

Supplementary Material

N-Heterocyclic Carbenes-Cu^I Complexes as Catalysts: A Theoretical Insight

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Table S1. Thermodynamic data of dimerization of NHCs computed at the B3LYP/def2-SVP level.

Species	Total enthalpy (a.u.)	Entropy (cal K ⁻¹ mol ⁻¹)	Actvation enthalpy ΔH^\ddagger (kcal mol ⁻¹)	Actvation entropy ΔS^\ddagger (cal K ⁻¹ mol ⁻¹)	Actvation free energy ΔG^\ddagger (kcal mol ⁻¹)	Standard enthalpy ΔH° (kcal mol ⁻¹)	Standard free energy ΔG° (kcal mol ⁻¹)
1a	-301.864700	86.037	-	-	-	-	-
TSa	-603.727174	130.038	1.40	-42.036	13.93	-	-
2a	-603.810450	118.020	-	-	-	-52.26	-36.14
1b	-602.27297	78.919	-	-	-	-	-
TSb	-1204.549194	117.885	-2.04	-39.953	9.87	-	-
2b	-1204.658897	110.152	-	-	-	-70.88	-56.64
1c	-417.063365	104.742	-	-	-	-	-
TSc	-834.123525	167.816	2.01	-41.668	14.43	-	-
2c	-834.173416	161.141	-	-	-	-29.30	-14.89
1d	-717.464621	98.858	-	-	-	-	-
TSd	-1434.934738	155.976	-3.45	-41.74	8.99	-	-
2d	-1435.018418	152.780	-	-	-	-55.96	-42.56
1e	-394.095133	97.567	-	-	-	-	-
TSe	-788.188683	153.930	0.99	-41.204	13.27	-	-
2e	-788.233562	147.075	-	-	-	-27.17	-12.84

Table S2. Thermodynamic data of the coordination of NHCs to Cu(I) halides computed at the B3LYP/def2-SVP level.

Species	Total enthalpy (a.u.)	Entropy (cal K ⁻¹ mol ⁻¹)	ΔH° (kcal mol ⁻¹)	ΔS° (cal K ⁻¹ mol ⁻¹)	ΔG° (kcal mol ⁻¹)	ΔH^\ddagger (kcal mol ⁻¹)	ΔG^\ddagger (kcal mol ⁻¹)
1a	-301.864700	86.037	-	-	-	-	-
1b	-602.27297	78.919	-	-	-	-	-
1c	-417.063365	104.742	-	-	-	-	-
1d	-717.464621	98.858	-	-	-	-	-
1e	-394.095133	97.567	-	-	-	-	-
CuCl	-2076.726021	55.958	-	-	-	-	-
CuBr	-4167.537501	58.692	-	-	-	-	-
CuI	-8474.360680	60.919	-	-	-	-	-
1a-CuI	-8776.459022	105.839	-141.940	41.117	-129.715	-	-
1b-CuI	-9076.88196	103.139	-155.814	36.699	-145.080	-	-
1c-CuI	-8891.627575	130.896	-127.715	34.765	-117.577	-	-
1c-CuBr	-4584.783636	130.054	-114.688	33.380	-104.849		
1c-CuCl	-2493.980176	122.798	119.7207	37.902	-108.689		
1d-CuI	-9192.141722	121.263	-198.554	38.525	-187.224	-	-
1d-CuITS	-9191.837953	135.161	-	-	-	-7.94 (barrierless)	-0.60 (barrierless)
1d-CuBrTS	-4885.002847	131.968	-	-	-	-0.45 (barrierless)	7.18
1d-CuClTS	-2794.195746	131.377	-	-	-	-3.20 (barrierless)	3.79
1e-CuI	-8868.658723	123.317	-127.326	35.154	-116.890	-	-

Table S3. Cartesian Coordinates of the optimized geometries of different species computed at the B3LYP/def2-SVP level

