

DFT Prediction of Multi-topic N-Heterocyclic Carbenes Using Clar's Aromatic Sextet Theory

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HOMA calculation

HOMA is calculated using the equation

$$\text{HOMA} = 1 - \alpha/n \sum (R_{\text{opt}} - R_{ij})^2$$

where R_{opt} for CC and CN are 1.388 Å and 1.334 Å, respectively. α value is 257.7 for CC bond and 93.52 for CN bond. R_{ij} is the bond length in the molecule and n is the number of bonds. See reference 60 for more details.

Table S1. Thermodynamic parameters of NHC systems (all values in a.u.). M06L/6-311++G(d,p) level.

System	SCF Energy	ZPE correction	Thermal correction to energy	Thermal correction to enthalpy	Thermal correction to Gibbs free energy
1	-304.82828	0.12605	0.13314	0.13408	0.09482
2	-531.01925	0.20021	0.21213	0.21308	0.16307
3	-684.72577	0.24666	0.26122	0.26216	0.20621
4	-684.71899	0.24646	0.26109	0.26203	0.20540
5	-838.38387	0.29282	0.31017	0.31111	0.24875
6	-838.38324	0.29429	0.31116	0.31210	0.25094
7	-910.91989	0.32200	0.34089	0.34184	0.27442
8	-992.03743	0.33903	0.35911	0.36005	0.29148
9	-992.03974	0.34026	0.36003	0.36097	0.29302
10	-1444.46988	0.48852	0.51773	0.51867	0.42996
11	-607.11242	0.20950	0.22327	0.22421	0.16919
12	-988.26437	0.35436	0.37592	0.37687	0.30457
13	-1449.33600	0.49491	0.52393	0.52488	0.43662
14^a	-1599.18516	0.55613	0.58996	0.59091	0.48978
15	-833.99070	0.233915	0.249564	0.250508	0.192127
16	-1065.05181	0.31277	0.33313	0.33408	0.26446
17	-990.76062	0.31815	0.33732	0.33826	0.27199

^aDue to large memory requirement, frequency calculation is done at M06L/6-31+G(d,p) level.

Table S2. Thermodynamic parameters of protonated NHC systems (all values in a.u.).
M06L/6-311++G(d,p) level.

System	SCF Energy	ZPE correction	Thermal correction to energy	Thermal correction to enthalpy	Thermal correction to Gibbs free energy
1-H⁺	-305.25542	0.13965	0.14713	0.14807	0.10539
2-H⁺	-531.44750	0.21285	0.22520	0.22615	0.17495
3-H⁺	-685.15613	0.25993	0.27472	0.27567	0.21915
4-H⁺	-685.14712	0.25962	0.27455	0.27550	0.21772
5-H⁺	-838.81482	0.30616	0.32369	0.32464	0.26187
6-H⁺	-838.81558	0.30752	0.32461	0.32556	0.26391
7-H⁺	-911.34793	0.33559	0.35440	0.35534	0.28992
8-H⁺	-992.46897	0.35228	0.37260	0.37354	0.30438
9-H⁺	-992.47446	0.35339	0.37343	0.37438	0.30565
10-H⁺	-1444.90199	0.50191	0.53135	0.53229	0.44308
11-H⁺	-607.54101	0.22217	0.23633	0.23727	0.18101
12-H⁺	-988.69939	0.36685	0.38885	0.38979	0.31621
13-H⁺	-1449.77082	0.50863	0.53776	0.53870	0.45040
14-H⁺^a	-1599.62357	0.56792	0.60229	0.60323	0.50100
15-H⁺	-834.40496	0.245127	0.261797	0.262741	0.201653
16-H⁺	-1065.48414	0.32596	0.34655	0.34749	0.27747
17-H⁺	-991.19845	0.330785	0.350334	0.351278	0.284098

^aDue to large memory requirement, frequency calculation is done at M06L/6-31+G(d,p) level.

Table S3. Thermodynamic parameters of hydrogenated NHC systems (all values in a.u.).
M06L/6-311++G(d,p) level.

System	SCF Energy	ZPE correction	Thermal correction to energy	Thermal correction to enthalpy	Thermal correction to Gibbs free energy
1-H₂	-306.03309	0.14907	0.15627	0.15721	0.11824
2-H₂	-532.23749	0.22296	0.23519	0.23613	0.18557
3-H₂	-685.94178	0.26881	0.28431	0.28526	0.22677
4-H₂	-685.93726	0.26938	0.28442	0.28537	0.22831
5-H₂	-839.60680	0.31539	0.33362	0.33456	0.27002
6-H₂	-839.59993	0.31671	0.33416	0.33511	0.27270
7-H₂	-912.14331	0.34470	0.36409	0.36503	0.29887
8-H₂	-993.26367	0.36162	0.38265	0.38359	0.31261
9-H₂	-993.25460	0.36339	0.38355	0.38449	0.31590
10-H₂	-1445.68719	0.51161	0.54145	0.54239	0.45290
11-H₂	-608.33598	0.23225	0.24630	0.24724	0.19183
12-H₂	-989.47563	0.37768	0.39906	0.40000	0.32885
13-H₂	-1450.55118	0.51666	0.54681	0.54775	0.45638
14-H₂^a	-1600.39694	0.57952	0.61322	0.61416	0.51504
15-H₂	-835.20709	0.255138	0.272071	0.273015	0.211509
16-H₂	-1066.26762	0.33536	0.356601	0.357545	0.28552

17-H₂	-991.97106	0.34068	0.36029	0.36123	0.29396
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^aDue to large memory requirement, frequency calculation is done at M06L/6-31+G(d,p) level.

Table S4. Thermodynamic parameters of CuCl coordinated NHC systems (all values in a.u.).
M06L/6-311++G(d,p) level.

System	SCF Energy	ZPE correction	Thermal correction to energy	Thermal correction to enthalpy	Thermal correction to Gibbs free energy
1-CuCl	-2405.56617	0.12984	0.14038	0.14132	0.09183
2-CuCl	-2631.75645	0.20351	0.21914	0.22008	0.15944
3-CuCl	-2785.46319	0.25017	0.26836	0.26930	0.20293
4-CuCl	-2785.45602	0.25048	0.26849	0.26943	0.20382
5-CuCl	-2939.12105	0.29636	0.31733	0.31827	0.24556
6-CuCl	-2939.12070	0.29799	0.31846	0.31940	0.24834
7-CuCl	-3011.65539	0.32551	0.34795	0.34889	0.27274
8-CuCl	-3092.77448	0.34251	0.36626	0.36721	0.28818
9-CuCl	-3092.77734	0.34422	0.36752	0.36846	0.29096
10-CuCl	-3545.20617	0.49239	0.52545	0.52639	0.42690
11-CuCl	-2707.84902	0.21303	0.23033	0.23127	0.16631
12-CuCl	-3089.00238	0.35843	0.38363	0.38457	0.30207
13-CuCl	-3550.07379	0.50005	0.53264	0.53358	0.43563
14-CuCl^a	-3699.92392	0.56005	0.59740	0.59834	0.48862
15-CuCl	-2934.72352	0.237007	0.256412	0.257356	0.188247
16-CuCl	-3165.78889	0.316317	0.340294	0.341238	0.261286
17-CuCl	-3091.49879	0.321547	0.34442	0.345364	0.268424

^aDue to large memory requirement, frequency calculation is done at M06L/6-31+G(d,p) level.

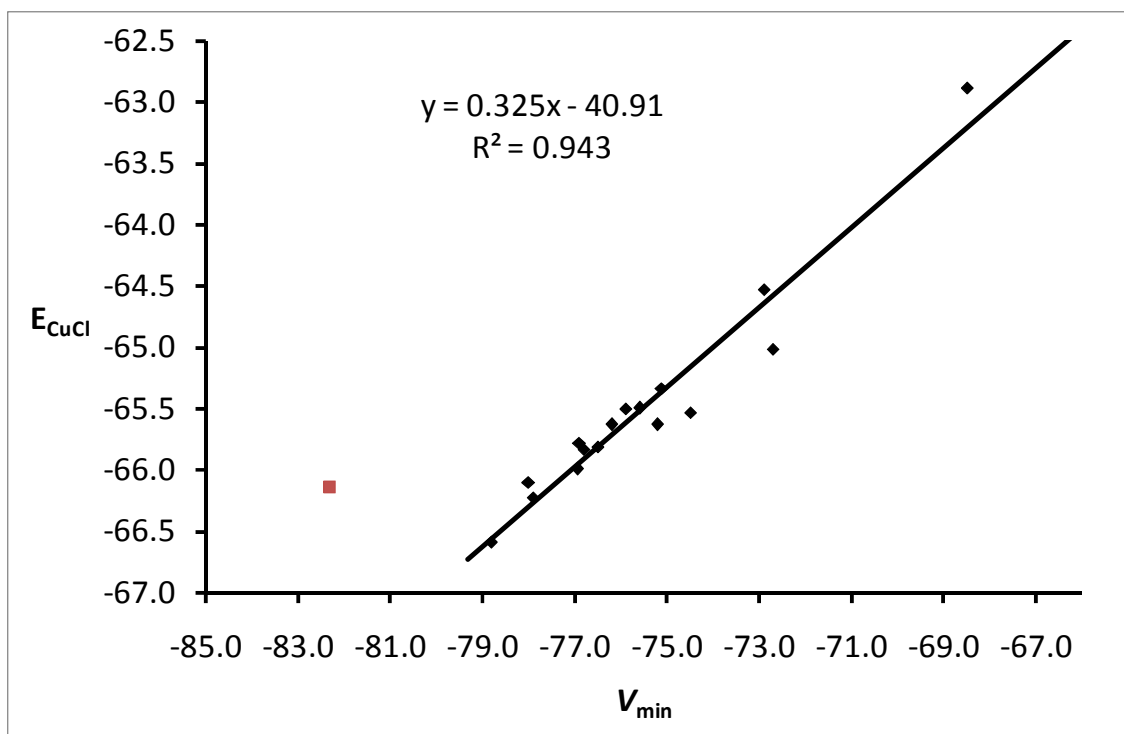


Figure S1. Correlation between $V_{\min}$ and CuCl binding energy (all values in kcal/mol). NHC coordination to the metal leads to electron deficiency on the ring. Except the case of **1**, this electron deficiency can be partially compensated by extended π -conjugation from annelated rings or inductive donation of electrons from the branches. Hence **1-CuCl** shows large deviation from the correlation plot.

Optimized geometries of NHC systems at M06L/6-311++G(d,p) level. All the X, Y, Z coordinates are given in Å.

1				2			
6	0.676937	1.209055	-0.000136	6	-0.675592	-0.000001	-0.000175
6	-0.676937	1.209055	0.000212	7	-1.085830	1.320230	-0.000176
7	1.059436	-0.121988	-0.000009	6	-0.000001	2.172055	-0.000582
6	0.000000	-0.988368	-0.000205	7	1.085830	1.320230	0.000031
7	-1.059436	-0.121988	-0.000036	6	0.675592	-0.000001	-0.000041
6	-2.435642	-0.565558	0.000038	6	-2.449487	1.797342	-0.000025
6	2.435642	-0.565558	0.000050	6	2.449485	1.797343	0.000364
1	-2.962540	-0.207564	0.888552	7	1.085829	-1.320230	0.000088
1	-2.433804	-1.653684	-0.000449	6	0.000001	-2.172057	-0.000134
1	2.962731	-0.207018	0.888230	7	-1.085829	-1.320230	-0.000095
1	2.433804	-1.653684	0.000224	6	2.449485	-1.797340	0.000561
1	-2.962877	-0.206761	-0.887950	6	-2.449483	-1.797342	-0.000218
1	2.962686	-0.207307	-0.888272	1	-2.987434	1.456688	-0.889129
1	1.381493	2.026043	-0.000210	1	-2.413324	2.885085	-0.000326
1	-1.381492	2.026043	0.000436	1	-2.987148	1.457176	0.889443
				1	2.987461	1.456974	-0.888833
				1	2.413322	2.885087	0.000400
				1	2.987121	1.456894	0.889738
				1	2.987673	-1.456665	-0.888388
				1	2.413326	-2.885084	0.000223
				1	2.986907	-1.457196	0.890183
				1	-2.987455	-1.456722	0.888886
				1	-2.413324	-2.885086	0.000046
				1	-2.987125	-1.457144	-0.889685

3				4			
6	-1.170442	0.703743	0.000008	6	0.692831	-2.128053	0.000013
6	-1.170442	-0.703743	0.000007	6	1.349373	-0.898114	0.000029
6	0.000000	-1.454822	-0.000004	6	0.702573	0.351679	0.000021
6	1.170442	-0.703743	-0.000012	6	-0.702572	0.351679	0.000001
6	1.170442	0.703743	-0.000011	6	-1.349377	-0.898113	-0.000022
6	0.000000	1.454822	-0.000001	6	-0.692836	-2.128052	-0.000014
7	2.510728	-1.071267	-0.000015	7	-1.736620	1.289906	0.000005
6	3.363981	0.000000	-0.000042	6	-2.984530	0.711751	-0.000008
7	2.510728	1.071266	-0.000016	7	-2.709045	-0.620242	-0.000028
7	-2.510728	1.071266	0.000016	7	2.709044	-0.620245	0.000013
6	-3.363981	0.000000	0.000033	6	2.984532	0.711745	-0.000010
7	-2.510728	-1.071267	0.000015	7	1.736622	1.289904	0.000002
1	0.000000	-2.539068	-0.000004	6	3.730241	-1.640798	0.000013
1	0.000000	2.539068	0.000001	6	-3.730248	-1.640790	-0.000058
6	-2.960488	-2.442561	0.000013	6	-1.612920	2.729417	0.000107
1	-2.602739	-2.972107	-0.888280	1	1.254920	-3.055118	0.000021
1	-2.602734	-2.972110	0.888302	1	-1.254925	-3.055117	-0.000032
1	-4.048411	-2.437452	0.000016	1	3.648543	-2.274148	-0.888192
6	-2.960487	2.442561	0.000013	1	3.648566	-2.274128	0.888234
1	-2.602743	2.972105	-0.888283	1	4.698481	-1.144166	-0.000006
1	-4.048411	2.437453	0.000022	1	-4.698485	-1.144151	-0.000073
1	-2.602728	2.972111	0.888299	1	-3.648547	-2.274123	-0.888275
6	2.960487	2.442561	-0.000004	1	-3.648584	-2.274140	0.888150
1	2.602742	2.972101	0.888294	1	-2.624166	3.131675	0.000054
1	4.048411	2.437453	-0.000012	1	-1.089238	3.086410	0.890121
1	2.602729	2.972116	-0.888289	1	-1.089090	3.086531	-0.889769
6	2.960488	-2.442561	-0.000007	6	1.612931	2.729415	-0.000060
1	2.602731	-2.972107	0.888283	1	1.089088	3.086505	0.889817
1	2.602742	-2.972110	-0.888299	1	2.624179	3.131667	0.000021
1	4.048411	-2.437452	-0.000001	1	1.089266	3.086441	-0.890073
5				6			
6	0.000000	-0.724373	-0.000006	6	-1.663267	1.962026	0.000006
6	0.000000	0.724373	0.000001	6	-2.398693	0.772640	-0.000053
6	1.230704	1.428316	0.000034	6	-1.791073	-0.478720	-0.000071
6	2.396847	0.707013	0.000059	6	-0.377986	-0.616791	-0.000041
6	2.396847	-0.707013	0.000041	6	0.377986	0.616792	0.000013
6	1.230704	-1.428316	0.000019	6	-0.292463	1.869349	0.000034
6	-1.230700	-1.428315	-0.000037	6	0.292463	-1.869349	-0.000066
6	-2.396846	-0.707012	-0.000063	6	1.663267	-1.962026	-0.000038
6	-2.396846	0.707012	-0.000047	6	2.398692	-0.772640	0.000020
6	-1.230700	1.428315	-0.000021	6	1.791073	0.478720	0.000043
7	3.738504	1.073959	0.000105	7	3.764484	-0.546130	0.000056
6	4.588465	0.000000	0.000113	6	4.080785	0.781050	0.000260
7	3.738504	-1.073959	0.000062	7	2.848303	1.389070	0.000061
7	-3.738501	-1.073962	-0.000111	7	-3.764485	0.546129	-0.000039
6	-4.588457	0.000000	-0.000097	6	-4.080785	-0.781050	-0.000222
7	-3.738501	1.073962	-0.000073	7	-2.848302	-1.389070	-0.000030
6	4.189130	2.444922	0.000123	6	2.753619	2.833033	-0.000043
6	4.189130	-2.444922	0.000121	6	4.757700	-1.594501	-0.000036
6	-4.189137	-2.444929	-0.000117	6	-2.753618	-2.833033	0.000061
6	-4.189137	2.444929	-0.000113	6	-4.757700	1.594500	0.000067
1	1.229662	2.513786	0.000046	1	-2.157994	2.927592	0.000029
1	1.229662	-2.513786	0.000028	1	0.287292	2.780997	0.000088
1	-1.229663	-2.513786	-0.000039	1	-0.287292	-2.780997	-0.000120
1	-1.229663	2.513786	-0.000020	1	2.157994	-2.927592	-0.000070
1	3.830356	2.974113	0.888020	1	3.771973	3.217217	0.000060
1	5.276957	2.440383	0.000181	1	2.234674	3.197111	-0.890767
1	3.830452	2.974107	-0.887817	1	2.234456	3.197198	0.890518
1	5.276956	-2.440383	-0.000250	1	4.661598	-2.225136	0.888514
1	3.830709	-2.973987	0.888237	1	4.661633	-2.224980	-0.888702
1	3.830099	-2.974234	-0.887600	1	5.738275	-1.122410	0.000026
1	-3.830587	-2.974069	0.887901	1	-2.234472	-3.197187	-0.890514
1	-5.276963	-2.440373	-0.000329	1	-3.771972	-3.217218	-0.000027
1	-3.830240	-2.974165	-0.887937	1	-2.234657	-3.197121	0.890771
1	-5.276963	2.440373	0.000025	1	-4.661576	2.225163	-0.888460
1	-3.830527	2.974061	-0.888112	1	-4.661656	2.224952	0.888756
1	-3.830300	2.974172	0.887726	1	-5.738276	1.122409	-0.000033

