	-4.2307305
C	2.2383929	2.1459012	-2.8371993
C	2.1141007	3.3398619	-1.8933654
N	0.6765685	4.6234237	-0.6014378
C	1.6960218	4.1625901	0.2447313
N	2.4571181	3.2324140	-0.4726083

O	1.8946463	4.5201393	1.4070741
C	3.7509149	2.7824700	0.0136879
C	3.1584208	-0.5694895	4.2589484
C	2.9916319	0.9687450	4.2693967
C	2.6791837	1.5655171	2.8756329
C	4.1430431	-1.0878636	3.1816383
C	3.7217368	-0.4723560	1.8483762
C	3.7639424	1.0603436	1.9270203
N	3.7636162	1.4144850	0.5053845
N	4.5103234	-0.7182308	0.6374333
C	4.7486104	-2.0489687	0.0965240
C	4.3956053	0.3922704	-0.2123460
O	4.7906576	0.4617541	-1.3770768
C	-0.9345375	3.2929630	4.1742622
C	-2.1704850	2.3643735	4.2244911
C	-2.5328773	1.7443306	2.8530553
C	-0.9993079	4.3668034	3.0604790
C	-1.3204935	3.6450203	1.7530740
C	-2.6591754	2.9021294	1.8654461
N	-2.9725004	2.6713449	0.4529615
N	-1.5190437	4.4058623	0.5161767
C	-0.5045736	5.2794148	-0.0574390
C	-2.4203134	3.7134830	-0.3039595
O	-2.6909010	3.9780382	-1.4764635
C	-3.0814572	0.1898747	-4.2041041
C	-2.9728117	-1.3523865	-4.1521926
C	-3.8417607	-2.0071677	-3.0495754
C	-2.8726844	0.8709757	-2.8298505
C	-3.8421284	0.2038319	-1.8565453
C	-3.5222414	-1.2932985	-1.7371766
N	-4.2414409	-1.6412222	-0.5072420
N	-3.9017969	0.5962129	-0.4456045
C	-4.1536415	1.9589497	-0.0019475
C	-4.3283803	-0.5008220	0.3084311
O	-4.7211976	-0.4728308	1.4757865
C	-2.1723226	-2.2008522	4.2342296
C	-0.7625214	-2.8375161	4.2767662
C	-0.0788032	-2.9258339	2.8893531
C	-3.1132645	-2.8211815	3.1715942
C	-2.3551199	-2.8185011	1.8458511
C	-1.0638764	-3.6382781	1.9662999
N	-0.7533845	-3.8979649	0.5521628
N	-2.9556061	-3.4110356	0.6439954
C	-4.2297046	-2.9708057	0.0778589
C	-1.9405580	-3.9206786	-0.1583646
O	-2.1136844	-4.3204769	-1.3296501
C	1.4005793	-2.7300626	-4.1360452
C	2.6654059	-1.8405370	-4.1015433
C	3.6804841	-2.2353692	-3.0002965
C	0.7158767	-2.8888955	-2.7567072
C	1.7911401	-3.3639071	-1.7822383
C	2.9092916	-2.3162185	-1.6842940
N	3.5881437	-2.7360923	-0.4545436
N	1.4933057	-3.5910996	-0.3620308
C	0.4850631	-4.5270534	0.0998415
C	2.6694786	-3.3857417	0.3770202
O	2.8583129	-3.7295107	1.5450928
H	0.0234068	2.8826696	-1.6115349
H	0.8124004	5.2787491	-3.3894242
H	-0.8691872	4.6965683	-3.0873436

H	0.1327062	3.6972914	-5.2212597
H	-0.4019775	2.4926176	-4.0244384
H	1.7729545	1.7737545	-4.9452901
H	2.5082711	3.3618707	-4.6212134
H	1.6013591	1.3087020	-2.4684773
H	3.2803602	1.7625228	-2.8765798
H	2.7125137	4.1805695	-2.3372641
H	3.4843288	-0.9183978	5.2638146
H	2.1641632	-1.0411755	4.0762908
H	3.9295519	1.4361236	4.6517319
H	2.1921317	1.2535964	4.9895030
H	1.6801710	1.2278880	2.5157147
H	2.6514974	2.6758265	2.9104463
H	5.1897214	-0.7902622	3.4219220
H	4.0975644	-2.1966696	3.1311401
H	2.6585716	-0.7731084	1.6577952
H	4.7547293	1.3592917	2.3638978
H	-0.0225816	2.6742669	4.0055978
H	-0.7955020	3.7850983	5.1625234
H	-2.0008441	1.5562667	4.9704918
H	-3.0500125	2.9431454	4.5934808
H	-1.7347770	1.0455658	2.5109309
H	-3.4735060	1.1556652	2.9139722
H	-1.7887685	5.1218286	3.2800189
H	-0.0224125	4.8910321	2.9863402
H	-0.5200679	2.8792518	1.5843771
H	-3.4200902	3.6161947	2.2827295
H	-4.0891844	0.4740806	-4.5893102
H	-2.3482042	0.5915338	-4.9385957
H	-3.2408400	-1.7812696	-5.1430650
H	-1.9096734	-1.6354908	-3.9703294
H	-4.9266118	-1.9028198	-3.2818057
H	-3.6049353	-3.0897905	-2.9787021
H	-1.8260765	0.7317038	-2.4719173
H	-3.0480810	1.9664478	-2.8927202
H	-4.8728351	0.3040148	-2.2914566
H	-2.4202936	-1.3931788	-1.5554045
H	-2.0725954	-1.1124064	4.0146872
H	-2.6457900	-2.2704743	5.2386671
H	-0.1149089	-2.2650093	4.9772750
H	-0.8367834	-3.8671525	4.6995325
H	0.8904716	-3.4645552	2.9511384
H	0.1438480	-1.9089831	2.4908434
H	-4.0415834	-2.2170494	3.0911411
H	-3.3925198	-3.8644773	3.4457247
H	-2.0709240	-1.7585544	1.6176795
H	-1.3167281	-4.6229262	2.4427945
H	0.6727653	-2.3186892	-4.8705181
H	1.6716069	-3.7452949	-4.5080640
H	2.3621621	-0.7813218	-3.9287917
H	3.1642419	-1.8605707	-5.0958759
H	4.4834734	-1.4701669	-2.9354664
H	4.1505198	-3.2205106	-3.2250685
H	-0.1202367	-3.6167096	-2.8256492
H	0.2894653	-1.9201180	-2.4067559
H	2.2278030	-4.3070223	-2.2025297
H	2.4291405	-1.3173267	-1.5115308
H	-4.5858811	2.5356214	-0.8482274
H	-4.8873198	1.9069326	0.8322488
H	5.5071472	-1.9425860	-0.7043748

H	5.1526419	-2.6910121	0.9041871
H	0.2426843	-5.2387520	-0.7171035
H	0.9173928	-5.0914201	0.9542231
H	4.0534219	3.4639747	0.8386202
H	4.4885778	2.8459968	-0.8158323
H	-0.9923291	5.8543006	-0.8696541
H	-0.1564621	5.9773977	0.7298101
H	-4.5096679	-3.7076334	-0.7003178
H	-4.9876493	-2.9803567	0.8862994
H	-1.4809542	-5.5682464	-2.1001981

Non-dissociated HI complex with cycHC[6] (a)

140

I	-4.3519849	-6.5246368	-2.2275844
C	0.7040483	3.7816972	-1.8107998
C	0.2466747	4.3748410	-3.1422469
C	0.3991307	3.2685365	-4.2149866
C	1.7956825	2.6030467	-4.2377667
C	2.2736824	2.1207378	-2.8463515
C	2.1646009	3.3174807	-1.9040510
N	0.7452808	4.6144106	-0.6052111
C	1.7671302	4.1484640	0.2346610
N	2.5162997	3.2104311	-0.4855685
O	1.9772758	4.5076553	1.3945023
C	3.8103514	2.7533734	-0.0074299
C	3.2078980	-0.5838483	4.2478848
C	3.0520753	0.9554966	4.2549518
C	2.7406488	1.5510623	2.8605088
C	4.1869751	-1.1113937	3.1698621
C	3.7664350	-0.4964766	1.8361281
C	3.8194537	1.0360331	1.9104624
N	3.8172049	1.3864200	0.4877535
N	4.5494941	-0.7506962	0.6229499
C	4.7824505	-2.0832965	0.0861832
C	4.4383730	0.3581030	-0.2297924
O	4.8277819	0.4202760	-1.3969388
C	-0.8509738	3.2853830	4.1760065
C	-2.0928482	2.3648454	4.2291563
C	-2.4653247	1.7511295	2.8575508
C	-0.9131381	4.3629056	3.0655198
C	-1.2457787	3.6475024	1.7573937
C	-2.5889278	2.9131618	1.8744394
N	-2.9114283	2.6892636	0.4629494
N	-1.4457267	4.4136374	0.5239245
C	-0.4275659	5.2797856	-0.0541035
C	-2.3564957	3.7298185	-0.2936255
O	-2.6310946	4.0003542	-1.4636672
C	-3.0517594	0.2402916	-4.2065498
C	-2.9558859	-1.3031796	-4.1671586
C	-3.8264646	-1.9586707	-3.0665018
C	-2.8327177	0.9085342	-2.8277553
C	-3.8031816	0.2409727	-1.8558820
C	-3.4937886	-1.2594478	-1.7496940
N	-4.2081086	-1.6114497	-0.5183299
N	-3.8534989	0.6229241	-0.4418758
C	-4.0982774	1.9834470	0.0118578
C	-4.2852008	-0.4771096	0.3058541
O	-4.6729831	-0.4543959	1.4749224