1a

6	-0.780630377	1.268663301	0.000042004
7	-1.087964442	-0.215725865	-0.000184618
6	-0.000018936	-1.100527988	-0.000057462
7	1.087955647	-0.215749416	0.000038396
6	0.780646379	1.268642245	-0.000027970
6	-2.505419547	-0.661468836	0.000066514
6	2.505411466	-0.661469048	0.000036085
1	3.040075627	-0.293543362	0.898483272
1	1.204245263	1.759825356	0.899054450
1	-1.204204320	1.759961719	-0.898987425
1	2.513117663	-1.764000263	-0.000051854
1	3.040072913	-0.293336714	-0.898313650
1	-1.204097337	1.759598878	0.899325458
1	1.204112122	1.759678027	-0.899256670
1	-2.513074916	-1.764000220	0.000529903
1	-3.039995219	-0.293057734	0.898352264
1	-3.040124121	-0.293836745	-0.898467222

1b

6	0.128765973	-1.257533692	-0.000068644
7	0.945782140	-0.150836633	-0.000263798
6	0.412864165	1.287831127	0.000400241

6	-1.138384683	1.174146529	-0.000394241
16	-1.534593501	-0.648746245	0.000147975
6	2.439909181	-0.289308126	-0.000039855
1	2.873142970	0.188413872	0.899766199
1	0.795296974	1.811141483	0.898986636
1	-1.571928464	1.653989281	-0.893324154
1	2.680863745	-1.364739235	-0.000395502
1	2.873435050	0.188980250	-0.899406438
1	-1.572877665	1.654883591	0.891575594
1	0.796160607	1.812312082	-0.897108364

1c

7	0.817067183	-0.415036359	-0.337463156
6	0.162034040	0.856225283	-0.142938195
6	-1.168117411	0.565897324	0.040535195
7	-1.270776189	-0.869956888	-0.041276760
6	-0.041860859	-1.552118486	-0.278703170
6	0.885961526	2.195027620	-0.186339023
6	-2.368341361	1.470500325	0.279021575
6	2.297735447	-0.569445198	-0.530174468
6	3.081389172	-0.581348061	0.818688159
1	-2.046468178	2.522483481	0.301853622
1	-2.860130888	1.240078098	1.240067605
1	-3.121344764	1.358090424	-0.520321825
1	1.651655700	2.269825428	0.604718323
1	1.387378777	2.349423195	-1.157538544

1	0.163447242	3.012282905	-0.041469244
1	2.445220687	-1.530987094	-1.056047809
1	4.155557085	-0.722120037	0.621900025
1	2.725376955	-1.406854484	1.452923327
1	2.943735316	0.365640332	1.361370191
1	2.662521223	0.249307540	-1.179819986
6	-2.563779119	-1.604466096	0.102254548
1	-2.343536791	-2.679560169	-0.004638344
1	-3.015446358	-1.418000549	1.094897410
1	-3.282131599	-1.296292581	-0.680783081

1d

6	-0.126255106	0.750806608	-0.148134200
6	-1.401091341	0.313422378	0.067921323
16	-1.464693816	-1.459458068	0.058363350
6	0.288192765	-1.705098839	-0.249516939
7	0.773718189	-0.390314370	-0.321039754
6	-2.659542759	1.150782909	0.285148458
6	2.259864560	-0.192605571	-0.528794089
6	3.031239515	-0.042383365	0.816939350
6	0.393345674	2.183567440	-0.253416477
1	-2.420479201	2.225071003	0.294394008
1	-3.142279683	0.898933184	1.245281741
1	-3.398826903	0.971805347	-0.515058094
1	1.187264828	2.383113804	0.485454156
1	0.803122431	2.389042040	-1.257439097

1	-0.429218304	2.890524533	-0.070944397
1	2.617165970	-1.090370007	-1.065823882
1	4.107501885	0.071143817	0.614128152
1	2.879741218	-0.938511546	1.437190485
1	2.683456009	0.838303622	1.376975147
1	2.417105611	0.693524505	-1.171578067