7				8			
6	-1.371522	0.328587	0.020771	6	-1.225679	0.725504	-0.000018
6	-0.401409	1.352106	0.015644	6	-1.225679	-0.725504	-0.000015
6	0.970999	1.023678	0.004474	6	2.460575	-1.434106	0.000024
6	1.372205	-0.327951	0.009678	6	3.620407	-0.710460	0.000047
6	0.401475	-1.352511	-0.021171	6	3.620407	0.710459	0.000037
6	-0.970222	-1.024313	-0.021742	6	2.460575	1.434106	0.000027
7	-2.161532	-1.759885	-0.036160	6	-2.460575	1.434106	-0.000034
6	-3.270852	-0.970542	0.011313	6	-3.620407	0.710460	-0.000052
7	-2.770926	0.295792	0.046685	6	-3.620407	-0.710459	-0.000039
7	2.605390	-0.990204	0.043975	6	-2.460575	-1.434106	-0.000021
6	2.477476	-2.346048	0.031827	7	4.963033	-1.074331	0.000063
7	1.130943	-2.547776	-0.014744	6	5.812625	0.000000	0.000059
7	-0.444255	2.751591	-0.007764	7	4.963033	1.074331	0.000030
6	0.793999	3.317847	-0.043936	7	-4.963033	1.074331	-0.000066
7	1.642282	2.252130	-0.030708	6	-5.812625	0.000000	-0.000069
6	-2.351556	-3.191906	-0.109339	7	-4.963033	-1.074331	-0.000037
6	0.652055	-3.912539	-0.025936	6	5.414260	-2.444846	-0.000022
6	3.062041	2.514717	-0.118897	6	5.414260	2.444846	0.000040
6	3.936328	-0.433951	0.151180	6	-5.414260	2.444846	-0.000007
6	-3.708327	1.392422	0.149589	6	-5.414261	-2.444846	0.000012
6	-1.592834	3.629708	-0.051466	1	2.459691	-2.519623	0.000005
1	-3.427450	-3.352224	-0.137140	1	2.459692	2.519622	0.000023
1	-1.941245	-3.701768	0.763670	1	-2.459692	2.519623	-0.000019
1	0.046408	-4.134614	0.854592	1	-2.459692	-2.519622	-0.000003
1	1.538910	-4.542597	-0.011019	1	5.054784	-2.973946	0.887818
1	3.597402	2.169463	0.766172	1	5.055536	-2.973627	-0.888360
1	3.164552	3.595269	-0.193280	1	6.502241	-2.440125	0.000435
1	4.040614	0.180098	1.047410	1	6.502241	2.440125	-0.000042
1	4.613434	-1.282433	0.224470	1	5.055093	2.973813	-0.888006
1	-4.695898	0.940351	0.212135	1	5.055227	2.973760	0.888172
1	-3.532589	1.985359	1.049094	1	-5.054870	2.973904	-0.887907
1	-2.212081	3.536498	0.842106	1	-6.502241	2.440125	-0.000360
1	-1.197327	4.642019	-0.102958	1	-5.055450	2.973668	0.888271
1	-1.908060	-3.610593	-1.014506	1	-6.502241	-2.440124	-0.000150
1	0.076164	-4.132216	-0.926043	1	-5.055293	-2.973719	0.888195
1	4.204584	0.156753	-0.725685	1	-5.055027	-2.973854	-0.887983
1	3.497772	2.056412	-1.008292	6	0.000000	1.395744	0.000000
1	-2.204437	3.444017	-0.936238	6	1.225679	0.725504	0.000016
1	-3.673196	2.042854	-0.725413	6	0.000000	-1.395744	-0.000001
				6	1.225679	-0.725504	0.000014
				1	0.000000	2.483256	0.000000
				1	0.000000	-2.483256	0.000001
9				10			
6	3.145122	2.052290	-0.000013	6	-3.719723	-0.711925	0.000173
6	3.647634	0.735694	-0.000009	6	-3.719723	0.711925	-0.000173
6	2.825531	-0.380578	-0.000009	6	-2.497676	1.382568	0.027121
6	-0.894488	-1.098827	0.000013	6	1.231072	0.720934	0.022992
6	-1.406514	0.254535	0.000009	6	1.231072	-0.720934	-0.022996
6	1.787080	2.212938	-0.000013	6	-2.497676	-1.382568	-0.027120
6	-1.787080	-2.212938	0.000019	6	2.497725	1.382550	0.027290
6	-3.145122	-2.052290	0.000013	6	3.719799	-0.711939	0.000094
6	-3.647634	-0.735694	0.000007	6	2.497725	-1.382550	-0.027293
6	-2.825531	0.380577	0.000012	7	4.694967	-1.706679	0.031249
7	-4.947195	-0.260920	-0.000001	6	4.162620	-2.968477	0.018410
6	-5.015385	1.104128	-0.000001	7	2.820469	-2.740636	-0.024061
7	-3.692225	1.470527	0.000014	7	-4.694953	1.706575	-0.031428
7	4.947195	0.260921	-0.000011	6	-4.162672	2.968405	-0.018848
6	5.015385	-1.104128	-0.000017	7	-2.820500	2.740641	0.023657
7	3.692225	-1.470527	-0.000012	6	1.913561	-3.868767	-0.044646
6	-3.312812	2.866341	0.000030	6	6.131070	-1.563100	0.133437
6	-6.118500	-1.106739	0.000000	6	-1.913669	3.868839	0.043967
6	3.312813	-2.866341	-0.000019	6	-6.131052	1.562779	-0.133438
6	6.118500	1.106739	-0.000011	1	2.531599	-4.764410	-0.029636
1	3.815318	2.905353	-0.000014	1	1.260658	-3.872271	0.832212
1	1.356145	3.209671	-0.000017	1	1.301549	-3.873817	-0.950601
1	-1.356146	-3.209672	0.000025	1	6.558176	-1.092447	-0.753704
1	-3.815318	-2.905353	0.000014	1	6.409881	-0.988260	1.018346
1	-4.232392	3.448413	0.000059	1	6.533144	-2.570184	0.223909
1	-2.730023	3.117677	0.890275	1	-1.301712	3.874209	0.949959

1	-2.730058	3.117710	-0.890229	1	-2.531770	4.764434	0.028654
1	-6.141460	-1.743910	-0.888498	1	-1.260715	3.872121	-0.832852
1	-6.141527	-1.743825	0.888558	1	-6.557984	1.092172	0.753816
1	-6.993302	-0.460007	-0.000063	1	-6.409875	0.987757	-1.018231
1	2.730062	-3.117706	0.890243	1	-6.533295	2.569786	-0.224007
1	4.232393	-3.448413	-0.000048	6	0.000032	1.381449	0.047945
1	2.730020	-3.117682	-0.890260	6	-1.231016	0.720947	0.022940
1	6.141504	1.743854	0.888526	6	0.000032	-1.381449	-0.047946
1	6.141483	1.743881	-0.888530	6	-1.231016	-0.720947	-0.022942
1	6.993302	0.460007	-0.000031	7	-4.694953	-1.706575	0.031431
6	0.488061	-1.305858	0.000010	6	-4.162672	-2.968405	0.018854
6	1.406514	-0.254536	-0.000002	7	-2.820500	-2.740641	-0.023654
6	-0.488061	1.305857	-0.000003	6	-1.913669	-3.868839	-0.043961
6	0.894488	1.098827	-0.000007	6	-6.131052	-1.562779	0.133439
1	0.834647	-2.332144	0.000019	1	-1.301712	-3.874212	-0.949952
1	-0.834648	2.332144	-0.000011	1	-2.531771	-4.764434	-0.028646
				1	-1.260715	-3.872119	0.832858
				1	-6.557983	-1.092173	-0.753816
				1	-6.409877	-0.987756	1.018231
				1	-6.533295	-2.569786	0.224009
				7	2.820469	2.740636	0.024050
				6	4.162619	2.968478	-0.018416
				7	4.694967	1.706679	-0.031245
				6	6.131071	1.563100	-0.133418
				6	1.913560	3.868767	0.044621
				1	6.558168	1.092446	0.753727
				1	6.533147	2.570184	-0.223886
				1	6.409890	0.988260	-1.018324
				1	1.301551	3.873830	0.950577
				1	1.260655	3.872258	-0.832236
				1	2.531599	4.764410	0.029597
				6	3.719799	0.711939	-0.000088
				1	0.000043	2.453857	0.089860
				1	0.000043	-2.453857	-0.089858
11				12			
6	0.715518	0.679722	-0.278456	6	-0.000517	-0.000279	1.336877
6	0.715518	-0.679724	-0.278454	6	-1.332111	0.348331	0.677905
7	2.005976	1.082914	-0.014751	6	-1.332348	0.348588	-0.677299
6	2.866986	0.000000	0.037067	6	-0.000993	0.000151	-1.336772
7	2.005976	-1.082913	-0.014745	6	0.363378	-1.327879	0.677532
6	2.482441	-2.448544	0.042933	6	0.363086	-1.327700	-0.677892
6	2.482441	2.448545	0.042919	6	0.966543	0.979181	-0.677605
1	1.866260	-3.032519	0.730353	6	0.966555	0.979265	0.677732
1	3.511178	-2.432758	0.397300	7	1.640155	2.116931	1.069243
1	1.866255	3.032525	0.730332	6	2.118905	2.838985	-0.000189
1	3.511176	2.432762	0.397293	7	1.639758	2.116918	-1.069457
1	2.451402	-2.917558	-0.943648	7	1.013479	-2.478545	-1.069799
1	2.451406	2.917551	-0.943665	6	1.400714	-3.254083	-0.000561
6	-0.715514	0.679716	0.278310	7	1.013905	-2.478781	1.068987
6	-0.715514	-0.679718	0.278308	7	-2.654368	0.361158	-1.068899
7	-2.005970	1.082969	0.014711	6	-3.519319	0.414359	0.000625
6	-2.866884	0.000000	-0.037941	7	-2.654041	0.360737	1.069872
7	-2.005970	-1.082968	0.014706	1	-0.000468	-0.000208	2.428776
6	-2.482481	-2.448605	-0.042543	1	-0.001264	0.000547	-2.428674
6	-2.482480	2.448606	-0.042530	6	1.890709	2.499007	2.440819
1	-1.866155	-3.032837	-0.729614	1	2.452789	3.430733	2.427628
1	-3.511131	-2.432913	-0.397162	1	0.952001	2.655057	2.981005
1	-1.866151	3.032842	-0.729594	1	2.474045	1.735386	2.963326
1	-3.511129	2.432916	-0.397153	6	1.889050	2.499334	-2.441171
1	-2.451689	-2.917281	0.944208	1	0.949783	2.654794	-2.980580
1	-2.451693	2.917274	0.944225	1	2.450527	3.431428	-2.428318
				1	2.472470	1.736119	-2.964181
				6	-3.108884	0.385492	2.441802
				1	-2.739256	1.272630	2.964078
				1	-4.196893	0.405094	2.429723
				1	-2.773123	-0.505303	2.981301
				6	-3.109580	0.386422	-2.440691
				1	-4.197583	0.406139	-2.428302
				1	-2.739988	1.273708	-2.962743

				1	-2.774047	-0.504220	-2.980598
				6	1.221058	-2.884176	-2.441666
				1	0.268578	-3.009157	-2.964911
				1	1.823912	-2.146686	-2.980047
				1	1.749474	-3.835561	-2.429506
				6	1.222219	-2.884503	2.440710
				1	1.750680	-3.835860	2.428237
				1	1.825326	-2.146986	2.978779
				1	0.270023	-3.009533	2.964458
13				14			
6	-0.000664	-0.000751	-1.286726	6	-3.556277	5.095959	3.641609
6	-1.330100	-0.451908	-0.704431	6	-3.272949	3.764003	2.907926
6	-1.330066	-0.451826	0.704549	6	-3.714732	3.747602	1.579180
6	-0.000595	-0.000604	1.286713	6	-4.390789	5.064964	1.131761
6	0.273208	1.376313	-0.704661	6	-2.926101	6.133585	2.737569
6	0.273242	1.376395	0.704475	6	-3.352481	6.117756	1.455216
6	1.054950	-0.926665	0.704643	6	-5.472023	5.272938	2.170390
6	1.054914	-0.926745	-0.704609	6	-5.045641	5.288794	3.452739
7	3.842010	-3.366065	-1.070910	7	-6.175425	5.268234	4.244786
6	4.485658	-3.929157	0.000095	6	-7.333177	5.268001	3.501469
7	3.842068	-3.365943	1.071070	7	-6.850945	5.242772	2.213162
7	0.996200	5.008866	1.070631	7	-2.522899	6.967780	0.752778
6	1.162238	5.847794	-0.000372	6	-1.579859	7.560831	1.560171
7	0.996151	5.008742	-1.071271	7	-1.847429	6.992911	2.784421
7	-4.837563	-1.641764	1.071293	6	-3.530597	2.617749	0.790235
6	-5.647205	-1.917167	0.000306	6	-2.644781	2.650639	3.454492
7	-4.837615	-1.641870	-1.070792	1	-3.208621	5.099900	4.676610
1	-0.000995	-0.000828	-2.379391	1	-4.732034	5.043301	0.094847
1	-0.000863	-0.000555	2.379378	6	-6.175736	5.283656	5.689897
6	4.182998	-3.662966	-2.441855	1	-7.211971	5.255463	6.020941
1	5.000711	-4.380873	-2.434380	1	-5.648248	4.412414	6.089545
1	3.329408	-4.094623	-2.973062	1	-5.699850	6.189793	6.075668
1	4.501792	-2.759520	-2.970558	6	-7.716538	5.225531	1.055997
6	4.183130	-3.662687	2.442030	1	-7.526746	4.341605	0.439816
1	3.329569	-4.094283	2.973334	1	-8.744467	5.197554	1.412014
1	5.000842	-4.380598	2.434593	1	-7.573233	6.119177	0.441807
1	4.501955	-2.759182	2.970613	6	-2.631142	7.252553	-0.659939
6	-5.265893	-1.788004	-2.441676	1	-2.512922	6.340201	-1.252106
1	-4.643225	-2.515625	-2.970830	1	-3.598363	7.703744	-0.899268
1	-6.296602	-2.136873	-2.434026	1	-1.837335	7.950492	-0.918627
1	-5.212877	-0.832625	-2.972358	6	-1.090485	7.309887	3.974018
6	-5.265788	-1.787733	2.442216	1	-0.304992	8.007535	3.690369
1	-6.296471	-2.136679	2.434653	1	-1.725255	7.773431	4.734652
1	-4.643046	-2.515233	2.971452	1	-0.634504	6.410107	4.397695
1	-5.212821	-0.832273	2.972756	6	-1.784659	0.203397	3.112990
6	1.083554	5.452008	2.441692	6	-2.460650	1.520785	2.665548
1	0.143273	5.272486	2.971647	6	-2.902434	1.504383	1.336802
1	1.886901	4.930708	2.971100	6	-2.619153	0.172407	0.603134
1	1.292913	6.519866	2.434764	6	-2.823028	-0.849340	2.789545
6	1.083438	5.451726	-2.442387	6	-3.249393	-0.865175	1.507185
1	1.292806	6.519584	-2.435591	6	-1.129801	-0.020501	0.792020
1	1.886754	4.930359	-2.971777	6	-0.703435	-0.004664	2.074372
1	0.143128	5.272151	-2.972273	7	0.675496	0.025165	2.031639
6	-2.447792	-0.830766	1.431361	6	1.157741	0.000000	0.743336
6	-2.447866	-0.830939	-1.431128	7	0.000000	0.000000	0.000000
6	-3.571291	-1.211597	0.699499	7	-4.328170	-1.724370	1.460356
6	-3.571318	-1.211679	-0.699139	6	-4.595841	-2.292188	2.684631
6	1.943384	-1.703637	1.431333	7	-3.652744	-1.699213	3.492011
6	1.943307	-1.703799	-1.431259	1	-1.443423	0.225054	4.149905
6	2.835724	-2.485161	0.699332	1	-2.966799	0.168473	-0.431871
6	2.835686	-2.485241	-0.699218	6	1.541071	0.042110	3.188822
6	0.504338	2.533828	1.431206	1	2.569014	0.069880	2.832829
6	0.736031	3.697112	0.698996	1	1.351464	0.926034	3.805063
6	0.504268	2.533662	-1.431538	1	1.397552	-0.851548	3.802946
6	0.735997	3.697032	-0.699473	6	0.000339	-0.015301	-1.445112
1	-2.445530	-0.830180	-2.517185	1	-0.527006	0.856049	-1.844711
1	-2.445391	-0.829878	2.517416	1	1.036586	0.012756	-1.776132
1	0.504663	2.531280	-2.517624	1	-0.475678	-0.921338	-1.830957
1	0.504786	2.531574	2.517292	6	-5.085130	-2.041311	0.270759

1	1.942256	-1.701623	-2.517329	1	-5.540968	-1.141489	-0.152983
1	1.942390	-1.701340	2.517402	1	-4.450410	-2.504994	-0.489833
				1	-5.870733	-2.738824	0.554432
				6	-3.544570	-1.983918	4.904746
				1	-4.338489	-2.681719	5.163462
				1	-2.577422	-2.435244	5.144122
				1	-3.662661	-1.071512	5.496857
				1	-2.301468	2.663388	4.487067
				1	-3.873917	2.604997	-0.242337

Optimized geometries of protonated NHC systems at M06L/6-311++G(d,p) level. All the X, Y, Z coordinates are given in Å.