C	-2.2283812	-2.2342745	4.2382773
C	-0.8023101	-2.8329878	4.2875750
C	-0.1024901	-2.8816153	2.9062686
C	-3.1418910	-2.8654967	3.1579353
C	-2.3715828	-2.8224246	1.8400878
C	-1.0580392	-3.6053557	1.9614281
N	-0.7287575	-3.8260911	0.5469191
N	-2.9483478	-3.4076658	0.6190769
C	-4.2184554	-2.9472796	0.0488889
C	-1.9122975	-3.8812502	-0.1729717
O	-2.0064282	-4.3035216	-1.3466395
C	1.4477076	-2.7694021	-4.1600400
C	2.7158294	-1.8840495	-4.1240378
C	3.7253279	-2.2771981	-3.0168484
C	0.7557402	-2.9138838	-2.7826006
C	1.8239722	-3.3885769	-1.7995871
C	2.9495677	-2.3484625	-1.7031490
N	3.6207281	-2.7673195	-0.4681944
N	1.5193074	-3.6032117	-0.3811932
C	0.4828788	-4.4993847	0.0926854
C	2.6901315	-3.3996747	0.3645561
O	2.8653366	-3.7322194	1.5378033
H	0.0719271	2.8774198	-1.6082145
H	0.8695857	5.2641453	-3.3948703
H	-0.8147960	4.6961623	-3.0816357
H	0.1660657	3.6854734	-5.2199691
H	-0.3714787	2.4873799	-4.0180134
H	1.7914465	1.7485326	-4.9508376
H	2.5421223	3.3309099	-4.6344165
H	1.6324998	1.2891688	-2.4719415
H	3.3126106	1.7296912	-2.8915621
H	2.7665395	4.1525525	-2.3538403
H	3.5334079	-0.9326712	5.2528973
H	2.2100830	-1.0491139	4.0680634
H	3.9941103	1.4171936	4.6340774
H	2.2561927	1.2477165	4.9760722
H	1.7384805	1.2194782	2.5036807
H	2.7208452	2.6616231	2.8925975
H	5.2361208	-0.8200806	3.4072266
H	4.1339187	-2.2200023	3.1225567
H	2.7007559	-0.7901420	1.6495265
H	4.8135370	1.3296896	2.3433895
H	0.0559926	2.6609759	4.0017175
H	-0.7043439	3.7738488	5.1649972
H	-1.9253946	1.5536106	4.9722558
H	-2.9668918	2.9484396	4.6035120
H	-1.6732453	1.0482095	2.5097039
H	-3.4093927	1.1681395	2.9208919
H	-1.6960957	5.1229816	3.2909001
H	0.0670854	4.8806218	2.9884774
H	-0.4514078	2.8768417	1.5820807
H	-3.3427080	3.6309363	2.2983111
H	-4.0585295	0.5354764	-4.5855741
H	-2.3181438	0.6420565	-4.9406958
H	-3.2320522	-1.7221109	-5.1599752
H	-1.8942089	-1.5962653	-3.9914536
H	-4.9110423	-1.8430428	-3.2926246
H	-3.6059890	-3.0456076	-3.0112027
H	-1.7858807	0.7582929	-2.4747648
H	-3.0001242	2.0057487	-2.8808725

H	-4.8348779	0.3520091	-2.2855578
H	-2.3914489	-1.3686235	-1.5747107
H	-2.1561736	-1.1407637	4.0337741
H	-2.7099431	-2.3301753	5.2366848
H	-0.1780717	-2.2537504	5.0036507
H	-0.8531578	-3.8705542	4.6941803
H	0.8788195	-3.3986926	2.9692721
H	0.0970356	-1.8531740	2.5254511
H	-4.0843572	-2.2839264	3.0780547
H	-3.3964341	-3.9194312	3.4145035
H	-2.1148758	-1.7522176	1.6308930
H	-1.2852894	-4.6063761	2.4167639
H	0.7257920	-2.3606711	-4.9016952
H	1.7210330	-3.7870768	-4.5254603
H	2.4144455	-0.8234930	-3.9572923
H	3.2185185	-1.9097314	-5.1162223
H	4.5302405	-1.5140702	-2.9525201
H	4.1937802	-3.2646739	-3.2352338
H	-0.0950480	-3.6268675	-2.8389082
H	0.3400296	-1.9371662	-2.4426920
H	2.2609923	-4.3365920	-2.2121219
H	2.4745234	-1.3463280	-1.5367052
H	-4.5350628	2.5668408	-0.8274726
H	-4.8258689	1.9284353	0.8511062
H	5.5443191	-1.9837764	-0.7124753
H	5.1803067	-2.7253136	0.8969527
H	0.1927581	-5.1901993	-0.7273477
H	0.9010769	-5.0800145	0.9437418
H	4.1232256	3.4346790	0.8137927
H	4.5428224	2.8095843	-0.8420375
H	-0.9151903	5.8593858	-0.8630259
H	-0.0690205	5.9741389	0.7317434
H	-4.5190919	-3.6733266	-0.7322898
H	-4.9764092	-2.9581958	0.8568569
H	-3.1543395	-5.3902468	-1.7719162

Non-dissociated HI complex with cycHC[6] (b)

140

I	-1.2355807	-7.2608955	-2.6558157
C	0.6444996	3.8028306	-1.8041867
C	0.1885642	4.3941434	-3.1369883
C	0.3560040	3.2910044	-4.2108491
C	1.7584413	2.6377538	-4.2274315
C	2.2328846	2.1569202	-2.8343325
C	2.1093994	3.3512850	-1.8908346
N	0.6727358	4.6343357	-0.5973142
C	1.6943019	4.1754452	0.2472746
N	2.4547844	3.2450431	-0.4706384
O	1.8953363	4.5347220	1.4086593
C	3.7495492	2.7965442	0.0141463
C	3.1603934	-0.5562155	4.2589740
C	2.9944728	0.9820741	4.2699456
C	2.6815503	1.5791044	2.8764611
C	4.1447689	-1.0747604	3.1814380
C	3.7239579	-0.4584873	1.8483978
C	3.7659822	1.0741955	1.9273977
N	3.7640795	1.4284532	0.5057189
N	4.5123135	-0.7035492	0.6370190

C	4.7546945	-2.0335703	0.0968662
C	4.3952240	0.4065631	-0.2129047
O	4.7877928	0.4755570	-1.3785522
C	-0.9318854	3.2946661	4.1778336
C	-2.1664303	2.3641888	4.2273338
C	-2.5286266	1.7454268	2.8552365
C	-0.9986346	4.3700313	3.0656331
C	-1.3199558	3.6501184	1.7572079
C	-2.6571920	2.9045500	1.8694023
N	-2.9716995	2.6762581	0.4567550
N	-1.5213050	4.4133328	0.5221700
C	-0.5085040	5.2887894	-0.0515502
C	-2.4228256	3.7214286	-0.2982540
O	-2.6958030	3.9886708	-1.4695354
C	-3.0815129	0.2158112	-4.2112948
C	-2.9639514	-1.3259180	-4.1656359
C	-3.8278861	-1.9899797	-3.0646553
C	-2.8739634	0.8923809	-2.8347654
C	-3.8383401	0.2167343	-1.8624183
C	-3.5114308	-1.2793174	-1.7499065
N	-4.2278189	-1.6356037	-0.5207691
N	-3.8963686	0.6025829	-0.4496262
C	-4.1516354	1.9622066	0.0012909
C	-4.3169674	-0.4994604	0.3004312
O	-4.7067486	-0.4783281	1.4689458
C	-2.1818065	-2.2296055	4.2312737
C	-0.7732410	-2.8686760	4.2797085
C	-0.0794820	-2.9484181	2.8968052
C	-3.1157838	-2.8413853	3.1575215
C	-2.3479812	-2.8283668	1.8374754
C	-1.0586579	-3.6517050	1.9605069
N	-0.7385563	-3.8974794	0.5464560
N	-2.9402237	-3.4080925	0.6248627
C	-4.2133861	-2.9684515	0.0564263
C	-1.9196049	-3.9089862	-0.1751918
O	-2.0736155	-4.2944594	-1.3544259
C	1.4233019	-2.7408968	-4.1469166
C	2.6798872	-1.8396748	-4.1083726
C	3.6945526	-2.2243242	-3.0030864
C	0.7342532	-2.9007947	-2.7698183
C	1.8089156	-3.3644234	-1.7890890
C	2.9200466	-2.3093841	-1.6893685
N	3.5972890	-2.7240017	-0.4568591
N	1.5067312	-3.5891933	-0.3701541
C	0.4981723	-4.5251469	0.0904428
C	2.6792574	-3.3768712	0.3728681
O	2.8651898	-3.7177903	1.5420008
H	0.0192312	2.8927791	-1.6060032
H	0.8049321	5.2892932	-3.3850182
H	-0.8759690	4.7061703	-3.0812138
H	0.1243956	3.7076411	-5.2163143
H	-0.4087963	2.5027579	-4.0190825
H	1.7654826	1.7845352	-4.9419975
H	2.5006041	3.3728625	-4.6187019
H	1.5963184	1.3197604	-2.4646382
H	3.2749132	1.7737962	-2.8746380
H	2.7064735	4.1921152	-2.3362534
H	3.4862171	-0.9056544	5.2636696
H	2.1658424	-1.0273378	4.0762764
H	3.9328485	1.4488760	4.6518550