1e

7	1.259800942	1.100367319	0.189866396
6	-0.072827345	1.010390962	-0.039915316
7	-0.454794275	-0.336614428	-0.340552074
6	0.654251641	-1.247300156	-0.311667802
7	1.651115616	-0.308465058	0.013703382
6	-1.864307070	-0.787418048	-0.604994167
6	-2.645084997	-1.098808067	0.708034587
6	3.102561877	-0.631416410	0.188613196
1	-2.381914334	-0.001005614	-1.187264605
1	-3.660479552	-1.444203729	0.459265990
1	-2.722295482	-0.201701226	1.340367479
1	-2.129638876	-1.888582663	1.274672759
1	-1.790863263	-1.698960664	-1.226877994
1	3.222863551	-1.715499289	0.024489366
1	3.710693239	-0.070335225	-0.545034447
1	3.432532647	-0.366559917	1.210252970
6	-1.024566271	2.201661667	-0.006465217
1	-1.521892834	2.338091880	-0.981944674

1	-1.803506752	2.069156091	0.763225234
1	-0.448521371	3.109925833	0.226092289

TSa

7	-1.851392859	1.065955362	0.135184483
6	-0.881972164	0.324534480	-0.556431057
7	-1.529333622	-0.905828200	-0.777602985
6	-2.954501782	-1.019645854	-0.279191943
6	-3.134029619	0.330831463	0.482066446
6	-1.003783962	-1.955199247	-1.688722291
6	-1.449007209	2.277498852	0.910978460
6	1.092724359	0.618663503	0.711273088
7	2.076008138	1.027780653	-0.239913571
6	2.890016745	-0.116756790	-0.824110241
6	2.663873091	-1.248325675	0.224411882
7	1.510318531	-0.689744163	1.022452441
6	1.735914498	2.136447985	-1.180443500
6	0.941562433	-1.492745926	2.133231746
1	0.929929466	1.829829283	-1.880595637
1	1.379932760	3.002454792	-0.597188204
1	2.635929696	2.429150791	-1.750143904
1	0.129898523	-0.907835041	2.596286435
1	0.530458414	-2.453434994	1.763429132
1	1.708280671	-1.717582353	2.902375462
1	0.030403001	-1.685391570	-1.958775538
1	-1.003668596	-2.944838111	-1.191001184

1	-1.610316960	-2.032791925	-2.614287420
1	-1.582780349	3.203116932	0.319000464
1	-2.056592735	2.348785362	1.829862441
1	-0.372891603	2.108496774	1.157282417
1	-3.661035183	-1.117130458	-1.128657225
1	-3.077119908	-1.902184291	0.380077443
1	-4.021431666	0.897050980	0.136031672
1	-3.217924412	0.184512777	1.577990448
1	3.553461883	-1.404291535	0.869319785
1	2.397767051	-2.218144496	-0.242265714
1	2.508257080	-0.406947532	-1.825141513
1	3.955463255	0.168212292	-0.922817504

2a

7	-1.472897387	1.257027402	0.232311798
6	-0.679752032	0.019176365	0.044418276
7	-1.513411165	-1.207855765	0.209477188
6	-2.837215285	-0.662694537	0.744521237
6	-2.925661542	0.814336872	0.245234872
6	0.679738083	-0.019182243	-0.044487192
7	1.513406328	1.207851108	-0.209517216
6	2.837164516	0.662651362	-0.744647959
6	2.925661426	-0.814303518	-0.245223065
7	1.472908155	-1.257037038	-0.232268867
6	1.715661180	1.874875088	1.149101236
6	1.192506228	-2.309942228	0.817485011