1-H⁺				2-H⁺			
6	-0.679215	1.231817	0.000093	6	-0.681381	-0.031822	-0.000084
6	0.679215	1.231817	-0.000092	7	-1.108315	1.276156	-0.000155
7	-1.084864	-0.084470	0.000096	6	0.000000	2.045608	-0.000111
6	0.000000	-0.862903	0.000207	7	1.108315	1.276156	0.000072
7	1.084864	-0.084469	0.000123	6	0.681381	-0.031822	0.000067
6	2.470877	-0.548106	-0.000123	6	-2.480004	1.773811	-0.000255
6	-2.470877	-0.548106	-0.000166	6	2.480004	1.773811	0.000148
1	2.978064	-0.182407	-0.892349	7	1.094490	-1.338699	0.000163
1	2.482983	-1.635474	0.002212	6	0.000000	-2.180508	0.000107
1	-2.978124	-0.182220	-0.892281	7	-1.094490	-1.338699	-0.000070
1	-2.482983	-1.635474	0.001939	6	2.463490	-1.829489	0.000466
1	2.979595	-0.178600	0.889653	6	-2.463490	-1.829489	-0.000333
1	-2.979535	-0.178787	0.889721	1	-3.000943	1.425421	-0.891957
1	-1.386289	2.044685	0.000136	1	-2.460473	2.861278	-0.000498
1	1.386289	2.044685	-0.000201	1	-3.000951	1.425815	0.891597
1	0.000000	-1.940943	0.000118	1	3.000928	1.425816	-0.891719
				1	2.460473	2.861278	0.000395
				1	3.000967	1.425419	0.891836
				1	2.995334	-1.495546	-0.892472
				1	2.412376	-2.915533	0.000208
				1	2.994792	-1.495942	0.893878
				1	-2.995304	-1.495548	0.892624
				1	-2.412376	-2.915533	-0.000078
				1	-2.994822	-1.495940	-0.893726
				1	0.000000	3.124000	-0.000180
3-H⁺				4-H⁺			
6	1.201136	0.711283	-0.000007	6	-0.660297	-2.150319	0.000476
6	1.201136	-0.711283	-0.000006	6	-1.315170	-0.919430	0.000618
6	0.037976	-1.463993	0.000000	6	-0.668164	0.335267	-0.000117
6	-1.128398	-0.703940	0.000006	6	0.735490	0.360273	-0.000270
6	-1.128398	0.703940	0.000006	6	1.378292	-0.894671	-0.001022
6	0.037976	1.463993	-0.000001	6	0.720470	-2.127744	-0.000708
7	-2.464572	-1.095450	0.000013	7	1.758559	1.294773	0.001064
6	-3.227703	0.000000	0.000015	6	3.007934	0.710454	0.000878
7	-2.464572	1.095450	0.000013	7	2.730936	-0.622134	-0.000709
7	2.530618	1.076165	-0.000014	7	-2.680748	-0.665735	0.000853
6	3.382747	0.000000	-0.000017	6	-2.865222	0.649713	-0.000462
7	2.530618	-1.076165	-0.000013	7	-1.689913	1.289642	-0.001127
1	0.036809	-2.547190	0.000001	6	-3.724441	-1.679937	0.001861
1	0.036809	2.547190	-0.000001	6	3.762984	-1.643021	-0.001485
6	2.993161	-2.450330	-0.000017	6	1.645481	2.739348	0.003773
1	2.641888	-2.976684	0.890926	1	-1.212738	-3.081798	0.000959
1	2.641887	-2.976681	-0.890962	1	1.288658	-3.050567	-0.001135
1	4.080100	-2.432696	-0.000018	1	-3.630954	-2.302322	0.892567
6	2.993161	2.450330	-0.000017	1	-3.632135	-2.302946	-0.888535
1	2.641892	2.976683	0.890928	1	-4.697971	-1.194411	0.002331
1	4.080100	2.432696	-0.000022	1	4.725622	-1.137529	-0.000889
1	2.641883	2.976682	-0.890960	1	3.683671	-2.271035	0.888656
6	-2.937304	2.471108	0.000016	1	3.683935	-2.269382	-0.892811
1	-2.574703	2.985872	-0.890692	1	2.660215	3.131160	0.009216
1	-4.024963	2.478851	0.000020	1	1.137410	3.101332	-0.892889
1	-2.574697	2.985871	0.890722	1	1.129116	3.097008	0.897418

6	-2.937304	-2.471108	0.000019
1	-2.574694	-2.985876	-0.890682
1	-2.574706	-2.985866	0.890731
1	-4.024963	-2.478851	0.000012
1	-4.306379	0.000000	0.000021
5-H⁺			
6	0.036231	0.728838	-0.000008
6	0.036225	-0.728846	-0.000044
6	1.265191	-1.433963	-0.000050
6	2.429315	-0.711299	0.000025
6	2.429330	0.711294	-0.000033
6	1.265194	1.433954	-0.000013
6	-1.186419	1.435245	0.000031
6	-2.349340	0.706097	0.000006
6	-2.349344	-0.706108	-0.000050
6	-1.186421	-1.435253	-0.000057
7	3.760966	-1.077229	0.000028
6	4.612538	-0.000016	-0.000016
7	3.760960	1.077222	-0.000080
7	-3.690693	1.098061	0.000106
6	-4.447879	0.000007	0.000064
7	-3.690701	-1.098056	0.000015
6	4.221902	-2.450078	0.000264
6	4.221896	2.450068	-0.000153
6	-4.165031	2.471713	0.000143
6	-4.165155	-2.471670	-0.000199
1	1.266082	-2.518714	-0.000093
1	1.266073	2.518705	-0.000067
1	-1.188379	2.519806	0.000104
1	-1.188375	-2.519814	-0.000168
1	3.868311	-2.977122	-0.889725
1	5.309150	-2.435122	0.000286
1	3.868223	-2.976819	0.890395
1	5.309145	2.435128	-0.000243
1	3.868175	2.976932	-0.890195
1	3.868324	2.976977	0.889923
1	-3.801624	2.987432	-0.890046
1	-5.252906	2.479638	0.000188
1	-3.801567	2.987450	0.890302
1	-5.253024	-2.479484	0.001067
1	-3.800786	-2.987867	0.889306
1	-3.802779	-2.987003	-0.891023
1	-5.527170	0.000012	0.000040
7-H⁺			
6	-0.025782	1.425206	-0.044115
6	1.184753	0.708043	-0.048608
6	1.184950	-0.707680	0.048485
6	-0.025368	-1.425188	0.044007
6	-1.239099	-0.706980	-0.013291
6	-1.239303	0.706634	0.013174
7	-2.232577	1.675652	0.108940
6	-1.733608	2.945683	0.107669
7	-0.385191	2.770790	-0.003475
7	-0.384372	-2.770878	0.003482
6	-1.732739	-2.946181	-0.107625
7	-2.232090	-1.676297	-0.108972
7	2.529726	1.092777	-0.098341
6	3.281977	0.000452	-0.000023
7	2.530013	-1.092068	0.098309
6	-3.657994	1.502755	0.339394
6	-3.657571	-1.503833	-0.339355
6	3.137950	-2.400939	0.302728
6	0.461812	-3.947545	-0.008263
8-H⁺			
6	1.186044	0.728398	-0.000037
6	1.186044	-0.728398	-0.000035
6	-2.493686	-1.438134	0.000145
6	-3.653023	-0.713702	0.000171
6	-3.653023	0.713701	0.000119
6	-2.493686	1.438134	0.000057
6	2.412534	1.440661	-0.000073
6	3.568903	0.709493	-0.000124
6	3.568903	-0.709492	-0.000134
6	2.412534	-1.440661	-0.000082
7	-4.987364	-1.077050	0.000203
6	-5.838213	0.000001	0.000283
7	-4.987364	1.077050	0.000129
7	4.913527	1.098714	-0.000192
6	5.668343	-0.000001	-0.000190
7	4.913525	-1.098715	-0.000166
6	-5.446707	-2.449221	0.000303
6	-5.446703	2.449223	-0.000004
6	5.388274	2.471456	0.000039

6	0.460621	3.947724	0.008392	6	5.388270	-2.471458	-0.000445
6	3.137361	2.401799	-0.302659	1	-2.493287	-2.522915	0.000175
1	-4.048789	2.490667	0.571199	1	-2.493287	2.522915	0.000007
1	-3.834355	0.841207	1.188116	1	2.413955	2.525300	-0.000047
1	-4.168955	-1.122158	0.543383	1	2.413956	-2.525299	-0.000069
1	-4.048124	-2.491884	-0.570984	1	-5.091501	-2.976443	-0.889133
1	2.755158	-2.852613	1.216203	1	-5.091847	-2.976184	0.890033
1	4.212335	-2.261286	0.405657	1	-6.534055	-2.436351	0.000091
1	1.039129	-4.041544	0.912502	1	-6.534050	2.436356	0.000108
1	-0.208299	-4.800737	-0.084512	1	-5.091576	2.976417	0.889481
1	-0.209759	4.800694	0.084755	1	-5.091758	2.976210	-0.889685
1	1.125156	3.952892	0.874762	1	5.024762	2.987244	0.890232
1	2.946166	3.055361	0.545339	1	6.476167	2.479667	-0.000327
1	4.211785	2.262391	-0.405500	1	5.024196	2.987721	-0.889644
1	-4.169328	1.121090	-0.543371	1	6.476163	-2.479670	-0.000785
1	-3.834153	-0.842469	-1.188168	1	5.024201	-2.987381	-0.890331
1	1.126330	-3.952606	-0.874645	1	5.024748	-2.987587	0.889545
1	2.946978	-3.054571	-0.545267	6	-0.039852	1.400295	-0.000008
1	2.754549	2.853409	-1.216156	6	-1.261789	0.728161	0.000037
1	1.037885	4.042023	-0.912373	6	-0.039852	-1.400294	0.000024
1	4.359984	0.000594	0.000005	6	-1.261789	-0.728161	0.000071
				1	-0.039996	2.486864	-0.000020
				1	-0.039997	-2.486863	0.000036
				1	6.747808	-0.000001	-0.000199
9-H⁺				10-H⁺			
6	-3.175077	-2.050603	0.000028	6	3.738487	-0.705764	-0.052494
6	-3.678162	-0.737157	0.000049	6	3.737683	0.713521	0.052891
6	-2.852927	0.383420	0.000048	6	2.512441	1.385561	0.081445
6	0.859104	1.095268	0.000004	6	-1.204134	0.713605	-0.011234
6	1.365950	-0.258784	-0.000020	6	-1.208472	-0.727562	0.017031
6	-1.816270	-2.218108	0.000007	6	2.512770	-1.379736	-0.076601
6	1.749198	2.213787	0.000004	6	-2.478675	1.355172	-0.064733
6	3.107425	2.080820	-0.000020	6	-3.709054	-0.746213	0.056769
6	3.606776	0.761902	-0.000045	6	-2.474227	-1.398758	0.071714
6	2.787232	-0.363052	-0.000045	7	-4.674382	-1.744054	0.157297
7	4.916190	0.314860	-0.000075	6	-4.122257	-2.991310	0.235620
6	4.906527	-1.019886	-0.000090	7	-2.778702	-2.748680	0.175212
7	3.642343	-1.461410	-0.000074	7	4.710165	1.700874	0.149140
7	-4.972540	-0.264842	0.000071	6	4.177919	2.959931	0.238793
6	-5.038724	1.101994	0.000080	7	2.834549	2.737772	0.189975
7	-3.715084	1.470903	0.000070	6	-1.860253	-3.871516	0.257072
6	3.285489	-2.873236	-0.000086	6	-6.115827	-1.618838	0.232615
6	6.100727	1.160158	-0.000084	6	1.933282	3.865099	0.285839
6	-3.341223	2.870344	0.000077	6	6.153137	1.557337	0.202818
6	-6.151762	-1.107309	0.000082	1	-2.472758	-4.763202	0.371120
1	-3.845848	-2.902845	0.000030	1	-1.264663	-3.965047	-0.653682
1	-1.390834	-3.216542	-0.000010	1	-1.201205	-3.777993	1.122921
1	1.310032	3.206391	0.000024	1	-6.418896	-1.017049	1.091802
1	3.769364	2.937918	-0.000019	1	-6.536314	-1.203072	-0.684861
1	4.197968	-3.466253	-0.000106	1	-6.502558	-2.627188	0.362718
1	2.706237	-3.112245	0.891958	1	1.331049	3.975532	-0.621392
1	2.706210	-3.112223	-0.892117	1	2.554750	4.751211	0.401019
1	6.105353	1.789810	-0.890279	1	1.278053	3.777013	1.157706
1	6.105421	1.789739	0.890160	1	6.548514	1.128743	-0.718192
1	6.989049	0.532656	-0.000144	1	6.457413	0.947012	1.053527
1	-2.763308	3.123584	0.892772	1	6.554516	2.560629	0.325745
1	-4.263371	3.447444	0.000089	6	0.019566	1.383669	0.014078
1	-2.763322	3.123596	-0.892625	6	1.252284	0.724501	0.028018
1	-6.176256	-1.740647	0.889951	6	0.021241	-1.384816	-0.005346
1	-6.176271	-1.740647	-0.889787	6	1.252156	-0.720592	-0.021859
1	-7.021497	-0.454807	0.000089	7	4.710283	-1.691180	-0.151774
6	-0.520135	1.303396	0.000027	6	4.176894	-2.951941	-0.239098
6	-1.439275	0.249678	0.000027	7	2.834667	-2.731171	-0.185537
6	0.456789	-1.312978	-0.000018	6	1.930566	-3.860001	-0.273966
6	-0.927407	-1.106105	0.000005	6	6.153030	-1.549663	-0.210517
1	5.780570	-1.650236	-0.000113	1	1.331663	-3.965519	0.634753
1	0.797714	-2.340941	-0.000034	1	2.551114	-4.746423	-0.388906
1	-0.869101	2.328370	0.000044	1	1.271726	-3.773318	-1.142211
				1	6.552843	-1.121829	0.709029