H	2.1954886	1.2671746	4.9905056
H	1.6824629	1.2415181	2.5167455
H	2.6538179	2.6894183	2.9115356
H	5.1916113	-0.7779444	3.4220543
H	4.0986583	-2.1835213	3.1305701
H	2.6607566	-0.7591345	1.6576424
H	4.7570513	1.3733456	2.3634382
H	-0.0190976	2.6775081	4.0080192
H	-0.7931716	3.7856686	5.1667028
H	-1.9953256	1.5553558	4.9722067
H	-3.0466123	2.9412355	4.5974751
H	-1.7298425	1.0480137	2.5119517
H	-3.4683639	1.1553531	2.9158945
H	-1.7888182	5.1238319	3.2867818
H	-0.0224141	4.8955996	2.9916221
H	-0.5183024	2.8861576	1.5859916
H	-3.4187444	3.6167855	2.2887285
H	-4.0916009	0.4956761	-4.5934363
H	-2.3520526	0.6247189	-4.9455742
H	-3.2306566	-1.7524538	-5.1578932
H	-1.8988987	-1.6033474	-3.9859740
H	-4.9134998	-1.8914199	-3.2957934
H	-3.5842113	-3.0713060	-2.9975655
H	-1.8261296	0.7567448	-2.4790258
H	-3.0545581	1.9872136	-2.8928477
H	-4.8704596	0.3140639	-2.2946396
H	-2.4088371	-1.3746585	-1.5693060
H	-2.0791086	-1.1397496	4.0199690
H	-2.6625956	-2.3055708	5.2317512
H	-0.1298584	-2.3019612	4.9887742
H	-0.8522087	-3.9010715	4.6947930
H	0.8881908	-3.4895054	2.9619859
H	0.1485731	-1.9292825	2.5074059
H	-4.0430452	-2.2359267	3.0752807
H	-3.3974540	-3.8865408	3.4218054
H	-2.0604100	-1.7669101	1.6210968
H	-1.3165797	-4.6402123	2.4258457
H	0.6954009	-2.3380988	-4.8860124
H	1.7075017	-3.7537916	-4.5160135
H	2.3658291	-0.7833013	-3.9378040
H	3.1825120	-1.8559091	-5.1008129
H	4.4907623	-1.4522754	-2.9364638
H	4.1739324	-3.2056731	-3.2249349
H	-0.1027236	-3.6289579	-2.8338585
H	0.3020315	-1.9326817	-2.4252058
H	2.2563435	-4.3053805	-2.2043158
H	2.4326047	-1.3136472	-1.5191063
H	-4.5880414	2.5414030	-0.8410826
H	-4.8828939	1.9037480	0.8371070
H	5.5148350	-1.9258145	-0.7023354
H	5.1583266	-2.6745851	0.9055294
H	0.2504184	-5.2305535	-0.7300563
H	0.9302664	-5.0965838	0.9401229
H	4.0520253	3.4781862	0.8389556
H	4.4863948	2.8610858	-0.8160178
H	-0.9978617	5.8638298	-0.8626870
H	-0.1601550	5.9864323	0.7359171
H	-4.4878983	-3.7011734	-0.7275995
H	-4.9744443	-2.9864701	0.8617907
H	-1.6533356	-5.7511891	-1.9669191

Non-dissociated HCOOH complex with cycHC[6] (a)

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C	1.8983185	1.6721040	3.1117203
C	3.2334394	2.3857794	3.3136323
C	4.2947465	1.6080345	2.4964215
C	4.3121902	0.0862431	2.7738504
C	2.9166338	-0.5775209	2.6750258
C	1.9922555	0.2179833	3.5926191
N	0.6968155	2.1321012	3.8199271
C	-0.1204563	1.0356148	4.0750364
N	0.5713327	-0.1243045	3.7484942
O	-1.2698217	1.0937426	4.5404675
C	0.0990145	-1.4481772	4.1384796
C	-4.0564872	-3.0986668	1.0262571
C	-4.1220730	-2.0518818	2.1619051
C	-2.7557806	-1.3980578	2.4826115
C	-2.9460448	-4.1605742	1.2175318
C	-1.6424996	-3.4090430	1.4797708
C	-1.7674483	-2.5340339	2.7351071
N	-0.3541811	-2.2720496	3.0342433
N	-0.4092530	-4.1481615	1.7685380
C	0.1658129	-5.1332363	0.8613400
C	0.4023664	-3.3739239	2.6040228
O	1.5685202	-3.6154489	2.9200944
C	-4.0778167	2.6762845	1.7584385
C	-4.0978454	3.1078546	0.2734786
C	-2.7116202	3.0284564	-0.4119367
C	-2.9797068	3.3732829	2.5991782
C	-1.6549736	3.1876328	1.8595229
C	-1.7423540	3.8208571	0.4623561
N	-0.3239242	3.9449072	0.1145200
N	-0.4216611	3.7941047	2.3718972
C	0.1449404	3.4784067	3.6717490
C	0.4136560	4.1165478	1.2889164
O	1.5842339	4.4931440	1.3650077
C	4.3773765	2.6024006	-1.9089963
C	4.3366018	1.5866228	-3.0753288
C	3.2387570	1.8809058	-4.1277342
C	2.9984710	2.8377811	-1.2461264
C	2.0273148	3.2056866	-2.3656356
C	1.9223791	2.0504828	-3.3717196
N	0.6958942	2.4080483	-4.0907529
N	0.6120095	3.4708985	-2.0938500
C	0.1472412	4.4775491	-1.1553163
C	-0.1316482	3.1506439	-3.2373512
O	-1.2996211	3.4759872	-3.4557144
C	-4.0484614	0.3486318	-3.4197966
C	-4.0785226	-1.1623795	-3.0885565
C	-2.6924903	-1.7390341	-2.7090217
C	-2.9637063	0.7447098	-4.4519169
C	-1.6385030	0.1631677	-3.9620987
C	-1.7348294	-1.3642243	-3.8379357
N	-0.3170809	-1.7324440	-3.7928194
N	-0.4218281	0.3072036	-4.7679422
C	0.1308301	1.5959838	-5.1603636
C	0.4148375	-0.7923898	-4.5280498
O	1.5812952	-0.9163943	-4.9056309
C	4.3831865	-2.7687332	-1.6342876

C	4.3508480	-3.2745346	-0.1723513
C	3.2667164	-4.3467531	0.0989342
C	2.9974916	-2.3283511	-2.1667807
C	2.0434176	-3.4966404	-1.9284163
C	1.9421536	-3.7947672	-0.4256849
N	0.7280282	-4.6145730	-0.3776633
N	0.6273149	-3.4157946	-2.2951733
C	0.1568357	-3.0970460	-3.6333005
C	-0.1049653	-4.2557776	-1.4488781
O	-1.2681850	-4.6232711	-1.6203525
H	1.6825913	1.6570486	2.0126934
H	3.4954802	2.4001822	4.3965668
H	3.1726096	3.4336466	2.9516108
H	5.3032319	2.0361567	2.6902592
H	4.0899038	1.7775686	1.4137096
H	5.0154690	-0.4139203	2.0716400
H	4.7186223	-0.0961874	3.7968537
H	2.5317379	-0.5409478	1.6295580
H	2.9581508	-1.6484831	2.9666731
H	2.4558936	0.2172676	4.6146665
H	-5.0434411	-3.6020608	0.9244920
H	-3.8738407	-2.5767993	0.0578990
H	-4.5042677	-2.5378171	3.0898484
H	-4.8626394	-1.2622972	1.9073238
H	-2.4025031	-0.7701120	1.6320790
H	-2.8559397	-0.7338176	3.3657945
H	-3.1773558	-4.8297003	2.0778034
H	-2.8577497	-4.7828290	0.3015184
H	-1.4623093	-2.7287431	0.6076952
H	-2.1893899	-3.1675896	3.5611488
H	-3.9129930	1.5752069	1.8170042
H	-5.0723861	2.8583789	2.2211543
H	-4.8304730	2.4854486	-0.2867702
H	-4.4682906	4.1578819	0.2013397
H	-2.3667480	1.9713119	-0.4910707
H	-2.7501017	3.4318440	-1.4464027
H	-3.1965613	4.4597583	2.7186811
H	-2.9478017	2.9191274	3.6111430
H	-1.4902543	2.0865077	1.7240107
H	-2.1657885	4.8545390	0.5768664
H	4.7582059	3.5800403	-2.2875042
H	5.1105252	2.2638005	-1.1431989
H	5.3315171	1.5466086	-3.5718610
H	4.1555341	0.5666645	-2.6627138
H	3.4707255	2.8092073	-4.6991493
H	3.1693187	1.0356995	-4.8454744
H	2.6431651	1.9147202	-0.7316840
H	3.0551672	3.6358835	-0.4743018
H	2.4557366	4.0954408	-2.9006487
H	1.7423355	1.1084086	-2.7907627
H	-3.8611658	0.9221402	-2.4818534
H	-5.0485240	0.6729576	-3.7836000
H	-4.8032086	-1.3505292	-2.2651046
H	-4.4652910	-1.7237236	-3.9716272
H	-2.7415564	-2.8396676	-2.5636268
H	-2.3304809	-1.3022657	-1.7500151
H	-2.8999135	1.8511670	-4.5255355
H	-3.2064572	0.3388289	-5.4611898
H	-1.4471636	0.5761990	-2.9371185
H	-2.1716332	-1.7636941	-4.7924094