6	-1.715629583	-1.874956476	-1.149106608
6	-1.192481875	2.310044883	-0.817336566
1	2.302924660	2.798424905	1.002863368
1	0.718937506	2.137842552	1.542709429
1	2.235120343	1.232268971	1.887332630
1	0.091525191	-2.384510949	0.903863317
1	1.620337307	-3.272412269	0.485425445
1	1.622235524	-2.050789614	1.806493963
1	-0.718881805	-2.137755058	-1.542767199
1	-2.302734008	-2.798596914	-1.002806085
1	-2.235240456	-1.232445452	-1.887314617
1	-0.091498434	2.384569603	-0.903745914
1	-1.622260576	2.051011043	-1.806353424
1	-1.620266927	3.272493318	-0.485156156
1	-3.681798680	-1.285569916	0.402601293
1	-2.796986845	-0.684504684	1.850349914
1	-3.512854409	1.454805250	0.930764021
1	-3.383725905	0.869176944	-0.765305250
1	3.512894541	-1.454816379	-0.930677268
1	3.383713363	-0.869038469	0.765327946
1	3.681777328	1.285582097	-0.402907397
1	2.796794034	0.684331664	-1.850473799
TSb			
7	1.805362280	0.864736665	-0.272231384
6	0.881831461	0.084069526	0.370337614

16	1.716658510	-1.373982300	0.939281600
6	3.402799008	-0.948378861	0.270173645
6	3.272588681	0.446608676	-0.409689392
6	1.363706858	2.139314951	-0.935152964
1	1.643892585	3.017094306	-0.323450757
6	-1.225306840	0.740562964	-0.632300983
16	-1.599608683	-0.781227019	-1.494785840
6	-2.844721273	-1.438365666	-0.282370060
6	-2.905375813	-0.416097077	0.890445874
7	-2.119408551	0.808766001	0.433774665
6	-1.971080989	1.887390633	1.461101391
1	-1.477409829	2.752370387	0.989453974
1	-1.353830717	1.541585599	2.314884368
1	-2.965475584	2.190716599	1.838645233
1	1.837008620	2.220592533	-1.929749071
1	0.248895635	2.001235122	-1.008724271
1	-3.943818657	-0.113299663	1.129126282
1	-2.442967535	-0.825961869	1.812281130
1	-2.542702307	-2.435603478	0.078572596
1	-3.829733958	-1.537313212	-0.769410305
1	3.909596870	1.210233226	0.078979744
1	3.532584915	0.414068378	-1.485965403
1	4.137598370	-0.923064058	1.091721224
1	3.725241782	-1.714454312	-0.454370608

2b

7	1.462111394	1.128690309	-0.001856386
6	0.625593148	-0.108159420	-0.018931057
16	1.591257954	-1.640222794	-0.061374266
6	3.166482895	-0.720820991	-0.268836183
6	2.775155770	0.745420399	-0.670641256
6	-0.736127036	-0.089867992	-0.015506850
7	-1.576038171	1.117315226	0.101294113
6	-3.016138151	0.758607469	-0.212180963
6	-3.255264566	-0.668764555	0.356394338
16	-1.705671806	-1.602444904	0.044312927
6	-1.102030412	2.285178595	-0.733181974
6	1.713661663	1.558962938	1.441730593
1	-0.000595821	2.324007733	-0.618136855
1	-1.358389780	2.163263169	-1.805081515
1	-1.576138799	3.208534585	-0.356595189
1	2.335974981	2.470860526	1.434997262
1	0.737743656	1.791977864	1.899868410
1	2.218056165	0.783286677	2.051615966
1	-3.475204876	-0.618540342	1.437630591
1	-4.104556908	-1.160514574	-0.146442068
1	-3.682016119	1.504869710	0.263312200
1	-3.208030109	0.772370015	-1.307995522
1	3.558159607	1.473884080	-0.393611939
1	2.616242730	0.793307924	-1.765023474
1	3.783699586	-1.184769524	-1.056662750

1	3.755164946	-0.725232112	0.665962350
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TSc