		1	6.455919	-0.940751	-1.062861		
		1	6.551752	-2.553953	-0.334266		
		7	-2.793171	2.707121	-0.183521		
		6	-4.117830	2.835646	-0.228104		
		7	-4.700023	1.635386	-0.145254		
		6	-6.147593	1.490908	-0.211221		
		6	-1.903941	3.856293	-0.290067		
		1	-6.425441	0.866985	-1.058616		
		1	-6.581699	2.479591	-0.346433		
		1	-6.534228	1.060057	0.710196		
		1	-1.238568	3.736164	-1.145061		
		1	-1.319992	3.973808	0.622945		
		1	-2.510860	4.747979	-0.437196		
		6	-3.702806	0.668628	-0.040224		
		1	-4.646507	3.769772	-0.322795		
		1	0.025562	-2.458013	-0.009205		
		1	0.026792	2.457419	0.027998		
11-H ⁺		12-H ⁺					
6	-0.764670	-0.684477	0.291164	6	0.027045	-0.070445	-1.344239
6	-0.764670	0.684473	0.291167	6	1.350182	-0.431997	-0.677872
7	-2.039403	-1.090899	0.001159	6	1.350327	-0.433106	0.676869
6	-2.891098	0.000000	-0.071158	6	0.027259	-0.072615	1.344065
7	-2.039403	1.090898	0.001168	6	-0.978993	-1.006177	-0.678874
6	-2.533363	2.456897	-0.055980	6	-0.978687	-1.007473	0.677368
6	-2.533365	-2.456896	-0.055999	6	-0.300368	1.263379	0.684184
1	-2.536746	2.906317	0.938556	6	-0.300511	1.264577	-0.682202
1	-3.550750	2.425267	-0.438078	7	-0.539316	2.545619	-1.091794
1	-2.536750	-2.906323	0.938534	6	-0.687275	3.320814	0.002861
1	-3.550751	-2.425264	-0.438100	7	-0.539266	2.543668	1.096147
1	-1.908202	3.053857	-0.721734	7	-2.069095	-1.750519	1.072195
1	-1.908201	-3.053854	-0.721755	6	-2.760794	-2.262218	-0.001559
6	0.688298	-0.680757	-0.166081	7	-2.070025	-1.747807	-1.074608
6	0.688297	0.680754	-0.166083	7	2.605371	-0.838479	1.072796
7	1.973956	-1.110711	-0.017054	6	3.424460	-1.098030	-0.001289
6	2.756194	0.000001	0.010702	7	2.605322	-0.836107	-1.074754
7	1.973954	1.110712	-0.017062	1	0.026355	-0.065303	-2.434741
6	2.470496	2.483798	0.012870	1	0.026813	-0.069223	2.434576
6	2.470501	-2.483795	0.012889	6	-0.620435	3.016196	-2.469826
1	2.414434	2.923131	-0.983103	1	-0.847137	4.079950	-2.471577
1	3.502860	2.484245	0.354922	1	0.333068	2.853607	-2.972984
1	2.414420	-2.923143	-0.983076	1	-1.409756	2.481763	-2.998435
1	3.502872	-2.484235	0.354919	6	-0.620528	3.011634	2.475047
1	1.862160	3.065699	0.704112	1	0.332844	2.847997	2.978072
1	1.862180	-3.065688	0.704152	1	-0.847055	4.075427	2.478777
1	3.829013	0.000002	-0.107779	1	-1.409994	2.476306	3.002541
				6	3.045187	-0.989132	-2.447295
				1	2.988768	-0.039117	-2.985711
				1	4.079682	-1.322910	-2.424715
				1	2.440596	-1.734034	-2.971124
				6	3.045422	-0.994131	2.444989
				1	4.079850	-1.328070	2.421656
				1	2.989255	-0.045059	2.985104
				1	2.440749	-1.739829	2.967563
				6	-2.430446	-2.049293	2.443915
				1	-1.635937	-2.606065	2.946287
				1	-2.634007	-1.132284	3.003887
				1	-3.331479	-2.658160	2.420579
				6	-2.432582	-2.043091	-2.446759
				1	-3.334191	-2.651159	-2.424273
				1	-2.635575	-1.124556	-3.004459
				1	-1.638978	-2.599459	-2.950934
				1	-0.920409	4.372209	0.003741
13-H ⁺		14-H ⁺					
6	-0.035800	0.006210	-1.289520	6	2.670540	-0.017130	1.324380
6	1.325230	-0.323970	-0.711850	6	1.257530	-0.053790	0.703340
6	1.325230	-0.324040	0.711820	6	1.257570	-0.053740	-0.703280
6	-0.035800	0.006080	1.289510	6	2.670620	-0.017050	-1.324240
6	-0.992730	-1.020030	-0.703500	6	3.371480	-1.188500	0.675610
6	-0.992730	-1.020100	0.703390	6	3.371520	-1.188460	-0.675500

6	-0.414260	1.357370	0.703610	6	3.284510	1.207220	-0.676820
6	-0.414260	1.357440	-0.703480	6	3.284470	1.207180	0.677070
7	-1.444900	4.909220	-1.072550	7	3.594360	2.492260	1.071450
6	-1.683630	5.729730	0.000290	6	3.836010	3.321570	0.000210
7	-1.444910	4.909110	1.073040	7	3.594420	2.492330	-1.071100
7	-3.539630	-3.702100	1.072540	7	3.972640	-2.364360	-1.072460
6	-4.129110	-4.320480	-0.000220	6	4.378150	-3.124040	0.000020
7	-3.539630	-3.701990	-1.072920	7	3.972590	-2.364430	1.072520
7	4.910420	-1.186810	1.094930	6	0.061270	-0.062590	-1.406510
6	5.656390	-1.365670	-0.000060	6	0.061190	-0.062670	1.406500
7	4.910430	-1.186660	-1.095040	1	2.660640	-0.019870	2.415840
1	-0.033890	0.005460	-2.381550	1	2.660770	-0.019710	-2.415700
1	-0.033890	0.005220	2.381540	6	3.741980	2.927870	2.443290
6	-1.578390	5.347310	-2.444150	1	3.990680	3.986860	2.429540
1	-1.892760	6.388560	-2.431390	1	2.811790	2.783790	3.001350
1	-0.625180	5.265700	-2.974440	1	4.542050	2.379350	2.946720
1	-2.328110	4.751520	-2.972170	6	3.742110	2.928020	-2.442910
6	-1.578400	5.347060	2.444690	1	2.811950	2.783980	-3.001020
1	-0.625180	5.265390	2.974980	1	3.990810	3.987000	-2.429080
1	-1.892760	6.388310	2.432030	1	4.542210	2.379530	-2.946320
1	-2.328120	4.751220	2.972640	6	4.204300	-2.765480	-2.443470
6	5.370080	-1.295800	-2.470430	1	3.261800	-2.857460	-2.990730
1	5.215120	-0.347690	-2.987340	1	4.845100	-2.045810	-2.959990
1	6.430310	-1.538920	-2.478890	1	4.700270	-3.733750	-2.424100
1	4.816470	-2.082980	-2.984030	6	4.204170	-2.765630	2.443520
6	5.370100	-1.295900	2.470310	1	4.700130	-3.733900	2.424120
1	6.430140	-1.539890	2.478750	1	4.844950	-2.045990	2.960120
1	5.215950	-0.347530	2.986980	1	3.261640	-2.857640	2.990730
1	4.815920	-2.082500	2.984160	6	-2.549520	-0.084780	1.328370
6	-3.860980	-4.028270	2.444280	6	-1.138280	-0.075200	0.697860
1	-2.975100	-4.383050	2.978840	6	-1.138240	-0.075160	-0.697930
1	-4.263840	-3.156920	2.968020	6	-2.549450	-0.084710	-1.328510
1	-4.610940	-4.816120	2.431870	6	-3.208370	1.111990	0.681790
6	-3.860960	-4.028040	-2.444680	6	-3.208330	1.112030	-0.681900
1	-4.610970	-4.815860	-2.432350	6	-3.249590	-1.259340	-0.676510
1	-4.263770	-3.156630	-2.968360	6	-3.249630	-1.259370	0.676260
1	-2.975100	-4.382830	-2.979250	7	-3.861420	-2.428250	1.073770
6	2.465060	-0.599060	1.440750	6	-4.263360	-3.187150	-0.000200
6	2.465060	-0.598930	-1.440810	7	-3.861360	-2.428200	-1.074110
6	3.615120	-0.876610	0.699330	7	-3.733030	2.306440	-1.094050
6	3.615120	-0.876530	-0.699420	6	-4.057740	3.023240	-0.000020
6	-0.738070	2.492080	1.433480	7	-3.733090	2.306380	1.093980
6	-0.738070	2.492220	-1.433230	1	-2.541920	-0.080250	2.419180
6	-1.070760	3.629250	0.701740	1	-2.541790	-0.080110	-2.419320
6	-1.070760	3.629320	-0.701380	6	-4.070620	-2.845510	2.445390
6	-1.801750	-1.879360	1.433190	1	-4.574370	-3.809370	2.421870
6	-2.619040	-2.737100	0.701400	1	-3.118440	-2.953200	2.971170
6	-1.801740	-1.879230	-1.433390	1	-4.697140	-2.128540	2.982910
6	-2.619040	-2.737030	-0.701680	6	-4.070490	-2.845380	-2.445760
1	6.705420	-1.615400	-0.000080	1	-3.118290	-2.953040	-2.971500
1	2.465530	-0.598530	-2.525590	1	-4.574250	-3.809240	-2.422320
1	2.465530	-0.598750	2.525530	1	-4.696990	-2.128390	-2.983280
1	-1.804130	-1.874770	-2.519170	6	-3.918940	2.744060	-2.472280
1	-1.804140	-1.875000	2.518970	1	-2.953940	2.789200	-2.977830
1	-0.740810	2.489700	-2.519050	1	-4.574350	2.048320	-2.996330
1	-0.740800	2.489450	2.519300	1	-4.370590	3.733610	-2.476110
				6	-3.919070	2.743920	2.472230
				1	-4.370730	3.733460	2.476080
				1	-4.574500	2.048140	2.996200
				1	-2.954100	2.789040	2.977830
				1	0.060770	-0.064350	2.494010
				1	0.060900	-0.064210	-2.494010
				1	-4.535370	3.988930	-0.000010

Optimized geometries of hydrogenated NHC systems at M06L/6-311++G(d,p) level . All the X, Y, Z coordinates are given in Å.

1-H₂		2-H₂	
6	0.719543 1.215028 0.295779	6	0.648240 -0.246990 -0.277058
6	-0.538680 1.215992 -0.159720	7	1.551169 0.792413 -0.206790
7	1.178647 -0.124563 0.492865	6	0.916032 1.988301 0.042300
6	-0.052126 -0.908206 0.415864	7	-0.408971 1.611619 0.186763
7	-1.000181 -0.098334 -0.358614	6	-0.571146 0.260717 -0.024225
6	-2.389458 -0.391048 -0.104213	6	2.973874 0.693559 -0.436548
6	2.207657 -0.517476 -0.466898	6	-1.462746 2.567615 0.435961
1	-2.643002 -0.337230 0.970000	7	-1.518862 -0.755044 0.207563
1	-2.628719 -1.397431 -0.457577	6	-0.778797 -1.910796 -0.406391
1	2.528395 -1.542131 -0.264712	7	0.665924 -1.667455 -0.273950
1	1.877074 -0.447769 -1.515758	6	-2.844920 -0.601658 -0.360111
1	-3.027101 0.310979 -0.645011	6	1.229972 -2.214192 0.968979
1	3.076923 0.132144 -0.341950	1	3.463331 0.111406 0.349958
1	1.391826 2.047802 0.439001	1	3.379656 1.703743 -0.434218
1	-1.170497 2.057475 -0.407028	1	3.179300 0.218938 -1.399523
1	-0.457366 -1.060880 1.437613	1	-2.042210 2.285597 1.319632
1	0.121583 -1.888417 -0.039203	1	-0.993530 3.534758 0.608061
		1	-2.140143 2.647180 -0.419682
		1	-3.342589 0.269096 0.070341
		1	-3.447270 -1.479552 -0.115066
		1	-2.826408 -0.489139 -1.458386
		1	2.294687 -1.977593 1.011584
		1	1.133290 -3.301734 0.959807
		1	0.748481 -1.815713 1.874204
		1	-1.027196 -1.941963 -1.481613
		1	-1.067265 -2.855088 0.062371
3-H₂		4-H₂	
6	-1.241460 -0.695626 0.036837	6	0.789314 -2.088115 0.220976
6	-1.241442 0.695561 -0.036919	6	1.441164 -0.869933 0.086381
6	-0.056188 1.441975 -0.089665	6	0.752861 0.348222 -0.058832
6	1.114086 0.704120 -0.060723	6	-0.631966 0.338616 -0.054838
6	1.114097 -0.704311 0.060705	6	-1.291399 -0.887486 0.090578
6	-0.056237 -1.442079 0.089618	6	-0.608010 -2.096338 0.216446
7	2.434883 1.133880 -0.188051	7	-1.577538 1.403442 -0.158687
6	3.323416 0.000036 0.000792	6	-2.813644 0.689841 -0.479832
7	2.434850 -1.134130 0.188422	7	-2.674269 -0.641997 0.119167
7	-2.580286 -1.067723 0.054947	7	2.791345 -0.535807 0.007825
6	-3.438508 0.000015 0.000070	6	3.006883 0.797317 -0.186681
7	-2.580238 1.067704 -0.055225	7	1.736299 1.317292 -0.221394
1	-0.059345 2.523077 -0.172377	6	3.856576 -1.504338 0.099630
1	-0.059482 -2.523181 0.172344	6	-3.578871 -1.652162 -0.369363
6	-3.027216 2.435991 -0.135263	6	-1.681130 2.189899 1.076531
1	-2.658515 3.020107 0.714090	1	1.346671 -3.014201 0.311960
1	-2.679636 2.910417 -1.058776	1	-1.148207 -3.031461 0.317400
1	-4.115491 2.433826 -0.122546	1	-2.912134 0.602828 -1.578483
6	-3.027359 -2.435953 0.135451	1	3.835119 -2.018960 1.065277
1	-2.679657 -2.910090 1.059066	1	4.801161 -0.973893 -0.004149
1	-4.115637 -2.433691 0.122945	1	3.773756 -2.252955 -0.694370
1	-2.658876 -3.020393 -0.713773	1	-4.610106 -1.327116 -0.212672
6	2.867084 -2.427547 -0.266223	1	-3.441315 -1.864848 -1.443393
1	2.930340 -2.498861 -1.364475	1	-3.440799 -2.582630 0.184844
1	3.851025 -2.659129 0.149068	1	-1.992560 1.588024 1.943056
1	2.177381 -3.195782 0.087187	1	-0.712504 2.636204 1.303027
6	2.866701 2.427880 0.265267	1	-3.688474 1.218851 -0.090625
1	3.850961 2.658925 -0.149547	1	-2.398153 3.000774 0.930721
1	2.177217 3.195614 -0.089621	6	1.485325 2.726068 -0.437075
1	2.929165 2.500568 1.363494	1	1.279847 3.246343 0.503835
1	3.981467 0.146401 0.879112	1	2.379421 3.160536 -0.881104
1	3.982770 -0.146294 -0.876522	1	0.634792 2.862446 -1.107222
5-H₂		6-H₂	
6	-0.075676 0.721186 -0.018555	6	1.693989 -1.955928 0.276561
6	-0.075675 -0.721185 0.018543	6	2.442899 -0.778108 0.123099
6	1.168349 -1.420128 0.052487	6	1.854499 0.473196 -0.018782
6	2.336045 -0.710583 0.046842	6	0.442114 0.630908 -0.030081
6	2.336044 0.710588 -0.046869	6	-0.318445 -0.592137 0.094505
6	1.168347 1.420130 -0.052508	6	0.326801 -1.849072 0.259333
6	-1.299051 1.423875 -0.035791	6	-0.245447 1.861646 -0.130503
6	-2.472832 0.702783 -0.018062	6	-1.626026 1.934170 -0.123148
6	-2.472831 -0.702784 0.018061	6	-2.359022 0.746265 -0.030030