H	5.1054191	-1.9266038	-1.7227094
H	4.7738307	-3.5790567	-2.2939076
H	4.1602620	-2.4100584	0.5055860
H	5.3510234	-3.6723855	0.1093531
H	3.2012490	-4.5484632	1.1892698
H	3.5118018	-5.3023413	-0.4200510
H	3.0484639	-2.0549738	-3.2424881
H	2.6300240	-1.4272661	-1.6234423
H	2.4866931	-4.3974181	-2.4319659
H	1.7484300	-2.8231721	0.1009025
H	0.9822943	5.1768880	-0.9345574
H	-0.6869798	5.0287336	-1.6416748
H	0.9662245	-5.6594183	1.4181619
H	-0.6257125	-5.8567909	0.5830505
H	0.9909976	-3.2471307	-4.3528303
H	-0.6740193	-3.7970459	-3.8701323
H	-0.7376032	-1.3031511	4.8552943
H	0.9324483	-1.9872184	4.6395547
H	0.9567962	4.2078716	3.8628889
H	-0.6419700	3.5936242	4.4432254
H	0.9255106	1.3953121	-5.9059079
H	-0.6737406	2.1945212	-5.6315231
H	-2.8744717	0.9245400	4.9473898
O	-3.8470682	0.8396768	5.1813915
C	-3.9874378	0.5914973	6.4980928
O	-5.0538676	0.4416522	7.0448386
H	-2.9977778	0.5381238	7.0421678

Non-dissociated HCOOH complex with cycHC[6] (b)

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C	1.8269590	1.7032127	3.1297131
C	3.1568122	2.4284679	3.3250777
C	4.2268460	1.6377540	2.5318380
C	4.2485160	0.1221586	2.8413025
C	2.8562358	-0.5496930	2.7487752
C	1.9245432	0.2620192	3.6446836
N	0.6172665	2.1704536	3.8184042
C	-0.1983299	1.0758357	4.0848388
N	0.5039130	-0.0854182	3.8053813
O	-1.3685004	1.1618811	4.5102246
C	0.0442180	-1.4260942	4.1625230
C	-4.0823337	-3.0247100	0.9868014
C	-4.1497901	-1.9724175	2.1176989
C	-2.7809337	-1.3298022	2.4504095
C	-2.9825952	-4.0950387	1.1923156
C	-1.6757884	-3.3523196	1.4637998
C	-1.8072001	-2.4753451	2.7170898
N	-0.3946373	-2.2244829	3.0333118
N	-0.4505382	-4.0992059	1.7641485
C	0.1258338	-5.0904156	0.8655447
C	0.3576023	-3.3321646	2.6092072
O	1.5186400	-3.5838696	2.9363659
C	-4.1029784	2.6181154	1.6636543
C	-4.1105472	3.0541047	0.1794731
C	-2.7141762	3.0016733	-0.4873409
C	-3.0302031	3.3329462	2.5224021
C	-1.6930670	3.1777680	1.7985294
C	-1.7716483	3.8103985	0.4010781

N	-0.3507109	3.9584553	0.0748743
N	-0.4817581	3.8094311	2.3305768
C	0.0647912	3.5125355	3.6433993
C	0.3663044	4.1430477	1.2603928
O	1.5291681	4.5381534	1.3541203
C	4.3770228	2.6317797	-1.8808096
C	4.3549356	1.6098611	-3.0421813
C	3.2713211	1.8957935	-4.1114912
C	2.9884356	2.8652621	-1.2378358
C	2.0325720	3.2265169	-2.3723736
C	1.9439560	2.0674702	-3.3755162
N	0.7274629	2.4211477	-4.1137775
N	0.6129529	3.4891605	-2.1215705
C	0.1317357	4.4936499	-1.1898166
C	-0.1136578	3.1640296	-3.2745864
O	-1.2794690	3.4859708	-3.5098208
C	-4.0282456	0.3662847	-3.5175303
C	-4.0631393	-1.1424697	-3.1761460
C	-2.6831948	-1.7166603	-2.7712843
C	-2.9271140	0.7554885	-4.5347754
C	-1.6099948	0.1787164	-4.0182615
C	-1.7076505	-1.3480077	-3.8868331
N	-0.2908003	-1.7153098	-3.8163701
N	-0.3800785	0.3191546	-4.8039178
C	0.1805755	1.6059166	-5.1907130
C	0.4527428	-0.7792178	-4.5444281
O	1.6251887	-0.9044930	-4.9025064
C	4.3821174	-2.7509672	-1.5874105
C	4.3294305	-3.2504408	-0.1238314
C	3.2384835	-4.3180336	0.1380983
C	3.0048391	-2.3084951	-2.1396316
C	2.0435002	-3.4722791	-1.9081207
C	1.9225199	-3.7638308	-0.4055707
N	0.7047223	-4.5784865	-0.3690702
N	0.6323592	-3.3874021	-2.2926778
C	0.1812677	-3.0786412	-3.6396704
C	-0.1137446	-4.2209261	-1.4511789
O	-1.2763949	-4.5837943	-1.6355405
H	1.6187315	1.6625588	2.0294866
H	3.4115853	2.4672199	4.4091576
H	3.0935066	3.4681690	2.9404414
H	5.2321870	2.0741402	2.7234497
H	4.0289899	1.7835286	1.4443483
H	4.9573436	-0.3898064	2.1533724
H	4.6501902	-0.0371411	3.8699902
H	2.4769562	-0.5366039	1.7007821
H	2.9014934	-1.6146777	3.0606105
H	2.3835345	0.2866610	4.6681376
H	-5.0725345	-3.5202789	0.8780402
H	-3.8862470	-2.5081849	0.0181173
H	-4.5443375	-2.4500622	3.0444738
H	-4.8811581	-1.1784151	1.8475748
H	-2.4132294	-0.7068004	1.6022375
H	-2.8782392	-0.6687551	3.3360105
H	-3.2270453	-4.7583391	2.0532516
H	-2.8919550	-4.7216270	0.2794431
H	-1.4834532	-2.6754741	0.5914236
H	-2.2448834	-3.0982715	3.5410972
H	-3.9167683	1.5200287	1.7187524
H	-5.1095355	2.7825120	2.1084723

H	-4.8244069	2.4204802	-0.3921687
H	-4.4989796	4.0974844	0.1061734
H	-2.3490561	1.9512334	-0.5640111
H	-2.7468862	3.4065320	-1.5214366
H	-3.2715481	4.4141263	2.6436942
H	-2.9876256	2.8726778	3.5321059
H	-1.5036128	2.0803045	1.6650486
H	-2.2146167	4.8366941	0.5096097
H	4.7592537	3.6089019	-2.2592409
H	5.1011058	2.2995971	-1.1036848
H	5.3566923	1.5696920	-3.5246868
H	4.1707924	0.5916528	-2.6265777
H	3.5097588	2.8209838	-4.6852995
H	3.2135160	1.0460441	-4.8249205
H	2.6288939	1.9428443	-0.7252362
H	3.0322970	3.6664650	-0.4682731
H	2.4662891	4.1153984	-2.9045765
H	1.7561045	1.1275806	-2.7935889
H	-3.8557098	0.9463860	-2.5808886
H	-5.0225285	0.6876877	-3.8994553
H	-4.8002959	-1.3252915	-2.3626152
H	-4.4364113	-1.7097991	-4.0612132
H	-2.7344070	-2.8163299	-2.6199397
H	-2.3362034	-1.2747436	-1.8090405
H	-2.8631283	1.8614179	-4.6159586
H	-3.1528160	0.3415935	-5.5447903
H	-1.4368547	0.5982391	-2.9927198
H	-2.1287447	-1.7531529	-4.8459829
H	5.1082740	-1.9116034	-1.6702585
H	4.7784268	-3.5654351	-2.2384806
H	4.1330557	-2.3824512	0.5481017
H	5.3246550	-3.6501934	0.1722922
H	3.1583433	-4.5148606	1.2283074
H	3.4869943	-5.2764772	-0.3739371
H	3.0705557	-2.0403647	-3.2158990
H	2.6335320	-1.4036608	-1.6051870
H	2.4894336	-4.3767924	-2.4025723
H	1.7259437	-2.7892870	0.1146651
H	0.9595417	5.1981244	-0.9585509
H	-0.6997645	5.0396785	-1.6865805
H	0.9166257	-5.6214514	1.4314315
H	-0.6679089	-5.8087526	0.5801749
H	1.0257998	-3.2337955	-4.3459513
H	-0.6462050	-3.7801793	-3.8837166
H	-0.7866132	-1.3349141	4.8934172
H	0.8902361	-1.9647684	4.6407666
H	0.8720886	4.2469308	3.8351318
H	-0.7333348	3.6360421	4.4018956
H	0.9883680	1.4023836	-5.9212003
H	-0.6148074	2.2036238	-5.6782850
H	-2.2581884	0.1544111	5.4017449
O	-2.7797047	-0.5433908	5.9299208
C	-3.5559834	0.0236216	6.8709354
O	-4.2642599	-0.5975131	7.6274256
H	-3.4776777	1.1518119	6.8819466

I- on the opening of cycHC[6]