7	-1.796564735	1.425054704	0.048334837
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6	-0.773856844	0.604616662	0.637649838
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7	-1.472652023	-0.649971476	0.652935377
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6	-2.794425606	-0.597419921	0.074874747
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6	-2.982941497	0.699671232	-0.334017032
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6	-0.902629196	-1.857781642	1.329357915
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6	-1.290372670	-1.942430131	2.839439068
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6	-3.711793277	-1.808388703	-0.024266494
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6	-1.411109736	2.758996294	-0.491605362
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6	0.847171135	0.626399662	-0.732081444
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7	2.029022574	0.825638510	0.060869951
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6	2.945723520	-0.286121757	0.041016073
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6	2.411755417	-1.215683318	-0.816992802
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7	1.163473521	-0.661375796	-1.282311211
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6	2.040401764	1.924422404	1.075233956
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6	2.419476595	3.307507405	0.465321882
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6	0.286304126	-1.339614450	-2.278287019
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6	2.933999740	-2.568887045	-1.276585746
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1	0.197148829	-1.793532798	1.228732972
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1	-1.250528232	-2.763538466	0.796948425
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1	-1.238521333	3.480229843	0.328731267
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1	-0.460740364	2.601292859	-1.049646590
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1	-2.199599162	3.144693033	-1.157501380
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1	-3.263746563	-2.606318022	-0.642030436
1	-3.931009260	-2.235822180	0.969416096
1	-4.665898963	-1.515362866	-0.487611798
1	0.819097186	-1.496419987	-3.235952935
1	-0.060939779	-2.320750266	-1.901843633
1	-0.587083120	-0.688819944	-2.449515204
1	3.904203358	-2.777760962	-0.801261828
1	2.238047291	-3.382776428	-1.008014866
1	3.075182341	-2.596468334	-2.371288370
1	2.748674195	1.656095010	1.880053702
1	1.003022619	1.936048698	1.483706705
1	2.351830343	4.087787286	1.239486975
1	3.446513013	3.292023832	0.069760946
1	1.731356609	3.561657304	-0.354093935
1	-0.827413175	-2.831460970	3.295438925
1	-0.935149398	-1.045452379	3.368228319
1	-2.381926728	-2.012220048	2.958753700
6	4.243704536	-0.308485454	0.836998782
1	4.860730268	0.580146919	0.620118328
1	4.055017382	-0.331405541	1.924760342
1	4.826635330	-1.204064570	0.574158903
6	-4.172666957	1.356593398	-1.020732462
1	-4.530465788	2.230446787	-0.449722275
1	-3.918698824	1.699137240	-2.039319019
1	-5.001139730	0.636825544	-1.101239345

2c

7	1.611819533	-0.856467461	0.006418040
6	0.692897392	0.301192406	-0.072979848
7	1.458384357	1.554844781	0.083528579
6	2.861373502	1.113963322	0.177628102
6	2.950749571	-0.240543234	0.132846990
6	-0.672941409	0.234176061	-0.023538575
7	-1.465438131	-1.002419219	-0.223006113
6	-2.843135096	-0.509494172	-0.440031289
6	-2.894491759	0.845820367	-0.389417575
7	-1.556246926	1.422324806	-0.135919916
6	-1.323739148	-2.025379512	0.907128176
6	-3.945452121	-1.510781768	-0.774778740
6	-4.070916787	1.785951016	-0.634423592
6	-1.492190374	2.345602096	1.077363143
6	1.178712307	2.587974405	-1.000452416
6	3.952573042	2.159026041	0.387451283
6	4.191872583	-1.113394213	0.295918776
6	1.422811892	-1.847908962	-1.151154111
1	-1.848605846	-2.943964709	0.584389084
1	-4.950240007	1.216833591	-0.970292599
1	-3.821477063	2.532437808	-1.407403616
1	-4.346624923	2.331339864	0.284651231
1	-3.635805165	-2.169186715	-1.603980365
1	-4.187262110	-2.150666946	0.091134003