6	-1.299049	-1.423875	0.035785
7	3.651754	-1.128945	0.163690
6	4.545138	0.000002	-0.000041
7	3.651752	1.128959	-0.163716
7	-3.814890	1.071789	-0.027740
6	-4.667711	-0.000003	-0.000006
7	-3.814888	-1.071792	0.027746
6	4.097523	-2.450189	-0.177285
6	4.097508	2.450183	0.177369
6	-4.263737	2.441367	-0.065116
6	-4.263733	-2.441371	0.065129
1	1.163697	-2.504343	0.106059
1	1.163694	2.504346	-0.106077
1	-1.298392	2.509602	-0.065051
1	-1.298389	-2.509602	0.065048
1	3.406810	-3.190410	0.229812
1	4.172684	-2.609673	-1.264428
1	5.078386	-2.639174	0.265704
1	5.078439	2.639150	-0.265473
1	3.406881	3.190442	-0.229809
1	4.172513	2.609629	1.264528
1	-3.908502	2.945705	-0.969513
1	-5.352037	2.438390	-0.060087
1	-3.900329	2.996784	0.805377
1	-5.352033	-2.438396	0.060093
1	-3.908503	-2.945704	0.969531
1	-3.900317	-2.996791	-0.805358
1	5.203648	-0.125061	-0.881293
1	5.203711	0.125055	0.881163
7-H₂			
6	-0.333744	1.323446	-0.016261
6	-1.321948	0.332120	-0.100773
6	-0.927089	-1.001619	-0.033799
6	0.420127	-1.341056	-0.046521
6	1.429356	-0.361431	-0.072279
6	1.041441	0.990600	-0.023809
7	1.705398	2.214103	0.112885
6	0.855349	3.273492	0.262407
7	-0.380104	2.709696	0.166840
7	1.066312	-2.569837	-0.106034
6	2.420928	-2.446752	-0.194065
7	2.623578	-1.092811	-0.159370
7	-2.736116	0.404327	-0.140407
6	-3.139415	-1.009427	-0.368719
7	-2.064275	-1.856071	0.116927
6	3.130816	2.433397	0.196588
6	3.969762	-0.581047	-0.277342
6	-2.255528	-2.240938	1.523140
6	0.401789	-3.850099	-0.230399
6	-1.561246	3.502850	0.446984
6	-3.345913	1.252851	-1.153356
1	3.272264	3.498359	0.369955
1	3.637904	2.153631	-0.729234
1	4.061017	0.100862	-1.126181
1	4.615637	-1.441431	-0.441465
1	-1.380710	-2.790262	1.873850
1	-3.123236	-2.899711	1.602199
1	-0.263689	-3.859695	-1.096029
1	1.177244	-4.603739	-0.354513
1	-1.255158	4.342570	1.068416
1	-2.008512	3.904237	-0.466796
1	-3.024993	2.285108	-1.061231
1	-3.109350	0.904498	-2.172898
1	3.569826	1.875435	1.027094
1	4.292739	-0.066707	0.630554
1	-0.188896	-4.085263	0.657742
1	-2.400010	-1.374823	2.186179
1	-4.431733	1.229717	-1.031445
1	-2.301623	2.905872	0.981938
1	-3.265119	-1.165634	-1.455028
6	-1.715935	-0.474734	0.075213
7	-3.742194	0.539183	-0.083431
6	-3.920352	-0.825475	0.429973
7	-2.674511	-1.528620	0.130893
7	3.813055	-0.569066	0.094193
6	4.147292	0.745146	-0.059603
7	2.921199	1.362969	-0.124193
6	-2.736331	-2.322948	-1.100412
6	-4.637681	1.537331	0.445184
6	2.829495	2.795581	-0.298550
6	4.793058	-1.622117	0.216704
1	2.182825	-2.914522	0.416177
1	-0.292850	-2.727272	0.406303
1	0.315314	2.783409	-0.206246
1	-2.123075	2.895557	-0.204010
1	-4.778850	-1.322393	-0.031792
1	-4.079225	-0.794768	1.524936
1	-3.036691	-1.729462	-1.976947
1	-1.755210	-2.753960	-1.303240
1	-3.444903	-3.143567	-0.968969
1	-4.442870	2.504946	-0.020670
1	-5.669924	1.263779	0.215087
1	-4.546641	1.653414	1.538534
1	2.289262	3.049135	-1.214974
1	3.847463	3.175134	-0.367308
1	2.328896	3.268075	0.551124
1	4.692133	-2.142164	1.173931
1	5.779391	-1.165818	0.159252
1	4.686666	-2.353124	-0.590213
8-H₂			
6	1.304397	-0.723308	0.010470
6	1.304397	0.723289	-0.010414
6	-2.394034	1.427682	-0.036810
6	-3.556521	0.715420	-0.040319
6	-3.556536	-0.715457	0.040181
6	-2.394033	-1.427718	0.036798
6	2.535553	-1.431176	0.021591
6	3.699459	-0.707956	0.011028
6	3.699457	0.707952	-0.011019
6	2.535546	1.431164	-0.021553
7	-4.870772	1.126970	-0.151448
6	-5.765503	0.000099	0.000697
7	-4.870765	-1.126996	0.150875
7	5.043159	-1.073181	0.016796
6	5.893718	0.000002	-0.000017
7	5.043156	1.073182	-0.016798
6	-5.320866	2.458615	0.137783
6	-5.321068	-2.458593	-0.138159
6	5.492851	-2.442980	0.039439
6	5.492841	2.442984	-0.039431
1	-2.388985	2.512225	-0.078209
1	-2.388982	-2.512261	0.078198
1	2.534797	-2.516964	0.037856
1	2.534782	2.516952	-0.037822
1	-5.388419	2.661659	1.217583
1	-4.636049	3.184286	-0.304301
1	-6.305780	2.623470	-0.305329
1	-6.306054	-2.623201	0.304876
1	-5.388538	-2.661816	-1.217922
1	-4.636471	-3.184360	0.304132
1	5.131444	-2.987913	-0.838393
1	6.581082	-2.439635	0.037288
1	5.134920	-2.957364	0.936964
1	6.581072	2.439644	-0.037266
1	5.131419	2.987914	0.838396
1	5.134920	2.957366	-0.936960
6	0.070466	-1.392924	0.019348
6	-1.148035	-0.723668	0.010466
6	0.070462	1.392897	-0.019298
6	-1.148030	0.723633	-0.010459

1	-4.085267	-1.237184	0.130230	1	0.070851	-2.480787	0.036603
				1	0.070839	2.480761	-0.036555
				1	-6.424720	-0.114000	-0.881209
				1	-6.422695	0.114451	0.884158
9-H₂				10-H₂			
6	3.185752	-2.061516	0.238551	6	3.771726	0.663051	0.075595
6	3.699589	-0.754956	0.103326	6	3.741973	-0.760167	0.024871
6	2.887485	0.362291	-0.003653	6	2.505384	-1.401979	0.005228
6	-0.822821	1.120326	-0.053849	6	-1.196415	-0.646147	0.013749
6	-1.340810	-0.224003	0.046106	6	-1.175915	0.794249	-0.002060
6	1.827577	-2.210743	0.257370	6	2.565134	1.361454	0.056339
6	-1.727691	2.215637	-0.116124	6	-2.443737	-1.308119	0.074444
6	-3.088951	2.034384	-0.090856	6	-3.656579	0.751055	0.008188
6	-3.589540	0.717934	-0.013398	6	-2.446718	1.444338	-0.034286
6	-2.742481	-0.367405	0.053423	7	-4.650787	1.704723	-0.193002
7	-4.914585	0.273224	-0.060480	6	-4.147965	2.968232	-0.343306
6	-4.843957	-1.117272	0.409453	7	-2.801611	2.781737	-0.214705
7	-3.493702	-1.578224	0.090162	7	4.693525	-1.777091	-0.028806
7	5.004175	-0.294721	0.050459	6	4.130281	-3.025380	-0.081283
6	5.084645	1.062452	-0.086205	7	2.794129	-2.765912	-0.054472
7	3.764032	1.438842	-0.115661	6	-1.897881	3.904400	-0.337182
6	-3.419709	-2.342360	-1.159587	6	-6.061848	1.455494	-0.414503
6	-5.969351	1.077459	0.503419	6	1.855413	-3.867351	-0.114492
6	3.398464	2.831695	-0.248692	6	6.134686	-1.666476	-0.081444
6	6.167469	-1.147113	0.128332	1	-2.510527	4.787657	-0.508359
1	3.849790	-2.915432	0.323280	1	-1.312616	4.047249	0.575779
1	1.387772	-3.198073	0.358993	1	-1.215834	3.772015	-1.181875
1	-1.316658	3.219073	-0.178200	1	-6.204834	0.495186	-0.912386
1	-3.762460	2.883837	-0.143574	1	-6.628932	1.469463	0.520509
1	-3.827760	-1.793151	-2.021617	1	-6.440894	2.253602	-1.050520
1	-2.377947	-2.582765	-1.374814	1	1.233880	-3.915392	0.782924
1	-3.966381	-3.281177	-1.046807	1	2.449042	-4.776867	-0.185825
1	-5.893976	1.167806	1.600320	1	1.209420	-3.790847	-0.992964
1	-5.953459	2.080269	0.072972	1	6.542357	-1.222570	0.828461
1	-6.937913	0.632676	0.263309	1	6.458050	-1.082101	-0.944919
1	2.808326	3.002057	-1.153373	1	6.515587	-2.681223	-0.178689
1	4.324035	3.400731	-0.313825	6	0.009640	-1.349784	0.022437
1	2.827676	3.175452	0.618267	6	1.252150	-0.715905	0.013040
1	6.176357	-1.873700	-0.689279	6	0.068462	1.429068	0.012394
1	6.193902	-1.689237	1.078145	6	1.281714	0.731645	0.019246
1	7.048316	-0.512649	0.053901	7	4.768688	1.634392	0.151392
6	0.562941	1.313094	-0.071583	6	4.265835	2.907205	0.175784
6	1.465506	0.252094	0.012715	7	2.919001	2.711701	0.111328
6	-0.440188	-1.288450	0.154784	6	2.039056	3.861177	0.121006
6	0.940615	-1.095581	0.142346	6	6.200309	1.454447	0.250972
1	-5.602579	-1.744608	-0.068271	1	1.431625	3.909149	-0.786890
1	-5.001563	-1.147590	1.504772	1	2.678336	4.740838	0.166679
1	0.923607	2.331714	-0.148943	1	1.381233	3.854041	0.994349
1	-0.825798	-2.296879	0.278132	1	6.615855	0.990399	-0.645169
				1	6.466244	0.856543	1.124525
				1	6.626215	2.449753	0.360585
				7	-2.638141	-2.723017	0.026561
				6	-3.998002	-2.874075	0.512856
				7	-4.705929	-1.590871	0.256066
				6	-5.737880	-1.375793	1.257536
				6	-2.448929	-3.258754	-1.327031
				1	-6.197565	-0.398184	1.157342
				1	-5.334773	-1.466510	2.279992
				1	-6.520819	-2.127917	1.134619
				1	-1.431435	-3.047605	-1.660528
				1	-3.144132	-2.823462	-2.060835
				1	-2.582311	-4.342687	-1.310103
				6	-3.655783	-0.658679	0.152601
				1	-3.986229	-3.048992	1.603917
				1	-4.508137	-3.712488	0.030637
				1	0.093825	2.503319	0.032390
				1	-0.059433	-2.425224	0.081626
11-H₂				12-H₂			

6	-0.782304	-0.677100	0.320133	6	-0.232357	0.312635	1.236087
6	-0.782426	0.677336	0.320111	6	0.823900	-0.753279	0.955902
7	-2.062883	-1.082546	0.005086	6	0.971910	-1.095556	-0.346442
6	-2.921342	-0.000145	-0.083681	6	0.063445	-0.356481	-1.322143
7	-2.063036	1.082536	0.005115	6	0.200207	1.445896	0.303000
6	-2.534437	2.447878	-0.073334	6	0.321574	1.112725	-0.994420
6	-2.533700	-2.448054	-0.073783	6	-1.325874	-0.584919	-0.741445
1	-2.540750	2.920073	0.912520	6	-1.474974	-0.242759	0.560391
1	-3.548550	2.435100	-0.468440	7	-2.833039	-0.170418	0.793522
1	-2.539674	-2.920613	0.911898	6	-3.575015	-0.510883	-0.313614
1	-3.547857	-2.435634	-0.468790	7	-2.596827	-0.717634	-1.259746
1	-1.890183	3.029971	-0.736906	7	1.165537	2.036218	-1.687902
1	-1.889243	-3.029611	-0.737645	6	1.149496	3.164393	-0.759284
6	0.658170	-0.679377	-0.203875	7	0.948792	2.592715	0.594918
6	0.658248	0.679694	-0.204004	7	1.743198	-2.237991	-0.366331
7	1.887194	-1.153554	0.260573	6	2.136182	-2.629956	0.893955
6	2.773027	-0.000068	0.045018	7	1.505578	-1.701028	1.690477
7	1.887332	1.153753	0.260772	1	-0.353093	0.590910	2.285983
6	2.421315	2.434907	-0.141994	1	0.179948	-0.621623	-2.375631
6	2.420754	-2.435040	-0.141488	6	-3.436501	0.144643	2.068033
1	2.730612	2.446975	-1.199343	1	-4.516798	0.123254	1.937807
1	3.288636	2.686610	0.473431	1	-3.152979	-0.585568	2.831638
1	2.729457	-2.448086	-1.198997	1	-3.136231	1.141200	2.406783
1	3.288422	-2.686251	0.473632	6	-2.898709	-1.091995	-2.623116
1	1.662884	3.204567	0.006509	1	-2.471449	-2.068708	-2.867482
1	1.662379	-3.204547	0.008137	1	-3.981473	-1.140906	-2.720993
1	3.159586	0.000180	-1.004125	1	-2.507920	-0.351549	-3.326962
1	3.630197	-0.000248	0.728685	6	1.618693	-1.706769	3.131239
				1	0.635572	-1.808127	3.600605
				1	2.236100	-2.557888	3.411360
				1	2.087243	-0.787229	3.493322
				6	2.170279	-2.922891	-1.564740
				1	2.773259	-3.777031	-1.262734
				1	1.310282	-3.276605	-2.141069
				1	2.771355	-2.266053	-2.200670
				6	2.508653	1.478612	-1.901570
				1	2.997521	1.145311	-0.973651
				1	2.435273	0.621094	-2.575271
				1	3.135733	2.228066	-2.388809
				6	0.437435	3.540897	1.560581
				1	-0.490041	4.031508	1.218009
				1	0.234030	3.041035	2.510116
				1	1.185169	4.315045	1.748445
				1	2.064891	3.759272	-0.820277
				1	0.280878	3.805680	-0.999573
13-H₂				14-H₂			
6	0.044334	0.014626	1.285085	6	2.583028	-0.076536	1.363152
6	-1.356584	0.007269	0.696147	6	1.182731	-0.136547	0.708662
6	-1.356583	-0.007221	-0.696163	6	1.216624	-0.175983	-0.690624
6	0.044331	-0.014640	-1.285114	6	2.645740	-0.151264	-1.279984
6	0.752645	-1.205933	0.718860	6	3.311417	-1.259368	0.766045
6	0.752344	-1.222041	-0.690927	6	3.343123	-1.296654	-0.583087
6	0.752669	1.205897	-0.718897	6	3.246738	1.091435	-0.655103
6	0.752366	1.221998	0.690897	6	3.217141	1.128748	0.697357
7	2.613891	4.429224	1.021253	7	3.503135	2.428872	1.061327
6	3.044356	5.156655	-0.057434	6	3.755699	3.233660	-0.025705
7	2.614889	4.405251	-1.120052	7	3.546858	2.370528	-1.077049
7	2.613099	-4.429701	-1.021253	7	3.948217	-2.486342	-0.932835
6	3.043373	-5.157241	0.057444	6	4.325412	-3.220647	0.167369
7	2.614056	-4.405726	1.120051	7	3.898192	-2.428067	1.207690
7	-5.054416	0.109243	-1.145536	6	0.035757	-0.195415	-1.423664
6	-5.944008	0.000526	0.000015	6	-0.033063	-0.120080	1.383039
7	-5.054394	-0.108453	1.145542	1	2.547859	-0.047603	2.454023
1	0.042946	0.027127	2.377986	1	2.662120	-0.184746	-2.371191
1	0.042924	-0.027164	-2.378014	6	3.583390	2.907263	2.422585
6	2.843352	4.833520	2.387420	1	3.834380	3.965526	2.388095
1	3.390851	5.773956	2.369964	1	2.625374	2.782729	2.936512
1	1.897229	4.977230	2.918352	1	4.354765	2.373073	2.984323
1	3.432764	4.083762	2.924028	6	3.679677	2.775477	-2.457753

6	2.845885	4.779365	-2.494590	1	2.743705	2.616005	-3.002504
1	1.900410	4.909343	-3.030139	1	3.923076	3.836021	-2.470434
1	3.391474	5.721111	-2.497076	1	4.475753	2.217886	-2.958997
1	3.437854	4.019205	-3.013445	6	4.192534	-2.927569	-2.287099
6	-5.485840	0.440281	2.402291	1	3.255343	-3.028933	-2.842315
1	-5.579048	1.538586	2.381657	1	4.841323	-2.225607	-2.818956
1	-6.455635	0.020422	2.681501	1	4.682829	-3.897834	-2.235751
1	-4.777210	0.171655	3.187176	6	4.078620	-2.795684	2.593542
6	-5.486117	-0.439564	-2.402162	1	4.562960	-3.770133	2.616806
1	-6.454834	-0.017949	-2.682512	1	4.708497	-2.069269	3.115293
1	-4.776300	-0.173090	-3.186686	1	3.116683	-2.861290	3.110340
1	-5.581620	-1.537653	-2.380653	6	-2.644279	-0.060996	1.230258
6	2.842448	-4.834083	-2.387414	6	-1.213901	-0.128695	0.648775
1	1.896297	-4.976944	-2.918527	6	-1.180048	-0.161734	-0.750350
1	3.432577	-4.084767	-2.923856	6	-2.578587	-0.100056	-1.400971
1	3.389130	-5.774998	-2.369942	6	-3.211530	1.173471	0.552491
6	2.845096	-4.779789	2.494602	6	-3.199086	1.144486	-0.790696
1	3.389710	-5.722102	2.497119	6	-3.328428	-1.241254	-0.759216
1	3.437978	-4.020099	3.013108	6	-3.359494	-1.221167	0.588510
1	1.899651	-4.908685	3.030465	7	-4.085789	-2.325845	0.985977
6	-2.551369	-0.001636	-1.421357	6	-4.528175	-3.067261	-0.084565
6	-2.551368	0.001944	1.421333	7	-4.035380	-2.357684	-1.155626
6	-3.736117	0.014407	-0.701585	7	-3.295447	2.463389	-1.336656
6	-3.736124	-0.013851	0.701552	6	-3.793395	3.201304	-0.176823
6	1.348084	2.216903	-1.456108	7	-3.293488	2.489368	1.025309
6	1.347519	2.249267	1.405459	1	-2.661813	-0.043619	2.322453
6	1.942718	3.252512	-0.735589	1	-2.549716	-0.112683	-2.492715
6	1.942205	3.268285	0.662043	6	-4.366383	-2.688295	2.355980
6	1.347397	-2.249363	-1.405487	1	-4.962451	-3.598734	2.342054
6	1.942085	-3.268375	-0.662064	1	-3.442524	-2.873380	2.912069
6	1.347954	-2.216988	1.456088	1	-4.928879	-1.899399	2.864057
6	1.942597	-3.252594	0.735573	6	-4.255526	-2.758452	-2.526443
1	-6.602997	-0.885234	-0.086140	1	-3.308277	-2.965005	-3.033281
1	-6.602795	0.886434	0.086159	1	-4.857744	-3.664742	-2.513646
1	-2.545912	-0.008196	2.507357	1	-4.787582	-1.980670	-3.081405
1	-2.545900	0.008431	-2.507382	6	-1.994499	2.948360	-1.817133
1	1.347605	-2.258501	-2.491609	1	-1.203224	2.918109	-1.051779
1	1.348738	-2.201585	2.542139	1	-1.673570	2.333418	-2.661663
1	1.347599	2.258453	2.491580	1	-2.104048	3.973304	-2.177671
1	1.348733	2.201576	-2.542159	6	-4.051720	2.763052	2.226052
				1	-3.916097	3.807327	2.518209
				1	-5.132078	2.578685	2.093876
				1	-3.693369	2.140450	3.048567
				1	-0.060383	-0.087432	2.470222
				1	0.062228	-0.215141	-2.511633
				1	-3.477811	4.247934	-0.191872
				1	-4.898509	3.154633	-0.175670

Optimized geometries of CuCl coordinated NHC systems at M06L/6-311++G(d,p) level .All the X, Y, Z coordinates are given in Å.