I	0.0526217	0.0063145	6.6442038
C	0.6675737	3.6731284	-1.7895788
C	0.2040339	4.2561227	-3.1241812
C	0.3203025	3.1353544	-4.1858880
C	1.7007992	2.4370927	-4.2157100
C	2.1821682	1.9614640	-2.8235717
C	2.1154789	3.1742111	-1.8979306
N	0.7465956	4.5283340	-0.6051013
C	1.7808030	4.0617283	0.2256152
N	2.4898198	3.0845306	-0.4873266
O	2.0318571	4.4564949	1.3625831
C	3.7850956	2.6067834	-0.0267660
C	3.3182932	-0.7757704	4.2042361
C	3.1858418	0.7620069	4.2439255
C	2.8131587	1.3780700	2.8734272
C	4.2247233	-1.3142614	3.0694062
C	3.7538215	-0.6713486	1.7666169
C	3.8331367	0.8581370	1.8643798
N	3.7886492	1.2332031	0.4413378
N	4.4883552	-0.9134984	0.5147443
C	4.7129185	-2.2364615	-0.0426077
C	4.3790711	0.2127999	-0.3084432
O	4.7532796	0.2956352	-1.4840264
C	-0.9074694	3.2667186	4.2249582
C	-2.1712920	2.3832193	4.2888794
C	-2.5396031	1.7473049	2.9264788
C	-0.9142309	4.3176377	3.0873762
C	-1.2571671	3.5855255	1.7918368
C	-2.6187594	2.8877669	1.9152226
N	-2.9464935	2.6580304	0.4982734
N	-1.4381863	4.3397649	0.5420086
C	-0.4181070	5.1980291	-0.0349000
C	-2.3727452	3.6795117	-0.2631268
O	-2.6531893	3.9609004	-1.4341804
C	-3.0258768	0.2599823	-4.1591413
C	-2.9423289	-1.2846462	-4.1351608
C	-3.8410712	-1.9469780	-3.0621942
C	-2.8316730	0.9092243	-2.7681209
C	-3.8351845	0.2444710	-1.8282371
C	-3.5459247	-1.2595912	-1.7300365
N	-4.3081056	-1.6211198	-0.5339965
N	-3.9195945	0.6089310	-0.4145535
C	-4.1434536	1.9684294	0.0540743
C	-4.4014109	-0.4951508	0.3033302
O	-4.8462286	-0.4783068	1.4493262
C	-2.3153656	-2.4618063	4.2656066
C	-0.9142422	-3.1095750	4.3005775
C	-0.2015200	-3.0971218	2.9259344
C	-3.2384501	-2.9843274	3.1369007
C	-2.4531614	-2.9011049	1.8296773
C	-1.1644093	-3.7295843	1.9248449
N	-0.8243948	-3.8856536	0.5006579
N	-3.0347314	-3.4254495	0.5841254
C	-4.2976839	-2.9668456	0.0304594
C	-2.0079959	-3.8958828	-0.2419113
O	-2.1297820	-4.2705856	-1.4139786
C	1.2282034	-2.7414527	-4.1887945
C	2.5230859	-1.8941192	-4.1790826
C	3.5607456	-2.3420596	-3.1204664
C	0.5862760	-2.9015489	-2.7895662

C	1.6767027	-3.4390511	-1.8649606
C	2.8346377	-2.4348425	-1.7790071
N	3.5444640	-2.9158875	-0.5932461
N	1.4216989	-3.6981606	-0.4486685
C	0.3638052	-4.5745737	0.0313179
C	2.6278175	-3.5636940	0.2540565
O	2.8515249	-3.9614262	1.3956457
H	0.0180629	2.7876316	-1.5624886
H	0.8414980	5.1300540	-3.3956561
H	-0.8504222	4.5980426	-3.0510876
H	0.0846178	3.5451417	-5.1940522
H	-0.4642442	2.3740120	-3.9701546
H	1.6682032	1.5744058	-4.9188891
H	2.4597778	3.1432601	-4.6290677
H	1.5227462	1.1535579	-2.4301857
H	3.2098697	1.5417392	-2.8711529
H	2.7277885	3.9881834	-2.3754015
H	3.6819273	-1.1400231	5.1894205
H	2.2976280	-1.2093318	4.0961343
H	4.1480354	1.2150515	4.5862479
H	2.4086147	1.0159229	5.0020143
H	1.7865251	1.0664714	2.5743237
H	2.8152890	2.4886859	2.9213754
H	5.2947044	-1.0518417	3.2479092
H	4.1432793	-2.4214245	3.0089766
H	2.6795915	-0.9498317	1.6166036
H	4.8524465	1.1251805	2.2544000
H	-0.0239474	2.5996993	4.1018347
H	-0.7572788	3.7673570	5.2062414
H	-1.9906073	1.5854944	5.0466002
H	-3.0396257	2.9911652	4.6425058
H	-1.7605351	1.0134662	2.6172281
H	-3.5005729	1.1920098	2.9919568
H	-1.6742792	5.1122181	3.2771053
H	0.0842348	4.8011804	3.0092961
H	-0.4802543	2.7955538	1.6298748
H	-3.3534467	3.6376132	2.3166494
H	-4.0229609	0.5672820	-4.5558708
H	-2.2732977	0.6639841	-4.8732426
H	-3.1949136	-1.6904458	-5.1407874
H	-1.8875543	-1.5856933	-3.9352815
H	-4.9200336	-1.8282181	-3.3168328
H	-3.6113326	-3.0317298	-2.9960399
H	-1.7964591	0.7376935	-2.3916856
H	-2.9801797	2.0097952	-2.8090991
H	-4.8536518	0.3728703	-2.2879461
H	-2.4518559	-1.3823651	-1.5208419
H	-2.1849095	-1.3613519	4.1532153
H	-2.8083223	-2.5943657	5.2534136
H	-0.3032802	-2.5571749	5.0520506
H	-0.9964008	-4.1685309	4.6474430
H	0.7619384	-3.6494368	2.9713372
H	0.0371221	-2.0522939	2.6210389
H	-4.1581296	-2.3627708	3.0789296
H	-3.5415029	-4.0424404	3.3205908
H	-2.1623635	-1.8305397	1.6730284
H	-1.4373127	-4.7448294	2.3218786
H	0.4924429	-2.2916249	-4.8929373
H	1.4577238	-3.7573933	-4.5899917
H	2.2573111	-0.8311917	-3.9730212

H	2.9875884	-1.9057611	-5.1908832
H	4.3857079	-1.5997855	-3.0631922
H	3.9957877	-3.3345098	-3.3831510
H	-0.2927576	-3.5811237	-2.8211665
H	0.2214686	-1.9209077	-2.4065419
H	2.0705349	-4.3829577	-2.3318032
H	2.3949039	-1.4266084	-1.5615796
H	-4.5895252	2.5643889	-0.7727936
H	-4.8574317	1.9043933	0.9041810
H	5.4664024	-2.1284617	-0.8488740
H	5.1144310	-2.8908482	0.7567537
H	0.0574222	-5.2525746	-0.7958861
H	0.7885988	-5.1680804	0.8702804
H	4.0987938	3.2716985	0.8074156
H	4.5139189	2.6802808	-0.8646290
H	-0.9042173	5.7934406	-0.8340829
H	-0.0404969	5.8764084	0.7564157
H	-4.5849952	-3.6817614	-0.7667069
H	-5.0599028	-2.9814886	0.8353559

Transition state of forming of I- and cycHC[6] inclusion complex

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I	0.0116717	-0.0372544	2.5652001
C	-1.7357415	3.2299948	-1.7682305
C	-2.4883765	3.3944195	-3.0894678
C	-1.6599581	2.6817757	-4.1856689
C	-0.1726419	3.1044989	-4.2222302
C	0.5200411	3.0374629	-2.8404416
C	-0.3371345	3.8544870	-1.8764260
N	-2.2398502	3.8698337	-0.5547187
C	-1.1581718	4.2202212	0.2695019
N	0.0210738	4.0125542	-0.4667222
O	-1.2333542	4.6711885	1.4110465
C	1.2923283	4.5815603	-0.0286815
C	3.2296833	1.9135521	4.2804337
C	2.3698057	3.1973449	4.3294785
C	1.6001985	3.4614508	3.0124871
C	4.1902897	1.8582579	3.0673261
C	3.3477023	2.0928338	1.8171741
C	2.6323908	3.4496068	1.8925120
N	2.2472661	3.6217980	0.4825189
N	4.0082382	2.2156744	0.5047480
C	4.9694453	1.2732718	-0.0391356
C	3.2384676	3.0478136	-0.3128540
O	3.4223883	3.2604203	-1.5184131
C	-3.3068083	1.7765343	4.2662693
C	-3.9886877	0.3886524	4.2878296
C	-3.8242232	-0.3897247	2.9599077
C	-3.7270834	2.6548044	3.0621043
C	-3.4985348	1.8263796	1.8014247
C	-4.3192870	0.5289219	1.8499844
N	-4.2666043	0.1307277	0.4340088
N	-3.9233150	2.3570517	0.4928374
C	-3.5840922	3.6690447	-0.0291263
C	-4.2550796	1.2875669	-0.3443218
O	-4.5200034	1.3599972	-1.5511316
C	-2.5470517	-1.6289151	-4.2712312
C	-1.4447281	-2.7135644	-4.2412007