1	-4.861970008	-0.981411808	-1.074284977
1	-0.243705268	-2.245690876	0.988413321
6	-1.861269656	-1.555079905	2.293478090
1	-0.428951609	2.576248826	1.261705149
1	-2.037157722	3.277083168	0.847118799
1	-1.925680862	1.887231843	1.987728868
1	4.912951235	1.670345584	0.607851698
1	4.085607652	2.785285878	-0.511665682
1	3.698777131	2.826279652	1.228475024
1	5.047591263	-0.493894850	0.603085483
1	4.031285592	-1.888837234	1.063103647
1	4.460468899	-1.617888603	-0.648245612
1	0.081672268	2.659119433	-1.104249162
1	1.590777519	3.561641212	-0.684320297
1	1.618169623	2.307155300	-1.977390015
1	0.334979061	-1.846419608	-1.357626029
1	1.952305928	-1.498052499	-2.061387362
6	1.878147177	-3.293344187	-0.791761858
1	1.584939048	-3.977513500	-1.603545926
1	2.967301389	-3.357169996	-0.663581491
1	1.396609861	-3.629181252	0.138329505
1	-1.701815258	-2.345404988	3.043447576
1	-1.326571458	-0.650128176	2.619102727
1	-2.937207682	-1.330249256	2.242633554

TSd

16	-1.480629127	-1.205723546	-1.509689366
6	-0.934195085	0.339115319	-0.762221253
7	-1.981353817	0.658382812	0.120651884
6	-3.125557708	-0.235283789	0.247133961
6	-2.994597611	-1.306396073	-0.589910557
6	-3.957214266	-2.476686106	-0.777101198
1	-4.268251704	-2.572571579	-1.831915479
1	-4.862104911	-2.342074855	-0.165241289
6	-4.262770904	0.096234934	1.212252360
1	-3.936697704	0.018614890	2.264006282
1	-5.096383163	-0.605434199	1.062027300
1	-4.638704126	1.119613432	1.046431918
6	-1.730020098	1.813772526	1.058755662
1	-0.644825243	1.684714265	1.307604221
1	-2.348290835	1.676266008	1.963151971
1	-1.758970269	4.000366141	1.099389987
1	-3.085410052	3.289297230	0.134463243
6	-2.020981271	3.191999611	0.398932959
1	-1.419023380	3.308169696	-0.514493108
6	0.934196884	0.339118316	0.762224025
16	1.480631063	-1.205720313	1.509692626
6	2.994597611	-1.306395247	0.589910694
6	3.125556994	-0.235283863	-0.247135144
7	1.981354489	0.658384114	-0.120651211
6	3.957213271	-2.476686185	0.777100838

1	4.862102948	-2.342076918	0.165239052
1	3.485554583	-3.430635626	0.482606214
1	4.268252614	-2.572570695	1.831914648
6	4.262768353	0.096232376	-1.212256588
1	5.096380395	-0.605437062	-1.062031857
1	4.638702623	1.119610913	-1.046438908
1	3.936692941	0.018610404	-2.264009680
6	1.730019881	1.813772680	-1.058756106
1	2.348290322	1.676265543	-1.963152501
1	0.644825090	1.684713768	-1.307604354
6	2.020980615	3.192000643	-0.398935060
1	-3.485557340	-3.430635748	-0.482604399
1	1.758968967	4.000366231	-1.099392929
1	1.419023068	3.308171506	0.514491138
1	3.085409464	3.289299051	-0.134465917

2d

7	1.475710599	0.796269914	-0.064786199
6	0.685521514	-0.452876690	-0.050309906
16	1.736974821	-1.905598379	-0.194944829
6	3.179538264	-0.855304827	-0.343200751
6	2.903207398	0.467955275	-0.226429217
6	-0.678460384	-0.489848561	-0.088332712
7	-1.547532726	0.714861111	-0.090953101
6	-2.955768971	0.273962586	0.025186080
6	-3.137955744	-1.067109572	0.127412067