1-CuCl				2-CuCl			
6	-2.904009	0.677299	0.000167	6	-1.646689	0.676593	0.000111
6	-2.904021	-0.677270	0.000191	7	-2.962137	1.087852	0.000194
7	-1.581965	1.071583	0.000123	6	-3.811558	0.000003	-0.000091
6	-0.738266	-0.000005	0.000043	7	-2.962139	-1.087849	-0.000030
7	-1.581985	-1.071576	0.000105	6	-1.646690	-0.676592	-0.000025
6	-1.131786	-2.449642	0.000141	6	-3.441582	2.453178	0.000407
6	-1.131742	2.449641	0.000097	6	-3.441587	-2.453173	-0.000011
1	-1.490193	-2.970159	0.890393	7	-0.335520	-1.097970	-0.000050
1	-0.041418	-2.449049	-0.000130	6	0.495877	-0.000002	-0.000072
1	-1.490414	2.970288	0.890165	7	-0.335517	1.097968	0.000150
1	-0.041374	2.449030	0.000153	6	0.146612	-2.464054	-0.000265
1	-1.490644	-2.970341	-0.889822	6	0.146617	2.464051	0.000490
1	-1.490316	2.970222	-0.890050	1	-3.102370	2.988857	0.890540
1	-3.718173	1.383179	0.000201	1	-4.528728	2.413529	0.000497
1	-3.718199	-1.383135	0.000252	1	-3.102529	2.989058	-0.889664
29	1.145104	-0.000003	-0.000081	1	-3.102653	-2.988891	0.890205

17	3.251725	-0.000009	-0.000249	1	-4.528733	-2.413523	-0.000251
				1	-3.102258	-2.989017	-0.889998
				1	-0.194396	-2.995683	0.890658
				1	1.236961	-2.431355	0.000021
				1	-0.193936	-2.995231	-0.891639
				1	-0.194381	2.995741	-0.890401
				1	1.236966	2.431350	0.000210
				1	-0.193939	2.995168	0.891896
				29	2.376583	-0.000001	-0.000118
				17	4.482957	0.000001	-0.000221
3-CuCl				4-CuCl			
6	-2.889771	0.704939	0.000014	6	-1.532882	2.343103	0.000036
6	-2.889771	-0.704940	0.000013	6	-0.568568	1.336407	0.000018
6	-1.721100	-1.456849	0.000008	6	-0.853290	-0.041307	0.000007
6	-0.552091	-0.703652	0.000003	6	-2.203182	-0.427772	0.000015
6	-0.552092	0.703653	0.000004	6	-3.164102	0.600792	0.000033
6	-1.721101	1.456850	0.000009	6	-2.864628	1.962987	0.000043
7	0.781448	-1.083226	-0.000003	7	-2.939805	-1.610545	0.000011
6	1.612089	0.000001	-0.000008	6	-4.297437	-1.393620	0.000025
7	0.781448	1.083228	-0.000002	7	-4.396191	-0.036405	0.000037
7	-4.227383	1.071712	0.000020	7	0.812147	1.448367	0.000008
6	-5.081350	-0.000001	0.000023	6	1.411718	0.231305	-0.000010
7	-4.227383	-1.071714	0.000019	7	0.386078	-0.677104	-0.000009
1	-1.719876	-2.540644	0.000007	6	1.529722	2.704281	0.000014
1	-1.719878	2.540644	0.000009	6	-5.659766	0.665093	0.000054
6	-4.679198	-2.443593	0.000020	6	-2.431076	-2.964175	-0.000006
1	-4.322563	-2.972150	-0.888899	1	-1.244419	3.387567	0.000043
1	-4.322556	-2.972151	0.888935	1	-3.657146	2.702577	0.000057
1	-5.766923	-2.436278	0.000024	1	1.282739	3.287725	0.890237
6	-4.679200	2.443592	0.000022	1	1.282720	3.287744	-0.890191
1	-4.322566	2.972149	-0.888898	1	2.597669	2.483272	0.000001
1	-5.766925	2.436275	0.000027	1	-6.452733	-0.079791	0.000060
1	-4.322557	2.972149	0.888937	1	-5.755500	1.294795	0.889007
6	1.237891	2.455223	-0.000002	1	-5.755520	1.294801	-0.888893
1	0.880749	2.979520	0.890092	1	-3.296123	-3.623930	0.000005
1	2.328363	2.451965	-0.000007	1	-1.831470	-3.165491	-0.890649
1	0.880741	2.979522	-0.890092	1	-1.831440	-3.165501	0.890614
6	1.237892	-2.455221	-0.000005	6	0.654366	-2.100082	-0.000025
1	0.880748	-2.979521	0.890086	1	0.243836	-2.577712	-0.891270
1	0.880746	-2.979518	-0.890097	1	1.738152	-2.226952	-0.000044
1	2.328364	-2.451962	-0.000007	1	0.243866	-2.577727	0.891227
29	3.491504	0.000001	-0.000017	29	3.261568	-0.119331	-0.000030
17	5.596494	-0.000002	-0.000027	17	5.334649	-0.484295	-0.000053
5-CuCl				6-CuCl			
6	-1.781868	-0.725385	-0.000001	6	-0.394103	2.396774	-0.000005
6	-1.781870	0.725388	0.000007	6	0.550162	1.364485	-0.000006
6	-0.552994	1.429932	0.000033	6	0.190146	0.020755	0.000000
6	0.611939	0.706458	0.000051	6	-1.170594	-0.384960	0.000009
6	0.611940	-0.706450	0.000044	6	-2.142631	0.685713	0.000010
6	-0.552990	-1.429927	0.000033	6	-1.720470	2.042493	0.000003
6	-3.012031	-1.429148	-0.000041	6	-1.592292	-1.739631	0.000018
6	-4.177909	-0.707384	-0.000070	6	-2.922780	-2.085863	0.000026
6	-4.177911	0.707380	-0.000032	6	-3.867522	-1.055751	0.000026
6	-3.012035	1.429147	-0.000006	6	-3.504740	0.288384	0.000018
7	1.947580	1.085851	0.000074	7	-5.250075	-1.089056	0.000034
6	2.774547	0.000007	0.000083	6	-5.808471	0.156419	0.000032
7	1.947584	-1.085838	0.000066	7	-4.711596	0.984705	0.000020
7	-5.517470	-1.073995	-0.000119	7	1.930466	1.413324	-0.000014
6	-6.368596	-0.000006	-0.000137	6	2.466821	0.163206	-0.000014
7	-5.517473	1.073987	-0.000038	7	1.390783	-0.683764	-0.000005
6	2.404487	2.457326	0.000152	6	-4.890925	2.421416	0.000009
6	2.404498	-2.457311	0.000178	6	-6.032791	-2.304106	0.000042
6	-5.969613	-2.445222	-0.000091	6	1.571972	-2.122760	-0.000002
6	-5.969622	2.445212	-0.000035	6	2.715430	2.628868	-0.000024
1	-0.551886	2.515046	0.000046	1	-0.089766	3.437196	-0.000010
1	-0.551880	-2.515040	0.000055	1	-2.463565	2.826832	0.000004
1	-3.011559	-2.514512	-0.000043	1	-0.854425	-2.528682	0.000018
1	-3.011565	2.514511	0.000005	1	-3.227596	-3.126611	0.000033

1	2.046209	2.981364	0.889944	1	-5.963435	2.605896	0.000012
1	3.494968	2.455090	0.000135	1	-4.451271	2.877142	0.891235
1	2.046189	2.981472	-0.889568	1	-4.451278	2.877128	-0.891227
1	3.494979	-2.455069	-0.000337	1	-5.821610	-2.904829	-0.888894
1	2.046643	-2.981211	0.890224	1	-5.821601	-2.904822	0.888981
1	2.045786	-2.981598	-0.889289	1	-7.082949	-2.020326	0.000047
1	-5.611885	-2.973604	0.888530	1	1.131150	-2.572146	0.892331
1	-7.057422	-2.438986	-0.000405	1	2.645691	-2.318058	-0.000011
1	-5.611370	-2.973781	-0.888397	1	1.131134	-2.572150	-0.892326
1	-7.057430	2.438971	0.000191	1	2.502044	3.224991	0.890320
1	-5.611824	2.973630	-0.888606	1	2.502048	3.224975	-0.890381
1	-5.611453	2.973738	0.888321	1	3.769279	2.348471	-0.000019
29	4.652637	0.000003	0.000026	29	4.294010	-0.290490	-0.000024
17	6.756803	-0.000014	-0.000144	17	6.342325	-0.781170	-0.000031
7-CuCl				8-CuCl			
6	0.199303	-0.703894	0.050474	6	0.603372	0.726083	0.000113
6	1.416442	-1.415236	0.040957	6	0.603202	-0.725423	0.000108
6	2.633243	-0.704949	-0.008477	6	4.287654	-1.434830	0.000141
6	2.633269	0.704804	0.009338	6	5.447426	-0.711122	0.000074
6	1.416588	1.415221	-0.041766	6	5.447609	0.710583	-0.000033
6	0.199352	0.704002	-0.051681	6	4.288007	1.434578	-0.000046
7	-1.144005	1.079867	-0.105689	6	-0.629572	1.436192	0.000155
6	-1.963278	0.000075	-0.000448	6	-1.788038	0.710678	0.000115
7	-1.144031	-1.079748	0.104596	6	-1.788203	-0.709478	0.000096
7	3.627599	1.682441	0.097972	6	-0.629896	-1.435249	0.000100
6	3.123742	2.948622	0.102851	7	6.788544	-1.074982	0.000076
7	1.776631	2.766386	0.000816	6	7.638684	-0.000546	-0.000142
7	1.776272	-2.766412	-0.002405	7	6.788802	1.074116	-0.000056
6	3.123472	-2.948786	-0.103172	7	-3.125258	1.087279	0.000122
7	3.627534	-1.682686	-0.096550	6	-3.950907	0.000858	0.000012
6	-1.722263	2.391406	-0.322406	7	-3.125489	-1.085788	0.000136
6	0.927460	3.938416	0.032239	6	7.240839	-2.445858	0.000294
6	5.050410	-1.511726	-0.306788	6	7.241437	2.444875	-0.000220
6	5.050148	1.511383	0.310368	6	-3.582376	2.458524	0.000586
6	-1.722123	-2.391125	0.322825	6	-3.582855	-2.456950	0.000099
6	0.926842	-3.938173	-0.037092	1	4.286660	-2.520157	0.000213
1	-2.797499	2.247609	-0.442278	1	4.287296	2.519907	-0.000123
1	-1.324665	2.845180	-1.230811	1	-0.630179	2.521243	0.000237
1	0.344269	4.043931	-0.883274	1	-0.630751	-2.520300	0.000108
1	1.595083	4.792430	0.123660	1	6.882388	-2.974181	0.888731
1	5.243815	-0.863652	-1.163625	1	6.882314	-2.974466	-0.887943
1	5.448106	-2.502880	-0.514236	1	8.328671	-2.439878	0.000249
1	5.552273	1.109211	-0.570192	1	8.329267	2.438627	0.000211
1	5.447623	2.502510	0.518372	1	6.883436	2.973207	-0.888835
1	-2.797153	-2.247159	0.444367	1	6.882727	2.973659	0.887837
1	-1.554271	-3.052488	-0.526500	1	-3.224624	2.981943	0.890997
1	0.256669	-3.920064	-0.898558	1	-3.222691	2.983071	-0.888369
1	1.594276	-4.792068	-0.131057	1	-4.672839	2.456592	-0.000580
1	-1.552970	3.052300	0.527002	1	-4.673328	-2.454846	0.000156
1	0.257308	3.923033	0.893781	1	-3.224186	-2.981048	0.889736
1	5.242178	0.863329	1.167528	1	-3.224278	-2.980943	-0.889636
1	5.551204	-1.109626	0.574562	6	1.828784	1.396690	0.000078
1	0.343697	-4.046347	0.878142	6	3.053723	0.725797	0.000047
1	-1.323070	-2.844418	1.230838	6	1.828450	-1.396330	0.000134
29	-3.851018	0.000046	0.000205	6	3.053547	-0.725737	0.000113
17	-5.955470	-0.000078	0.001284	1	1.828752	2.483929	0.000058
9-CuCl				10-CuCl			
6	-4.306098	-2.371171	0.000044	6	4.832084	-0.404815	-0.110916
6	-5.058126	-1.179977	0.000068	6	4.271752	-1.701901	0.060992
6	-4.472127	0.077435	0.000069	6	2.884759	-1.828074	0.145312
6	-0.968390	1.512826	0.000022	6	-0.270868	0.258851	0.078488
6	-0.202418	0.286959	-0.000001	6	0.301954	1.581363	0.041965
6	-2.942897	-2.263194	0.000021	6	3.976667	0.696684	-0.148663
6	-0.313047	2.782249	0.000022	6	-1.696247	0.162345	0.068146
6	1.048399	2.897794	0.000001	6	-1.982546	2.572685	0.121508
6	1.798859	1.704528	-0.000020	6	-0.593736	2.694969	0.091043