C	-1.6672687	-3.8058549	-3.1670889
C	-2.8507351	-1.0201845	-2.8819758
C	-3.1475747	-2.1877514	-1.9437915
C	-1.9130330	-3.0939303	-1.8364530
N	-2.2318285	-3.8699855	-0.6397102
N	-3.4811309	-1.9808956	-0.5344487
C	-4.6137573	-1.1700968	-0.0975501
C	-3.0824760	-3.1188752	0.1877455
O	-3.4482709	-3.4261829	1.3209287
C	0.0708003	-3.8479581	4.2144724
C	1.6140065	-3.7561675	4.2534330
C	2.2198784	-3.1897264	2.9461999
C	-0.4717711	-4.6182301	2.9856631
C	0.1460074	-3.9782695	1.7464255
C	1.6789824	-4.0446259	1.8073184
N	2.0096385	-3.7615979	0.4008671
N	-0.0899877	-4.5794493	0.4210082
C	-1.3889644	-4.9388840	-0.1189084
C	1.0093197	-4.3123895	-0.3998343
O	1.0908690	-4.5506136	-1.6116192
C	2.7390290	-1.3160571	-4.2657492
C	3.1225670	0.1813907	-4.2045439
C	4.1625923	0.5187459	-3.1088307
C	2.3435309	-1.9077948	-2.8917589
C	3.4872750	-1.5943329	-1.9295576
C	3.6504960	-0.0734464	-1.7950867
N	4.4646131	0.0194155	-0.5846420
N	3.4530080	-2.0088845	-0.5267970
C	3.3146212	-3.4021817	-0.1127500
C	4.2276993	-1.1057413	0.2217499
O	4.6611012	-1.2875158	1.3579455
H	-1.6097787	2.1328319	-1.5800863
H	-2.6069587	4.4787018	-3.3239452
H	-3.4962882	2.9339930	-3.0166163
H	-2.1262218	2.8532156	-5.1826842
H	-1.7177091	1.5838285	-4.0021639
H	0.3791863	2.4698877	-4.9518702
H	-0.0993057	4.1509250	-4.6056223
H	0.5868986	1.9857670	-2.4790071
H	1.5606422	3.4207761	-2.8879399
H	-0.4522292	4.8796955	-2.3274623
H	3.8113081	1.8106852	5.2253075
H	2.5433038	1.0375874	4.2188960
H	3.0248191	4.0754426	4.5547964
H	1.6430461	3.1198966	5.1689716
H	0.8447805	2.6618635	2.8399001
H	1.0594395	4.4318025	3.0628259
H	4.9855319	2.6394431	3.1474820
H	4.6837441	0.8621322	3.0223795
H	2.5609438	1.2957897	1.7704122
H	3.4092808	4.2294380	2.1319861
H	-2.2051787	1.6202614	4.2138387
H	-3.5185584	2.3173735	5.2173669
H	-3.5644683	-0.2153912	5.1209158
H	-5.0782969	0.5131034	4.5077923
H	-2.7534849	-0.6442619	2.7899749
H	-4.3969630	-1.3417913	2.9913267
H	-4.8015973	2.9518825	3.1362410
H	-3.1106738	3.5800244	3.0365480
H	-2.4157197	1.5431321	1.7603112

H	-5.3847269	0.8104608	2.0853688
H	-3.4875785	-2.0742956	-4.6757087
H	-2.2585778	-0.8219988	-4.9823648
H	-1.3521437	-3.1851239	-5.2459895
H	-0.4638580	-2.2251778	-4.0368921
H	-2.5471269	-4.4418293	-3.4227205
H	-0.7683583	-4.4541795	-3.0951645
H	-1.9757638	-0.4470929	-2.4983919
H	-3.6999021	-0.3058917	-2.9279399
H	-3.9754907	-2.7872528	-2.4166590
H	-1.0252637	-2.4443416	-1.6265847
H	-0.3387225	-2.8119753	4.1829628
H	-0.3043221	-4.3215728	5.1507166
H	1.9214785	-3.1130840	5.1080035
H	2.0421018	-4.7712296	4.4485577
H	3.3307251	-3.2151105	2.9872479
H	1.9111061	-2.1294847	2.8039534
H	-1.5811482	-4.5416167	2.9510251
H	-0.1980526	-5.7004663	3.0367814
H	-0.1471722	-2.8969835	1.7276252
H	1.9627330	-5.1149732	2.0158088
H	1.9070768	-1.4600251	-4.9919000
H	3.6028798	-1.8987508	-4.6670176
H	2.2042176	0.7805095	-4.0042550
H	3.4983678	0.5160156	-5.1980236
H	4.2716686	1.6200138	-3.0164058
H	5.1581348	0.0810411	-3.3581580
H	2.1523084	-2.9993504	-2.9587934
H	1.4032442	-1.4455896	-2.5148314
H	4.4284700	-2.0013851	-2.3940864
H	2.6396991	0.3659504	-1.5930953
H	-5.2917400	-1.0227905	-0.9684852
H	-5.1391686	-1.7417797	0.6962500
H	5.5161671	1.8009779	-0.8478782
H	5.6788462	0.9984962	0.7673915
H	3.5366185	-4.0481508	-0.9924232
H	4.0646265	-3.5845345	0.6858047
H	1.0660283	5.3108230	0.7774101
H	1.7533287	5.1067758	-0.8954466
H	-4.3055776	3.8881548	-0.8436189
H	-3.7130955	4.4101810	0.7858592
H	-1.2079460	-5.6615133	-0.9413275
H	-1.9730840	-5.4320574	0.6840672

HCOO- on the opening of cycHC[6]

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C	0.6978865	3.6986244	-1.7216805
C	0.2164676	4.2716859	-3.0545387
C	0.3277823	3.1459831	-4.1113340
C	1.7116169	2.4549982	-4.1512655
C	2.2109983	1.9918257	-2.7613813
C	2.1482259	3.2107691	-1.8433223
N	0.7824620	4.5613259	-0.5437629
C	1.8306585	4.1111453	0.2781163
N	2.5423098	3.1369168	-0.4368735
O	2.0927481	4.5203065	1.4078305
C	3.8521414	2.6815403	0.0075758
C	3.6322455	-0.5837935	4.3379725

C	3.6204791	0.9612959	4.3548059
C	3.1205932	1.5560384	3.0155645
C	4.4165641	-1.1921246	3.1501434
C	3.8747072	-0.5527145	1.8735230
C	4.0246233	0.9732749	1.9345502
N	3.8811902	1.3216752	0.5106911
N	4.5255354	-0.8405640	0.5844789
C	4.7135369	-2.1772338	0.0481543
C	4.4045894	0.2739973	-0.2508156
O	4.7250239	0.3288782	-1.4444325
C	-0.9419562	3.3958709	4.3261165
C	-2.2392139	2.5591843	4.3973804
C	-2.5670630	1.8656527	3.0528652
C	-0.9020539	4.4094787	3.1551811
C	-1.2364943	3.6441361	1.8762447
C	-2.6096213	2.9707017	2.0030317
N	-2.9247849	2.7098933	0.5871116
N	-1.4010986	4.3769183	0.6104924
C	-0.3815934	5.2304296	0.0288526
C	-2.3413395	3.7144097	-0.1866139
O	-2.6185262	3.9870547	-1.3615269
C	-3.0194029	0.3108486	-4.0629368
C	-2.9451291	-1.2342382	-4.0418838
C	-3.8454676	-1.8921149	-2.9677247
C	-2.8191799	0.9564430	-2.6712188
C	-3.8252161	0.2964364	-1.7303896
C	-3.5424971	-1.2086936	-1.6351590
N	-4.3034434	-1.5689549	-0.4385045
N	-3.9060809	0.6593578	-0.3167678
C	-4.1242173	2.0196006	0.1508223
C	-4.3904809	-0.4443399	0.4018244
O	-4.8362818	-0.4290645	1.5467434
C	-2.5058017	-2.8355308	4.4844938
C	-1.1135276	-3.5073180	4.5023865
C	-0.3295016	-3.3044493	3.1803751
C	-3.3699972	-3.1859608	3.2484965
C	-2.5189600	-2.9702443	1.9983047
C	-1.2435537	-3.8211059	2.0746530
N	-0.8390189	-3.8529462	0.6564486
N	-3.0481106	-3.3854786	0.6871884
C	-4.3003395	-2.9166780	0.1211561
C	-1.9977829	-3.8191143	-0.1237009
O	-2.0845628	-4.1400438	-1.3161104
C	1.2181254	-2.7447541	-4.0726059
C	2.5182624	-1.9058264	-4.0828431
C	3.5505847	-2.3356914	-3.0120266
C	0.5747924	-2.8681678	-2.6705629
C	1.6598975	-3.3923611	-1.7318870
C	2.8220018	-2.3917466	-1.6695281
N	3.5292650	-2.8482372	-0.4740251
N	1.4037055	-3.6215873	-0.3094965
C	0.3616527	-4.5147298	0.1807303
C	2.6112491	-3.4730919	0.3894994
O	2.8395323	-3.8491701	1.5373758
H	0.0572140	2.8101539	-1.4827007
H	0.8461202	5.1478439	-3.3376436
H	-0.8392233	4.6072152	-2.9709632
H	0.0790583	3.5487124	-5.1193766
H	-0.4500969	2.3817511	-3.8828194
H	1.6759599	1.5868351	-4.8476061