16	-1.625234076	-2.012761762	0.026803990
6	-1.231867183	1.634867964	-1.282589600
6	-4.049536047	1.343393558	0.101903508
6	-4.447568786	-1.825904491	0.340357624
6	4.533264892	-1.513619740	-0.604961723
6	3.882296139	1.641766869	-0.320356202
6	1.149295598	1.733143530	1.094013573
1	-0.137635716	1.548034343	-1.421759528
1	-5.306081549	-1.138883517	0.347399985
1	-4.440009880	-2.376442657	1.297633628
1	-4.607738621	-2.564097615	-0.464692849
1	-3.747217868	2.159474789	0.777353700
1	-4.264989770	1.779059610	-0.888800948
1	-4.981400392	0.904824504	0.486884448
1	-1.736012401	1.272439467	-2.202143790
6	-1.581259467	3.133831072	-1.037025575
1	5.337169019	-0.763309167	-0.625934732
1	4.771732640	-2.248719368	0.183355591
1	4.538821814	-2.049792083	-1.570440613
1	3.506884342	2.398900961	-1.028604402
1	4.023046524	2.133274371	0.657557264
1	4.864565030	1.295023180	-0.671811838
6	1.596510012	1.211891911	2.494688557
1	1.622817857	2.708816993	0.878313269
1	0.049832197	1.855984524	1.078512902

1	-1.123241736	3.739611188	-1.834725405
1	-2.663874980	3.315494012	-1.049022611
1	-1.178483131	3.471393932	-0.071021616
1	1.301513074	1.933743052	3.272091355
1	1.114109311	0.247112674	2.711627427
1	2.687793792	1.077008663	2.536522956

TSe

7	2.167143054	0.460678230	0.230316193
6	1.055086977	0.374193103	-0.649310232
7	1.173374798	-1.027447186	-0.975442552
6	2.242520490	-1.660097289	-0.263782972
7	2.890270734	-0.782564138	0.538249787
6	0.327098580	-1.708351120	-2.000460566
6	2.603751591	-3.135087100	-0.395652036
6	2.392736448	1.637696766	1.129394633
6	-0.693994710	0.840148614	0.478059098
7	-1.677605949	-0.214876064	0.405744138
6	-2.822957578	0.167543488	-0.364410055
7	-2.703388423	1.429626351	-0.839097033
7	-1.418444100	1.829733205	-0.240961159
6	-1.551375537	-1.496982005	1.174064438
6	-0.764467869	3.054983847	-0.786035329
6	-4.022530010	-0.733094024	-0.640515920
1	-0.473720839	-1.743425052	1.214983920
6	-2.126188878	-1.383137013	2.619739364

1	-2.075376538	-2.295021393	0.614189632
1	-0.502640084	3.750635909	0.032632592
1	0.160530410	2.743668522	-1.315366098
1	-1.466197473	3.543737463	-1.482326595
1	-3.717377986	-1.655207119	-1.164055076
1	-4.530976396	-1.020636686	0.295474157
1	-4.736666889	-0.187512989	-1.275518855
1	0.944600239	-2.056468596	-2.850443695
1	-0.200338842	-2.576739892	-1.562951072
1	-0.412144332	-0.975208560	-2.363395194
1	3.449253600	-3.357863107	0.272367333
1	1.752433183	-3.779868993	-0.118073936
1	2.896818297	-3.380557662	-1.430973674
1	3.001826066	1.280720678	1.980698156
6	3.104104534	2.817777557	0.403020066
1	1.386240770	1.940763032	1.493456113
1	3.213409662	3.666920703	1.095520781
1	4.102905732	2.511259494	0.057709931
1	2.513308257	3.143108544	-0.466015311
1	-1.990342025	-2.338800211	3.149505593
1	-1.598277628	-0.591472672	3.172006178
1	-3.199422253	-1.141653220	2.594246605
2e			
7	-1.550339889	0.978805775	0.042866787
6	-0.678921049	-0.227600259	0.037163374