6	1.213369	0.447426	-0.000021	7	-2.476188	3.871328	0.216584
7	3.166022	1.509175	-0.000040	6	-1.480837	4.810232	0.247991
6	3.475811	0.182641	-0.000054	7	-0.343444	4.064289	0.161860
7	2.266030	-0.457696	-0.000042	7	4.775094	-2.993185	0.191149
7	-6.425109	-0.971638	0.000091	6	3.790419	-3.930426	0.356074
6	-6.760517	0.353673	0.000118	7	2.646668	-3.192153	0.319477
7	-5.535317	0.974347	0.000090	6	0.942175	4.730912	0.198381
6	2.171418	-1.904219	-0.000049	6	-3.848017	4.313524	0.353260
6	4.152712	2.568273	-0.000043	6	1.371605	-3.855721	0.492524
6	-5.440003	2.418076	0.000092	6	6.155060	-3.430487	0.203424
6	-7.408092	-2.031588	0.000092	1	0.737495	5.793397	0.315311
1	-4.795619	-3.339395	0.000043	1	1.542644	4.387028	1.044435
1	-2.324522	-3.155147	0.000002	1	1.500276	4.578201	-0.729270
1	-0.933317	3.672819	0.000039	1	-4.436999	4.100437	-0.539948
1	1.537184	3.865771	0.000002	1	-4.326360	3.858826	1.223006
1	3.187860	-2.301446	-0.000063	1	-3.807957	5.391220	0.496546
1	1.651088	-2.259168	0.892159	1	0.836275	-3.466086	1.362689
1	1.651067	-2.259157	-0.892249	1	1.588626	-4.910135	0.652544
1	4.047371	3.192666	-0.890355	1	0.743307	-3.756278	-0.396919
1	4.047393	3.192651	0.890283	1	6.717539	-2.952823	1.007283
1	5.141805	2.108668	-0.000059	1	6.649202	-3.235313	-0.749732
1	-4.919102	2.779576	0.890918	1	6.133862	-4.504563	0.375557
1	-6.456921	2.805900	0.000115	6	0.593228	-0.837601	0.115011
1	-4.919140	2.779583	-0.890753	6	1.985350	-0.721328	0.078904
1	-7.305538	-2.660148	0.889006	6	1.691639	1.695625	-0.036632
1	-7.305558	-2.660135	-0.888834	6	2.556727	0.598065	-0.039748
1	-8.393056	-1.569078	0.000107	7	6.115489	0.110663	-0.268670
6	-2.363741	1.443551	0.000045	6	6.124944	1.473275	-0.405917
6	-3.056624	0.231161	0.000046	7	4.806492	1.805250	-0.324023
6	-0.892531	-0.925169	-0.000001	6	4.417520	3.193820	-0.452465
6	-2.288662	-0.994781	0.000022	6	7.375564	-0.598456	-0.334785
29	5.183066	-0.609615	-0.000077	1	3.751228	3.342917	-1.306535
17	7.083134	-1.519460	-0.000100	1	5.332991	3.759900	-0.613813
1	-0.351671	-1.863405	-0.000020	1	3.930843	3.560412	0.455619
1	-2.906664	2.380831	0.000063	1	7.386876	-1.316238	-1.156853
				1	7.597729	-1.114577	0.600502
				1	8.140137	0.154727	-0.512516
				7	-2.523335	-0.956320	0.010674
				6	-3.834604	-0.602206	-0.035200
				7	-3.840416	0.762267	0.005349
				6	-5.096718	1.479475	-0.089435
				6	-2.140651	-2.354359	-0.043590
				1	-5.304294	2.045171	0.818729
				1	-5.881200	0.732672	-0.222865
				1	-5.097996	2.148782	-0.950384
				1	-1.617580	-2.656590	0.866310
				1	-1.513078	-2.553192	-0.914743
				1	-3.059627	-2.937435	-0.129453
				6	-2.547453	1.267675	0.071313
				29	-5.320172	-1.758818	-0.152739
				17	-6.961581	-3.070079	-0.293399
				1	2.117519	2.678801	-0.100725
				1	0.169262	-1.821919	0.173746
11-CuCl				12-CuCl			
6	2.429859	0.680452	-0.276113	6	-1.345657	0.001060	-1.338529
6	2.429868	-0.680466	-0.276104	6	-1.813303	-1.292698	-0.677733
7	3.726869	1.084807	-0.060311	6	-1.813410	-1.292660	0.677735
6	4.587403	0.000011	-0.041788	6	-1.345826	0.001120	1.338535
7	3.726882	-1.084795	-0.060280	6	-2.226160	1.057579	-0.677831
6	4.208324	-2.450850	-0.026074	6	-2.226244	1.057608	0.677665
6	4.208294	2.450869	-0.026139	6	0.008872	0.235453	0.678767
1	3.617210	-3.039324	0.678872	6	0.008966	0.235422	-0.678588
1	5.248073	-2.433235	0.293069	7	1.318056	0.137253	-1.081306
1	3.617174	3.039353	0.678794	6	2.162818	0.111299	0.000253
1	5.248044	2.433276	0.293000	7	1.317909	0.137305	1.081663
1	4.145080	-2.912486	-1.014087	7	-2.825056	2.235597	1.070093
1	4.145041	2.912481	-1.014163	6	-3.256087	2.985488	-0.000186
6	1.022391	0.680137	0.325852	7	-2.824967	2.235530	-1.070385
6	1.022391	-0.680159	0.325843	7	-2.548487	-2.390282	1.070032
7	-0.267502	1.095971	0.110864	6	-2.994107	-3.131957	-0.000037

6	-1.107735	-0.000007	0.080273	7	-2.548339	-2.390330	-1.070079
7	-0.267501	-1.095984	0.110833	1	-1.343151	0.001100	-2.430057
6	-0.750019	-2.463583	0.070097	1	-1.343487	0.001227	2.430063
6	-0.750019	2.463571	0.070164	6	1.778325	0.112714	-2.455133
1	-0.167182	-3.039891	-0.650582	1	2.866955	0.048617	-2.445661
1	-1.797135	-2.449352	-0.232992	1	1.373962	-0.756769	-2.979383
1	-0.167181	3.039899	-0.650498	1	1.477304	1.021996	-2.980298
1	-1.797135	2.449350	-0.232926	6	1.778001	0.112885	2.455559
1	-0.669944	-2.930279	1.053713	1	1.373384	-0.756430	2.979888
1	-0.669946	2.930241	1.053794	1	2.866616	0.048569	2.446227
29	-2.984096	0.000004	0.003749	1	1.477103	1.022312	2.980545
17	-5.085240	0.000000	-0.142855	6	-2.791137	-2.778994	-2.442031
				1	-1.853251	-2.980346	-2.967352
				1	-3.393254	-3.685074	-2.427072
				1	-3.335950	-1.996588	-2.978359
				6	-2.791435	-2.778908	2.441967
				1	-3.393924	-3.684738	2.426973
				1	-1.853634	-2.980677	2.967284
				1	-3.335919	-1.996297	2.978326
				6	-3.057743	2.632266	2.441625
				1	-3.690332	1.906061	2.959675
				1	-2.114172	2.730890	2.986427
				1	-3.560990	3.596997	2.425470
				6	-3.057575	2.632107	-2.441956
				1	-3.560786	3.596859	-2.425893
				1	-2.113977	2.730670	-2.986722
				1	-3.690168	1.905893	-2.959989
				29	4.043806	0.057759	0.000136
				17	6.149629	-0.035501	-0.000274
13-CuCl				14-CuCl			
6	1.368415	-0.000057	-1.286911	6	-3.335603	-0.823124	1.323249
6	-0.034802	-0.000029	-0.705886	6	-2.090792	-0.152373	0.700670
6	-0.034816	0.000034	0.705888	6	-2.090815	-0.152422	-0.700586
6	1.368389	0.000058	1.286941	6	-3.335647	-0.823215	-1.323077
6	2.068540	1.217317	-0.704243	6	-4.489717	-0.086498	0.675701
6	2.068526	1.217380	0.704177	6	-4.489739	-0.086543	-0.675541
6	2.068523	-1.217319	0.704286	6	-3.356504	-2.191852	-0.675446
6	2.068536	-1.217381	-0.704133	6	-3.356483	-2.191807	0.675714
7	3.924776	-4.421175	-1.071134	7	-3.209709	-3.505638	1.071291
6	4.354794	-5.160003	0.000266	6	-3.138469	-4.366314	0.000202
7	3.924759	-4.421082	1.071596	7	-3.209737	-3.505709	-1.070942
7	3.924741	4.421185	1.071212	7	-5.517572	0.744724	-1.071011
6	4.354830	5.159983	-0.000180	6	-6.202419	1.270535	0.000061
7	3.924765	4.421091	-1.071518	7	-5.517538	0.744796	1.071148
7	-3.728073	0.000043	1.083077	6	-1.035417	0.415301	-1.403986
6	-4.560076	-0.000011	-0.000043	6	-1.035372	0.415399	1.403998
7	-3.728052	-0.000048	-1.083146	1	-3.326033	-0.817698	2.414871
1	1.367013	-0.000106	-2.379424	1	-3.326113	-0.817866	-2.414700
1	1.366967	0.000107	2.379454	6	-3.172682	-3.961883	2.442521
6	4.155411	-4.812355	-2.441956	1	-3.054955	-5.043506	2.427958
1	4.704046	-5.752048	-2.432554	1	-2.330601	-3.517426	2.981066
1	3.209637	-4.952948	-2.973850	1	-4.098462	-3.708920	2.967216
1	4.744608	-4.056908	-2.970248	6	-3.172749	-3.962041	-2.442144
6	4.155373	-4.812148	2.442455	1	-2.330699	-3.517598	-2.980748
1	3.209591	-4.952696	2.974346	1	-3.054995	-5.043660	-2.427516
1	4.704008	-5.751843	2.433139	1	-4.098554	-3.709135	-2.966822
1	4.744563	-4.056658	2.970693	6	-5.880954	1.023550	-2.442138
6	-4.184631	-0.000129	-2.455614	1	-5.054781	1.500116	-2.977816
1	-3.827401	-0.890225	-2.979644	1	-6.159702	0.106867	-2.969559
1	-5.275179	-0.000004	-2.452107	1	-6.733122	1.700165	-2.427297
1	-3.827194	0.889785	-2.979811	6	-5.880880	1.023711	2.442267
6	-4.184678	0.000098	2.455535	1	-6.733055	1.700317	2.427407
1	-5.275226	0.000150	2.452008	1	-6.159602	0.107061	2.969757
1	-3.827399	-0.889911	2.979679	1	-5.054695	1.500320	2.977887
1	-3.827310	0.890098	2.979633	6	1.266717	1.653188	1.324164
6	4.155328	4.812378	2.442039	6	0.019924	0.984507	0.699387
1	3.209538	4.952854	2.973934	6	0.019901	0.984457	-0.699448
1	4.744615	4.056994	2.970322	6	1.266675	1.653093	-1.324313
1	4.703854	5.752136	2.432647	6	2.414485	0.908453	0.677113

6	4.155383	4.812168	-2.442373	6	2.414464	0.908404	-0.677246
1	4.703907	5.751927	-2.433048	6	1.305441	3.019377	-0.675420
1	4.744683	4.056740	-2.970579	6	1.305461	3.019424	0.675170
1	3.209605	4.952597	-2.974302	7	1.214217	4.337634	1.071484
6	-1.212730	0.000065	1.433696	6	1.170842	5.199044	-0.000197
6	-1.212702	-0.000063	-1.433717	7	1.214184	4.337560	-1.071820
6	-2.397357	0.000037	0.698802	7	3.373248	0.011807	-1.082542
6	-2.397344	-0.000024	-0.698846	6	4.006999	-0.544877	-0.000037
6	2.658995	-2.239120	1.431631	7	3.373283	0.011887	1.082445
6	2.659022	-2.239245	-1.431379	1	1.259729	1.647810	2.415516
6	3.253508	-3.265426	0.699924	1	1.259651	1.647635	-2.415664
6	3.253520	-3.265487	-0.699571	6	1.190104	4.794743	2.443116
6	2.659003	2.239241	1.431433	1	1.109990	5.879671	2.428218
6	3.253516	3.265483	0.699637	1	0.332024	4.379358	2.979331
6	2.659031	2.239116	-1.431577	1	2.105792	4.510411	2.969271
6	3.253531	3.265422	-0.699858	6	1.190027	4.794579	-2.443481
29	-6.440350	-0.000007	-0.000064	1	0.331918	4.379175	-2.979636
17	-8.546052	0.000012	-0.000098	1	1.109934	5.879509	-2.428651
1	-1.212711	-0.000119	-2.519261	1	2.105689	4.510194	-2.969652
1	-1.212761	0.000105	2.519241	6	3.715789	-0.297073	-2.456057
1	2.658215	2.236882	2.517420	1	2.850427	-0.704088	-2.984765
1	2.658266	2.236662	-2.517563	1	4.068140	0.596195	-2.976809
1	2.658258	-2.236884	-2.517365	1	4.511250	-1.043142	-2.446602
1	2.658212	-2.236665	2.517618	6	3.715866	-0.296894	2.455972
				1	4.511327	-1.042965	2.446543
				1	4.068233	0.596411	2.976648
				1	2.850520	-0.703871	2.984735
				1	-1.035100	0.415254	2.491917
				1	-1.035179	0.415081	-2.491905
				29	5.413228	-1.796003	-0.000039
				17	6.967888	-3.220125	-0.000033

Geometries of cage complexes optimized using M06L/6-31G(d) method. All the X, Y, Z coordinates are given in Å.

(14) ₂ (CuCl) ₂				(14) ₃ (CuCl) ₄			
6	5.040205000	-2.554052000	-1.436883000	6	-0.086617000	2.616620000	1.515233000
6	5.055443000	-1.168161000	-0.752850000	6	-0.027076000	1.199940000	0.895042000
6	5.052657000	-1.229836000	0.648183000	6	0.022550000	1.199504000	-0.507149000
6	5.032461000	-2.669837000	1.209547000	6	0.081017000	2.614567000	-1.128928000
6	6.219768000	-3.274261000	-0.815907000	6	1.143047000	3.287837000	0.945747000
6	6.214814000	-3.333227000	0.535906000	6	1.235527000	3.275624000	-0.406391000
6	3.826630000	-3.288355000	0.532357000	6	-1.145233000	3.288247000	-0.560447000
6	3.829670000	-3.228158000	-0.821700000	6	-1.241457000	3.278361000	0.790862000
7	2.569117000	-3.592949000	-1.241675000	7	-2.510701000	3.716783000	1.101540000
6	1.765779000	-3.927055000	-0.174639000	6	-3.217937000	4.040856000	-0.035288000
7	2.573781000	-3.704015000	0.917128000	7	-2.341440000	3.746862000	-1.054921000
7	7.381077000	-3.970565000	0.907894000	7	2.507167000	3.696312000	-0.722484000
6	8.151158000	-4.339934000	-0.176324000	6	3.223887000	4.012316000	0.410873000
7	7.390171000	-3.877631000	-1.231506000	7	2.349814000	3.728465000	1.434767000
6	5.056156000	-0.061642000	1.404118000	6	-0.000053000	0.000523000	-1.212540000
6	5.056022000	0.061335000	-1.404067000	6	-0.000009000	0.000454000	1.600350000
1	5.044285000	-2.496658000	-2.531043000	1	-0.152497000	2.609299000	2.608457000
1	5.027580000	-2.706842000	2.304353000	1	0.146686000	2.605887000	-2.222202000
6	2.142776000	-3.716655000	-2.612278000	6	-3.048595000	3.903250000	2.426060000
1	1.073456000	-3.949992000	-2.591741000	1	-4.122889000	4.079297000	2.303807000
1	2.300830000	-2.778155000	-3.157034000	1	-2.893653000	3.007502000	3.038365000
1	2.672905000	-4.527470000	-3.125031000	1	-2.597731000	4.768483000	2.925459000
6	2.128743000	-3.961730000	2.269657000	6	-2.667484000	3.961206000	-2.448428000
1	1.752157000	-3.045415000	2.742807000	1	-3.027205000	3.035207000	-2.916106000
1	1.332340000	-4.713924000	2.215494000	1	-3.445052000	4.733629000	-2.491728000
1	2.954425000	-4.362204000	2.865392000	1	-1.784223000	4.316914000	-2.987521000
6	7.773705000	-4.258574000	2.266991000	6	3.050663000	3.868693000	-2.046396000
1	7.877348000	-3.336448000	2.852160000	1	2.921587000	2.958580000	-2.643918000
1	7.041288000	-4.909348000	2.759994000	1	2.586454000	4.715041000	-2.565442000
1	8.737587000	-4.768785000	2.225452000	1	4.118819000	4.069550000	-1.909351000