H	2.4621150	3.1624451	-4.5782505
H	1.5604584	1.1835511	-2.3546308
H	3.2393444	1.5756083	-2.8168051
H	2.7476251	4.0258679	-2.3357427
H	4.0412411	-0.9749416	5.2970488
H	2.5721709	-0.9149484	4.2672106
H	4.6445856	1.3513796	4.5787807
H	2.9546210	1.3040671	5.1765401
H	2.0616872	1.2430284	2.8707133
H	3.1613088	2.6669510	3.0286638
H	5.5112601	-0.9884581	3.2373384
H	4.2672665	-2.2939944	3.1243808
H	2.7848482	-0.7906511	1.8043840
H	5.0880578	1.1979398	2.2261432
H	-0.0866641	2.6933632	4.2099403
H	-0.7824311	3.9340617	5.2881825
H	-2.1201308	1.7710104	5.1715382
H	-3.0942179	3.2171622	4.6920633
H	-1.7753996	1.1146189	2.8304458
H	-3.5345853	1.3218124	3.1162532
H	-1.6474310	5.2266858	3.3054545
H	0.1088071	4.8679592	3.0814971
H	-0.4687708	2.8417339	1.7422458
H	-3.3360058	3.7495742	2.3654773
H	-4.0155134	0.6246292	-4.4574930
H	-2.2655774	0.7115839	-4.7777761
H	-3.2020291	-1.6369507	-5.0478875
H	-1.8920289	-1.5420870	-3.8437353
H	-4.9244541	-1.7663785	-3.2197979
H	-3.6210701	-2.9779543	-2.9034450
H	-1.7848067	0.7773294	-2.2962987
H	-2.9604081	2.0579725	-2.7097694
H	-4.8437242	0.4311033	-2.1894801
H	-2.4491161	-1.3371889	-1.4300353
H	-2.3343877	-1.7351997	4.5438008
H	-3.0629181	-3.1082341	5.4100592
H	-0.5328341	-3.0742188	5.3449092
H	-1.2143604	-4.6040732	4.6999550
H	0.6352070	-3.8571166	3.2033013
H	-0.1002363	-2.2217801	3.0455099
H	-4.2694783	-2.5324549	3.2230011
H	-3.7136107	-4.2484404	3.2778070
H	-2.2191548	-1.8943980	1.9600788
H	-1.5512550	-4.8672087	2.3531591
H	0.4850485	-2.3069337	-4.7872356
H	1.4417189	-3.7711825	-4.4502362
H	2.2595415	-0.8365782	-3.9021392
H	2.9842562	-1.9446226	-5.0935602
H	4.3801081	-1.5975565	-2.9706045
H	3.9789163	-3.3373472	-3.2504542
H	-0.3098630	-3.5399448	-2.6848164
H	0.2175443	-1.8764464	-2.3099277
H	2.0494441	-4.3482899	-2.1784305
H	2.3879578	-1.3764364	-1.4769642
H	-4.5778151	2.6135545	-0.6739563
H	-4.8306550	1.9569648	1.0071541
H	5.4573616	-2.1006216	-0.7711655
H	5.1157352	-2.8225298	0.8547185
H	0.0742755	-5.2040381	-0.6448340
H	0.8003838	-5.0931326	1.0223040

H	4.1778727	3.3679643	0.8187563
H	4.5592532	2.7450288	-0.8498366
H	-0.8687020	5.8243965	-0.7711659
H	-0.0005077	5.9109789	0.8169120
H	-4.5857945	-3.6233836	-0.6845221
H	-5.0699291	-2.9337204	0.9189283
O	0.3054912	-0.0480835	3.7511028
O	-1.0830619	-0.2111188	5.5601508
C	0.0177137	-0.0212739	4.9881660
H	0.9036720	0.2117112	5.6918470

Transition state of forming of HCOO⁻ and cycHC[6] inclusion complex

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C	3.7642252	0.1630062	-1.7283416
C	4.3029806	0.6652004	-3.0678892
C	3.3770799	0.1073424	-4.1758621
C	3.1482975	-1.4202935	-4.0907980
C	2.7203524	-1.9027476	-2.6842367
C	3.7584942	-1.3714233	-1.6992738
N	4.4793868	0.4682759	-0.4905519
C	4.2865217	-0.5799057	0.4240196
N	3.6603059	-1.6325056	-0.2627994
O	4.6340547	-0.5845813	1.6035243
C	3.6219453	-2.9780659	0.3004454
C	0.0983862	-3.4663199	4.3988855
C	1.5907481	-3.0816021	4.5218497
C	2.1664982	-2.5260506	3.1963065
C	-0.1942058	-4.4421511	3.2329943
C	0.3981575	-3.8228529	1.9691702
C	1.9062583	-3.5930933	2.1408643
N	2.3142645	-3.4212810	0.7366345
N	0.3896764	-4.5951305	0.7131810
C	-0.7960056	-5.1790634	0.1117567
C	1.5004506	-4.2338655	-0.0541284
O	1.7318298	-4.5908690	-1.2162948
C	2.7945254	2.7238518	4.1244528
C	1.7287148	3.8348062	3.9898221
C	0.9887810	3.8048359	2.6306738
C	3.7907513	2.6483531	2.9420443
C	2.9729562	2.5907810	1.6548259
C	2.0576745	3.8185573	1.5467994
N	1.7241598	3.7790311	0.1121192
N	3.6640908	2.6581288	0.3562842
C	4.7805080	1.8227068	-0.0462102
C	2.8298210	3.2802647	-0.5760388
O	3.0493159	3.3924979	-1.7885164
C	-0.3838863	2.6983831	-4.6698225
C	-1.8263527	2.1394684	-4.6579905
C	-2.7687696	2.8522628	-3.6580755
C	0.2461881	2.8087593	-3.2606856
C	-0.7273764	3.6138660	-2.4023498
C	-2.0670404	2.8694972	-2.3000595
N	-2.6881827	3.5509996	-1.1658081
N	-0.4551480	3.9061332	-0.9952734
C	0.7334785	4.6141801	-0.5371907
C	-1.6826801	4.0608268	-0.3285045
O	-1.8495789	4.5797979	0.7722610
C	-3.6384570	1.7554533	3.8328321

C	-4.0105306	0.2577624	3.9450471
C	-3.5924529	-0.5575444	2.6951885
C	-4.1374547	2.4328899	2.5334619
C	-3.6768330	1.5713560	1.3607237
C	-4.2279490	0.1467326	1.5041558
N	-4.0718056	-0.3498652	0.1250306
N	-4.1341110	1.8993257	-0.0030201
C	-4.0014895	3.1963810	-0.6379051
C	-4.2562832	0.7236317	-0.7462774
O	-4.5083972	0.6497760	-1.9566433
C	-1.9889787	-2.2478836	-4.3069120
C	-0.8115893	-3.2402973	-4.1568635
C	-1.0081461	-4.2875705	-3.0335630
C	-2.4171595	-1.5911770	-2.9731788
C	-2.6810776	-2.7292446	-1.9896053
C	-1.3920576	-3.5306337	-1.7622732
N	-1.7256943	-4.2699858	-0.5462112
N	-3.1097311	-2.4763228	-0.6151212
C	-4.3101470	-1.7188823	-0.2841037
C	-2.6769326	-3.5408007	0.1900255
O	-3.0790541	-3.8114597	1.3197197
H	2.7038792	0.5133499	-1.6377257
H	5.3518523	0.3128164	-3.2101282
H	4.2953193	1.7753479	-3.0929302
H	3.7847057	0.3727296	-5.1776517
H	2.3935542	0.6255775	-4.0955001
H	2.3864224	-1.7269758	-4.8425401
H	4.0910741	-1.9473532	-4.3740215
H	1.7157553	-1.5035324	-2.4155328
H	2.6433088	-3.0094970	-2.6389389
H	4.7649019	-1.7281310	-2.0543921
H	-0.2654702	-3.9030107	5.3567353
H	-0.4756689	-2.5313613	4.2133655
H	2.1869985	-3.9724206	4.8424509
H	1.7064959	-2.3154530	5.3203472
H	1.6264943	-1.5918556	2.9253584
H	3.2492197	-2.2956799	3.2967173
H	0.2638334	-5.4443413	3.4177919
H	-1.2924555	-4.5756419	3.1201173
H	-0.0836763	-2.8256824	1.8146703
H	2.3580702	-4.5572347	2.5074873
H	2.2605975	1.7519148	4.2029374
H	3.3584353	2.8535169	5.0764337
H	0.9784890	3.7015289	4.7972808
H	2.2092159	4.8351314	4.1296450
H	0.3558841	2.8925478	2.5845382
H	0.3067903	4.6782344	2.5405518
H	4.4588108	3.5430495	2.9208155
H	4.4276844	1.7417186	3.0404254
H	2.3280040	1.6769959	1.6885850
H	2.7014708	4.7261693	1.7181804
H	-0.3888030	3.7129631	-5.1356927
H	0.2585729	2.0634122	-5.3208653
H	-2.2581536	2.1873090	-5.6835962
H	-1.7918358	1.0587580	-4.3873685
H	-2.9815973	3.8969986	-3.9854196
H	-3.7295743	2.2999024	-3.5869030
H	0.3937604	1.7995115	-2.8119646
H	1.2482614	3.2847583	-3.2987165
H	-0.9117481	4.5873950	-2.9375747

H	-1.8479979	1.8072253	-2.0184295
H	-2.5245082	1.8228644	3.8720462
H	-4.0345319	2.3099645	4.7146912
H	-3.5113378	-0.1687626	4.8431441
H	-5.1125915	0.1440306	4.1057230
H	-3.9407504	-1.6106928	2.7782826
H	-2.4802098	-0.5688222	2.5988155
H	-3.7067644	3.4555647	2.4565261
H	-5.2512101	2.5215379	2.5154919
H	-2.5603635	1.5148494	1.3848584
H	-5.3328185	0.2318985	1.7033626
H	-1.7213840	-1.4607670	-5.0471827
H	-2.8692075	-2.7854559	-4.7344234
H	0.1162016	-2.6658296	-3.9318922
H	-0.6282888	-3.7567990	-5.1264672
H	-0.0648217	-4.8531563	-2.8759498
H	-1.8153293	-5.0094454	-3.2986618
H	-3.3146076	-0.9497992	-3.1042626
H	-1.6100667	-0.9330158	-2.5765506
H	-3.4339749	-3.4131042	-2.4732064
H	-0.5717102	-2.8021870	-1.5380219
H	1.2080741	5.1037449	-1.4168021
H	0.3995321	5.3838247	0.1911085
H	-0.4496286	-5.9204447	-0.6373019
H	-1.3709477	-5.6959365	0.9062387
H	-4.9740973	-1.7029386	-1.1780235
H	-4.8104521	-2.2554186	0.5500115
H	4.3040864	-2.9842466	1.1770362
H	3.9921380	-3.6892887	-0.4721976
H	5.2979293	2.3462989	-0.8760530
H	5.4691200	1.7259034	0.8172426
H	-4.7264795	3.2280290	-1.4773461
H	-4.2611812	3.9753292	0.1065654
O	-0.3529951	-0.4377104	2.8318047
O	-0.4628224	1.4335134	4.1409671
C	-0.0114667	0.3134653	3.7906604
H	0.8557213	-0.0854267	4.4416468

3. Collision Cross Section (CCS) Values of Computed Geometries

3.1 Anion@cycHC[6] complexes CCS values

#	Br@cycHC[6]	Cl@cycHC[6]	HCOO@cycHC[6]	I@cycHC[6]
1	186.1492	184.7408	187.347261	189.056
2	185.8304	184.7408	187.129941	189.056
3	185.8304	184.7408	187.129941	189.056
4	185.8304	184.8386	187.129941	187.615
5	186.1513	184.8386	187.126811	187.615
6	186.1513	185.1268	187.126811	187.615
7	186.1513	185.1268	187.39969	188.106
8	185.8879	185.1268	187.39969	188.106
9	185.8879	185.11	187.39969	188.598
10	185.655	185.11	187.870473	188.598
11	185.655	185.11	187.870473	188.598
12	185.655	185.913	187.870473	187.784
13	185.9726	185.913	186.740358	187.784
14	185.9726	185.913	186.740358	187.784
15	185.9726	185.2658	187.103887	187.825
16	184.9281	185.2658	187.103887	187.825
17	184.9281	184.6484	187.103887	188.689
18	185.4491	184.6484	186.64851	188.689
19	185.4491	184.6484	186.64851	188.689
20	185.4491	185.6784	186.64851	187.469
21	186.0547	185.6784	187.096018	187.469
22	186.0547	185.6784	187.096018	187.469
23	186.0547	185.1056	186.273905	187.705
24	185.4958	185.1056	186.273905	187.705
25	185.4958	185.2738	186.273905	186.864
26	185.4958	185.2738	187.453073	186.864
27	185.3183	185.2738	187.453073	186.864
28	185.3183	185.0758	187.98773	187.489
29	185.5202	185.0758	187.98773	187.489
30	185.5202	185.0758	187.98773	187.489
31	185.5202	185.2228	187.256754	188.74
32	185.5321	185.2228	187.256754	188.74
33	185.5321	185.2228	187.256754	188.74
34	185.5321	184.6092	186.738846	187.509
35	185.7548	184.6092	186.738846	187.509
36	185.7548	184.9171	186.592033	188.577
37	185.811	184.9171	186.592033	188.577
38	185.811	184.9171	186.592033	188.577
39	185.811	185.2311	187.461233	187.793

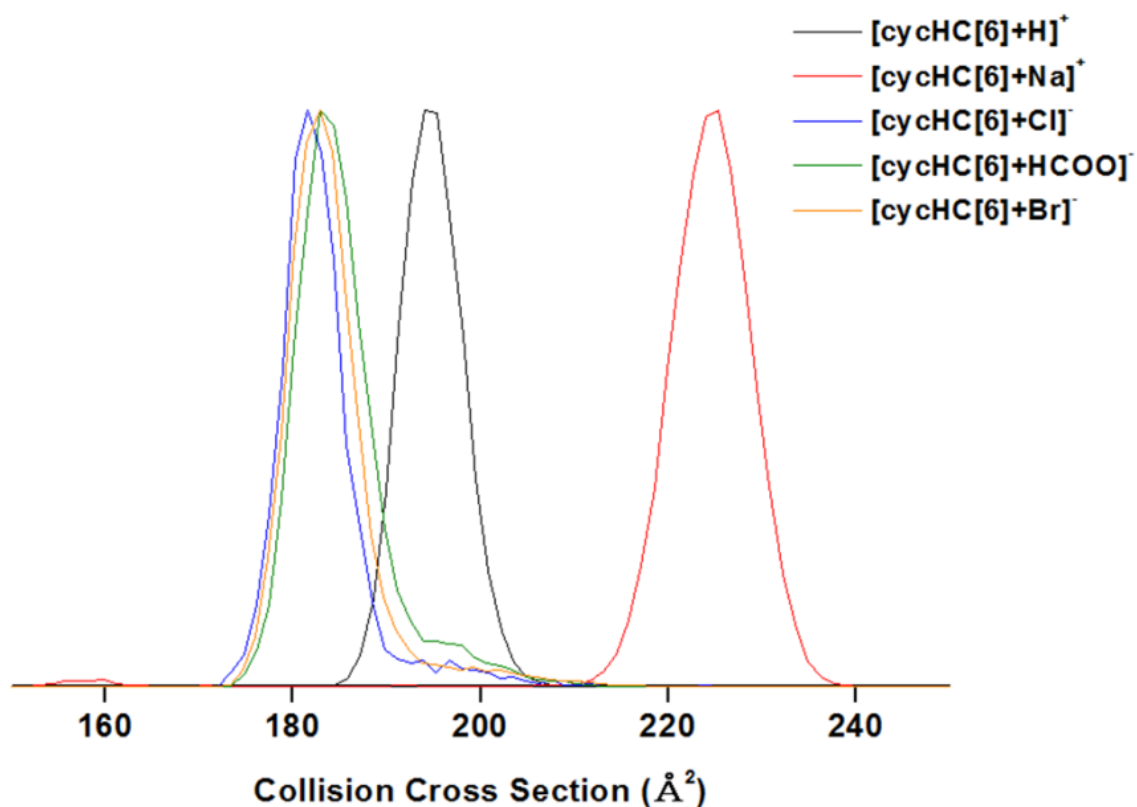
40	185.9879	185.2311	187.461233	187.793
41	185.9879	185.2311	187.461233	187.793
42	185.9879	184.8017	185.785629	188.269
43	185.5074	184.8017	185.785629	188.269
44	185.5074	184.9367	186.896476	188.141
45	186.4173	184.9367	186.896476	188.141
46	186.4173	184.9367	186.896476	188.141
47	186.4173	186.0009	186.790778	187.874
48	185.8517	186.0009	186.790778	187.874
49	185.8517	186.0009	186.790778	187.874
50	185.8517	185.7425	187.655851	188.069
Average	185.7626	185.1722	187.0623762	188.019

3.2 Protonated cycHC[6] CCS values

#	I	II	III	IV	V
1	195.3406	196.3798	190.7251	191.0945	202.8555
2	195.8562	196.6523	190.7251	191.0945	201.1847
3	195.8562	196.6523	190.7251	192.3648	201.1847
4	195.8562	196.6523	191.1684	192.3648	202.1472
5	196.5707	196.7405	191.1684	193.0691	202.1472
6	196.5707	196.7405	191.1684	193.0691	203.499
7	196.9409	196.0963	193.1016	193.0691	203.499
8	197.4769	196.0963	193.1016	192.7643	203.499
9	197.4769	197.4632	192.5144	192.7643	201.7679
10	197.4769	197.4632	192.5144	192.5683	201.7679
11	196.7879	197.2234	190.9652	192.5683	202.7387
12	196.7879	197.2234	190.9652	192.5683	202.7387
13	197.1287	197.2234	190.9652	194.2455	203.5634
14	197.1287	197.4359	191.8247	194.2455	203.5634
15	197.1287	197.4359	191.8247	193.5929	203.5634
16	196.8005	197.4359	191.8247	193.5929	201.1255
17	196.8005	195.9173	192.5422	193.5929	201.1255
18	197.6383	195.9173	192.5422	192.7392	202.038
19	197.6383	197.1715	191.866	192.7392	202.038
20	196.479	197.1715	191.866	192.7392	202.8721
21	196.479	197.1715	191.866	192.6291	202.8721
22	196.479	196.4357	190.9223	192.6291	202.749
23	197.358	196.4357	190.9223	193.1151	202.749
24	197.358	196.966	191.4637	193.1151	202.5654
25	196.6023	196.966	191.4637	193.1151	202.5654
26	196.6023	196.966	191.4637	193.3659	202.5654
27	196.565	195.6373	192.0929	193.3659	204.2827

28	196.565	195.6373	192.0929	193.2886	204.2827
29	197.0967	198.3219	190.9858	193.2886	203.0013
30	197.0967	198.3219	190.9858	193.2886	203.0013
31	196.7788	198.3219	190.9858	193.2745	203.143
32	196.7788	197.4209	191.5986	193.2745	203.143
33	197.5667	197.4209	191.5986	193.2745	202.5795
34	197.5667	196.6317	191.5986	193.4398	202.5795
35	196.7011	196.6317	190.9488	193.4398	202.5716
36	196.7011	195.4229	190.9488	192.8838	202.5716
37	196.1155	195.4229	192.5395	192.8838	203.141
38	196.1155	195.539	192.5395	192.8838	203.141
39	196.1155	195.539	192.5395	192.7657	203.0205
40	196.8213	194.7389	192.6581	192.7657	203.0205
41	196.8213	194.7389	192.6581	192.7657	203.0205
42	196.1282	196.3695	191.8192	193.6001	202.2142
43	196.1282	196.3695	191.8192	193.6001	202.2142
44	195.3392	196.3695	191.8192	191.5816	203.1286
45	195.3392	195.6157	190.085	191.5816	203.1286
46	195.3392	195.6157	190.085	191.5816	202.0786
47	196.4425	197.3961	190.085	191.4896	202.2285
48	196.4425	197.3961	190.796	191.4896	202.2285
49	196.861	196.8921	190.796	190.7104	203.6385
50	196.861	196.8921	193.082	190.7104	203.6385
Average	196.6581	196.6539	191.5872	192.7609	202.7197

4. Ion-Mobility Mass-spectra of studied cycHC[6] complexes



4.1. Detailed MS spectra of cycHC[6] complexes