6	7.799419000	-4.042528000	-2.605810000	6	2.685991000	3.939698000	2.826616000
1	8.754242000	-4.571258000	-2.598730000	1	3.539781000	4.627323000	2.857353000
1	7.064703000	-4.631134000	-3.168796000	1	1.843810000	4.401689000	3.350973000
1	7.927488000	-3.071596000	-3.100317000	1	2.942983000	2.991935000	3.317134000
6	5.032778000	2.669513000	-1.209517000	6	0.086640000	-2.615699000	1.515101000
6	5.052797000	1.229524000	-0.648132000	6	0.027037000	-1.199000000	0.894980000
6	5.055718000	1.167859000	0.752902000	6	-0.022632000	-1.198496000	-0.507207000
6	5.040809000	2.553778000	1.436916000	6	-0.081084000	-2.613520000	-1.129056000
6	3.827116000	3.288199000	-0.532197000	6	-1.143024000	-3.286933000	0.945621000
6	3.830325000	3.228103000	0.821859000	6	-1.235551000	-3.274657000	-0.406511000
6	6.220431000	3.273754000	0.815786000	6	1.145208000	-3.287196000	-0.560647000
6	6.215319000	3.332718000	-0.536027000	6	1.241487000	-3.277364000	0.790656000
7	7.381731000	3.969698000	-0.908167000	7	2.510628000	-3.716117000	1.101273000
6	8.152077000	4.338811000	0.175951000	6	3.217725000	-4.040372000	-0.035595000
7	7.391075000	3.876762000	1.231232000	7	2.341272000	-3.746115000	-1.055185000
7	2.569909000	3.593238000	1.241981000	7	-2.507111000	-3.695595000	-0.722585000
6	1.766461000	3.927306000	0.175014000	6	-3.223710000	-4.011883000	0.410771000
7	2.574288000	3.704021000	-0.916841000	7	-2.349666000	-3.727884000	1.434655000
1	5.027770000	2.706499000	-2.304323000	1	0.152558000	-2.608420000	2.608323000
1	5.045007000	2.496404000	2.531077000	1	-0.146783000	-2.604782000	-2.222327000
6	7.774253000	4.257633000	-2.267311000	6	3.048614000	-3.902653000	2.425746000
1	8.738340000	4.767465000	-2.225892000	1	4.122760000	-4.079476000	2.303303000
1	7.877444000	3.335500000	-2.852547000	1	2.894424000	-3.006669000	3.037898000
1	7.042013000	4.908721000	-2.760161000	1	2.597241000	-4.767468000	2.925407000
6	7.800557000	4.041530000	2.605481000	6	2.667197000	-3.960512000	-2.448711000
1	7.928323000	3.070556000	3.099984000	1	3.026708000	-3.034496000	-2.916514000
1	8.755580000	4.569896000	2.598270000	1	3.444878000	-4.732818000	-2.492017000
1	7.066139000	4.630422000	3.168559000	1	1.783944000	-4.316432000	-2.987683000
6	2.143890000	3.717197000	2.612664000	6	-3.050593000	-3.868020000	-2.046496000
1	2.300059000	2.778157000	3.157047000	1	-2.921542000	-2.957916000	-2.644034000
1	2.675733000	4.526709000	3.125694000	1	-2.586351000	-4.714363000	-2.565524000
1	1.075072000	3.952784000	2.592346000	1	-4.118743000	-4.068909000	-1.909468000
6	2.129099000	3.961651000	-2.269335000	6	-2.685753000	-3.939161000	2.826517000
1	1.332712000	4.713861000	-2.215122000	1	-3.539551000	-4.626772000	2.857283000
1	2.954715000	4.362074000	-2.865199000	1	-1.843554000	-4.401202000	3.350803000
1	1.752438000	3.045312000	-2.742381000	1	-2.942686000	-2.991410000	3.317090000
1	5.054877000	0.109530000	-2.494300000	1	0.000012000	0.000425000	2.691575000
1	5.055115000	-0.109836000	2.494351000	1	-0.000070000	0.000550000	-2.303765000
6	-5.041626000	-2.554611000	-1.435565000	6	-10.050861000	2.716935000	0.966627000
6	-5.055962000	-1.168291000	-0.752301000	6	-10.007093000	1.259319000	0.452462000
6	-5.052585000	-1.229170000	0.648777000	6	-9.908134000	1.153512000	-0.942308000
6	-5.031989000	-2.668839000	1.210930000	6	-9.848279000	2.517730000	-1.667039000
6	-3.830827000	-3.228683000	-0.820895000	6	-8.804141000	3.331238000	0.365923000
6	-3.826643000	-3.287735000	0.533189000	6	-8.699954000	3.227179000	-0.980580000
6	-6.214900000	-3.332515000	0.538538000	6	-11.082579000	3.238128000	-1.165365000
6	-6.220890000	-3.274197000	-0.813301000	6	-11.188295000	3.338044000	0.180606000
7	-7.391744000	-3.877498000	-1.227708000	7	-12.430394000	3.883605000	0.437666000
6	-8.152071000	-4.339040000	-0.171724000	6	-13.135935000	4.162378000	-0.715760000
7	-7.381040000	-3.969391000	0.911726000	7	-12.262171000	3.725439000	-1.690703000
7	-2.573619000	-3.703596000	0.917200000	7	-7.437436000	3.651647000	-1.322909000
6	-1.766686000	-3.927974000	-0.175102000	6	-6.724451000	4.038411000	-0.211183000
7	-2.570929000	-3.594807000	-1.241741000	7	-7.596841000	3.809008000	0.828036000
6	-5.056044000	-0.060585000	1.404101000	6	-9.870422000	-0.096364000	-1.553156000
6	-5.056160000	0.060866000	-1.404162000	6	-10.044452000	0.115857000	1.243763000
1	-5.046494000	-2.497822000	-2.529755000	1	-10.134499000	2.787743000	2.056683000
1	-5.026303000	-2.705230000	2.305752000	1	-9.760707000	2.426155000	-2.755114000
6	-7.802085000	-4.042983000	-2.601616000	6	-12.954213000	4.175683000	1.750573000
1	-8.757154000	-4.571254000	-2.593529000	1	-13.952498000	4.595814000	1.616167000
1	-7.930064000	-3.072267000	-3.096568000	1	-13.023537000	3.265322000	2.358849000
1	-7.068076000	-4.632256000	-3.164833000	1	-12.323616000	4.903679000	2.275608000
6	-7.772712000	-4.256648000	2.271259000	6	-12.567310000	3.817247000	-3.098692000
1	-7.876028000	-3.334200000	2.855979000	1	-12.556741000	2.826125000	-3.569116000
1	-8.736586000	-4.766953000	2.230671000	1	-13.566217000	4.247504000	-3.188342000
1	-7.039911000	-4.907088000	2.764133000	1	-11.847795000	4.461996000	-3.617736000
6	-2.127361000	-3.960386000	2.269504000	6	-6.897911000	3.770988000	-2.659758000
1	-1.749654000	-3.043906000	2.741443000	1	-6.500585000	2.810906000	-3.013596000
1	-2.952694000	-4.359762000	2.866461000	1	-7.673298000	4.118279000	-3.349300000
1	-1.331491000	-4.713144000	2.215174000	1	-6.098063000	4.520360000	-2.621001000
6	-2.146357000	-3.720458000	-2.612729000	6	-7.285226000	4.125653000	2.199494000
1	-1.079215000	-3.963458000	-2.593176000	1	-6.280692000	4.559951000	2.208807000
1	-2.683924000	-4.526026000	-3.125980000	1	-7.989385000	4.861519000	2.603331000

1	-2.296471000	-2.780042000	-3.156481000	1	-7.300865000	3.226670000	2.828036000
6	-5.031624000	2.669140000	-1.210968000	6	-10.011395000	-2.494260000	1.363666000
6	-5.052424000	1.229457000	-0.648838000	6	-9.994194000	-1.133647000	0.633533000
6	-5.055684000	1.168567000	0.752239000	6	-9.918574000	-1.240572000	-0.762309000
6	-5.041009000	2.554858000	1.435526000	6	-9.888396000	-2.699789000	-1.274830000
6	-6.214346000	3.333016000	-0.538439000	6	-11.168740000	-3.227801000	0.715488000
6	-6.220197000	3.274694000	0.813400000	6	-11.106693000	-3.331056000	-0.632904000
6	-3.830142000	3.228694000	0.820746000	6	-8.721597000	-3.305168000	-0.523243000
6	-3.826110000	3.287849000	-0.533338000	6	-8.778750000	-3.191624000	0.825101000
7	-2.573079000	3.703602000	-0.917458000	7	-7.566315000	-3.616608000	1.317041000
6	-1.765995000	3.927761000	0.174767000	6	-6.729344000	-4.019440000	0.301306000
7	-2.570132000	3.594536000	1.241465000	7	-7.475531000	-3.802947000	-0.834865000
7	-7.390822000	3.878348000	1.227945000	7	-12.287205000	-3.920756000	-1.037773000
6	-8.151163000	4.340064000	0.172046000	6	-13.119991000	-4.220364000	0.021955000
7	-7.380335000	3.970245000	-0.911491000	7	-12.386243000	-3.755741000	1.095021000
1	-5.026047000	2.705552000	-2.305790000	1	-10.060478000	-2.399786000	2.453884000
1	-5.045774000	2.498048000	2.529714000	1	-9.836173000	-2.772244000	-2.366801000
6	-2.126962000	3.960508000	-2.269787000	6	-7.188119000	-3.715018000	2.710091000
1	-1.331099000	4.713275000	-2.215481000	1	-6.371845000	-4.444781000	2.775296000
1	-1.749296000	3.044071000	-2.741839000	1	-6.858785000	-2.743103000	3.099456000
1	-2.952365000	4.359918000	-2.866622000	1	-8.032838000	-4.075319000	3.305175000
6	-2.145246000	3.719902000	2.612380000	6	-7.016334000	-4.132612000	-2.161584000
1	-2.297010000	2.779922000	3.156417000	1	-6.706401000	-3.236636000	-2.715208000
1	-1.077646000	3.960913000	2.592608000	1	-6.164365000	-4.810773000	-2.062346000
1	-2.681293000	4.526606000	3.125440000	1	-7.805227000	-4.644829000	-2.722148000
6	-7.800930000	4.043993000	2.601902000	6	-12.635001000	-4.234626000	-2.403108000
1	-7.929177000	3.073327000	3.096886000	1	-12.663051000	-3.329152000	-3.021833000
1	-7.066643000	4.633020000	3.165012000	1	-11.918790000	-4.940268000	-2.841681000
1	-8.755818000	4.572593000	2.593933000	1	-13.626055000	-4.691441000	-2.388603000
6	-7.772074000	4.257622000	-2.270979000	6	-12.863946000	-3.853456000	2.454069000
1	-8.735767000	4.768259000	-2.230284000	1	-13.851974000	-4.315645000	2.417872000
1	-7.039108000	4.907801000	-2.763951000	1	-12.196739000	-4.473417000	3.065004000
1	-7.875778000	3.335200000	-2.855673000	1	-12.945623000	-2.861437000	2.915348000
1	-5.055109000	0.108495000	-2.494420000	1	-10.111238000	0.197388000	2.329889000
1	-5.054903000	-0.108214000	2.494359000	1	-9.803603000	-0.177929000	-2.639282000
29	0.000311000	4.582547000	0.066631000	29	-4.982804000	-4.672247000	0.587554000
29	-0.000323000	-4.582514000	-0.066606000	29	-4.963086000	4.709579000	-0.289012000
17	0.000485000	-6.631739000	0.984291000	17	-4.908819000	6.644859000	-1.534031000
17	0.000676000	6.631750000	-0.984296000	17	-5.011092000	-6.554490000	1.909935000
E(SCF) = -7398.68847084 A.U.				6	10.050715000	-2.717312000	0.966561000
				6	10.007032000	-1.259690000	0.452408000
				6	9.908098000	-1.153866000	-0.942362000
				6	9.848192000	-2.518073000	-1.667106000
				6	8.803972000	-3.331548000	0.365829000
				6	8.699816000	-3.227469000	-0.980674000
				6	11.082445000	-3.238540000	-1.165416000
				6	11.188132000	-3.338474000	0.180554000
				7	12.430162000	-3.884186000	0.437628000
				6	13.135658000	-4.163097000	-0.715794000
				7	12.261982000	-3.725997000	-1.690743000
				7	7.437267000	-3.651813000	-1.323030000
				6	6.724214000	-4.038508000	-0.211321000
				7	7.596606000	-3.809178000	0.827919000
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				1	10.134330000	-2.788130000	2.056618000
				1	9.760645000	-2.426485000	-2.755182000
				6	12.953943000	-4.176300000	1.750542000
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				1	12.556728000	-2.826673000	-3.569126000
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				6	6.897755000	-3.771067000	-2.659896000
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				1	7.989191000	-4.861593000	2.603253000
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				6	10.011475000	2.493885000	1.363641000
				6	9.994238000	1.133275000	0.633496000
				6	9.918632000	1.240215000	-0.762347000
				6	9.888494000	2.699446000	-1.274853000
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				6	8.721711000	3.304833000	-0.523265000
				6	8.778858000	3.191292000	0.825077000
				7	7.566478000	3.616425000	1.317023000
				6	6.729552000	4.019351000	0.301285000
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				7	12.287547000	3.919902000	-1.037809000
				6	13.120449000	4.219240000	0.021905000
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				1	9.836269000	2.771915000	-2.366823000
				6	7.188339000	3.714943000	2.710078000
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				1	6.859039000	2.743057000	3.099543000
				1	8.033070000	4.075320000	3.305099000
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6	-5.031982000	-3.877727000	-1.216331000	6	-7.025645000	3.884775000	1.098187000
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6	-6.218651000	-4.537206000	-0.549639000	6	-10.224895000	5.786563000	0.249668000
6	-3.828048000	-4.499199000	-0.544287000	6	-3.678118000	5.641092000	0.594052000
6	-3.831325000	-4.456851000	0.811379000	6	-3.590979000	5.543258000	-0.802135000
7	-2.569168000	-4.821550000	1.226291000	7	-2.384899000	6.130416000	-1.146464000
6	-1.764854000	-5.137935000	0.155040000	6	-1.708933000	6.597772000	-0.048479000
7	-2.573446000	-4.904985000	-0.933858000	7	-2.530831000	6.297472000	1.004864000
7	-7.427305000	-5.082975000	-0.931822000	7	-11.388973000	6.490438000	0.527098000
6	-8.221551000	-5.418864000	0.145762000	6	-12.072842000	6.884276000	-0.599205000
7	-7.437033000	-5.017168000	1.208221000	7	-11.278782000	6.390222000	-1.608008000
6	-5.058968000	1.199251000	-1.439569000	6	-6.971277000	-1.167797000	1.465600000
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1	-7.148453000	-6.023702000	-2.793380000	1	-11.105540000	7.389463000	2.404906000
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6	-7.861531000	-5.167573000	2.579653000	6	-11.595372000	6.561671000	-3.004289000
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6	-5.050638000	2.443054000	0.642849000	6	-7.012146000	-2.453214000	-0.587903000
6	-5.054649000	2.400642000	-0.784092000	6	-6.962153000	-2.381682000	0.829533000
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6	-3.830598000	4.497554000	0.544087000	6	-3.678626000	-5.641047000	-0.593671000
6	-3.834091000	4.455359000	-0.811574000	6	-3.591686000	-5.543386000	0.802536000
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6	-6.221247000	4.534145000	0.549812000	6	-10.225628000	-5.785962000	-0.249921000
7	-7.430351000	5.078767000	0.932210000	7	-11.389772000	-6.489665000	-0.527491000
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7	-2.576210000	4.904149000	0.933488000	7	-2.531259000	-6.297314000	-1.004404000
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1	-5.052312000	1.308838000	2.458162000	1	-7.041714000	-1.360656000	-2.431723000
1	-5.060623000	1.162097000	-2.530380000	1	-6.947924000	-1.109939000	2.555127000
6	5.046956000	-3.799941000	1.431077000	6	6.984762000	3.837443000	-1.253912000
6	5.056261000	-2.402433000	0.778855000	6	6.984393000	2.427619000	-0.687193000
6	5.049371000	-2.441625000	-0.648209000	6	6.961498000	2.413301000	0.733229000
6	5.030394000	-3.872652000	-1.224763000	6	6.925166000	3.810925000	1.326784000
6	3.836280000	-4.457366000	0.805288000	6	3.658690000	5.631394000	-0.723511000
6	3.828620000	-4.495924000	-0.550432000	6	3.617959000	5.602238000	0.677444000
6	6.219301000	-4.533231000	-0.563195000	6	10.181867000	5.741716000	0.831536000
6	6.228844000	-4.495107000	0.790923000	6	10.216058000	5.751884000	-0.569539000
7	7.443396000	-5.016328000	1.189807000	7	11.373806000	6.439930000	-0.906178000
6	8.224806000	-5.415348000	0.124063000	6	12.089023000	6.876174000	0.184522000
7	7.427015000	-5.077596000	-0.950331000	7	11.321505000	6.425611000	1.233343000
7	2.573183000	-4.902108000	-0.936978000	7	2.436242000	6.226347000	1.036229000
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7	2.576148000	-4.825510000	1.223462000	7	2.497512000	6.273364000	-1.124791000
6	5.059756000	1.204720000	-1.436852000	6	6.991251000	-1.253735000	1.393861000
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6	6.226003000	4.498112000	-0.791058000	6	10.215574000	-5.752489000	0.569648000
6	3.833470000	4.458799000	-0.805111000	6	3.658134000	-5.631239000	0.723353000
6	3.825995000	4.497512000	0.550612000	6	3.617580000	-5.602400000	-0.677610000
7	2.570367000	4.902993000	0.937292000	7	2.435836000	-6.226476000	-1.036392000
6	1.765355000	5.139319000	-0.153522000	6	1.715031000	-6.632884000	0.056895000
7	2.573026000	4.825997000	-1.223128000	7	2.496830000	-6.272973000	1.124628000
7	7.440010000	5.020456000	-1.190135000	7	11.373216000	-6.440664000	2.906374000
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7	7.423890000	5.081755000	0.950005000	7	11.321032000	-6.426416000	-1.233147000
1	5.019163000	3.898865000	2.319812000	1	6.898308000	-3.802773000	-2.423079000
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6	2.119807000	5.137745000	2.292305000	6	1.997522000	-6.473043000	-2.390526000
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1	1.738479000	4.214147000	2.746776000	1	1.583209000	-5.564680000	-2.846977000
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6	2.149839000	4.964125000	-2.593413000	6	2.152162000	-6.544090000	2.496123000
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29	-0.001617000	5.790051000	-0.039942000	29	-0.002997000	-7.383563000	-0.084160000
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17	0.000150000	-7.829212000	-1.025904000	17	-0.043726000	9.403288000	1.111460000
17	-0.002968000	7.829262000	1.025922000	17	-0.043386000	-9.403087000	-1.111670000
6	-5.054404000	-1.284012000	-1.367221000	6	-7.021774000	1.308688000	1.341951000
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