7	-1.541679459	-1.416014066	0.147995944
6	-2.889252020	-0.842344446	0.183582312
7	-2.974413076	0.477967647	0.013984270
6	0.678911227	-0.227593366	-0.037177543
7	1.541676438	-1.416025591	-0.147963909
6	2.889251290	-0.842310102	-0.183517115
7	2.974390946	0.478004448	-0.013969352
7	1.550309615	0.978844405	-0.042913679
6	1.190505027	-2.384030456	-1.263502330
6	1.325075717	1.891175171	1.170032229
6	4.119604057	-1.738770938	-0.325181864
6	-1.190392397	-2.384170968	1.263343757
6	-4.119590426	-1.738812950	0.325295622
6	-1.325118967	1.891168900	-1.170044093
1	0.117874576	-2.626926893	-1.175636692
1	1.378807312	-1.954016880	-2.266773879
1	1.789771930	-3.302651653	-1.140818872
1	0.236395052	2.090241476	1.204289994
1	1.613815870	1.373342493	2.108265878
6	2.133492487	3.206742029	1.006717112
1	4.097605990	-2.546768774	0.424799083
1	4.162828848	-2.197401277	-1.327782083
1	5.024502895	-1.131039433	-0.176168257
1	-1.378762014	-1.954365989	2.266692635
1	-1.789527731	-3.302856561	1.140492920

1	-0.117723881	-2.626890147	1.175436674
1	-5.024507742	-1.130980244	0.176812227
1	-4.097882205	-2.546514013	-0.425017847
1	-4.162500520	-2.197846733	1.327721969
6	-2.133541124	3.206727534	-1.006685340
1	-0.236438261	2.090238190	-1.204303859
1	-1.613864554	1.373365295	-2.108292940
1	-1.970273829	3.856151180	-1.880793878
1	-3.206881768	2.980179875	-0.923985933
1	-1.815564336	3.743098683	-0.100544312
1	1.970190368	3.856154619	1.880827592
1	3.206837968	2.980206133	0.924050476
1	1.815541052	3.743121401	0.100571957

1a-CuI

6	1.789186152	-1.242191913	1.287275750
6	2.937151658	-0.157407128	1.270086094
7	2.717022061	0.622223633	-0.024879833
6	1.384596236	0.331199094	-0.459805438
7	1.130813072	-1.151677377	-0.089958908
6	3.098823610	2.074490944	0.039798761
6	1.761155062	-2.131818536	-1.069805073
1	1.544113447	-3.160546458	-0.730808450
1	1.033487200	-1.004996974	2.057780871
1	3.945777010	-0.615387399	1.263647071
1	1.314929474	-1.970672527	-2.064738985

1	2.855532724	-1.980233395	-1.131045725
1	2.859185439	0.505526137	2.155081512
1	2.171571516	-2.264334404	1.454837811
1	2.846130266	2.537718177	-0.928747136
1	2.569426467	2.618462195	0.848636167
1	4.187811174	2.152069874	0.208670266
29	-0.036637624	0.346533309	-0.789103547
53	-2.208033882	0.067801325	0.266967172

1b-CuI

16	-1.328074972	-1.508981380	-0.830290222
6	-1.357608524	0.429516244	-0.461880473
7	-2.676577245	0.645324263	0.009578943
6	-3.099507979	-0.428570001	1.004717870
6	-2.164756639	-1.677614267	0.813569094
6	-3.025220690	2.049196594	0.416520535
1	-2.547608081	2.343085832	1.373577172
1	-3.014369710	-0.046922110	2.042980037
1	-2.751734443	-2.611138551	0.801078584
1	-2.686599222	2.732231785	-0.380068713
1	-4.122308106	2.125102197	0.524531953
1	-1.427744629	-1.739195195	1.631855813
1	-4.161262690	-0.685067940	0.816927369
29	0.058776241	0.535136467	-0.701230532
53	2.205187157	-0.004637598	0.303864755

1c-CuI

6	0.767104124	0.169517932	-0.406250950
7	1.799399495	-0.864625205	-0.326990561
6	3.063049524	-0.340944999	0.093806043
6	2.928105727	1.021268005	0.223476678
7	1.557967921	1.347478362	-0.032002754
6	1.532476400	-2.308275314	-0.593946279
6	1.048682503	-3.100044623	0.663074450
6	4.284289611	-1.226419790	0.304097038
6	3.959481324	2.077416395	0.597122952
6	1.036640800	2.738419348	-0.123648720
1	4.938753458	1.599911690	0.748504624
1	3.684357453	2.600093564	1.529878928
1	4.065258469	2.834243024	-0.199239225
1	4.088423219	-2.009785738	1.056059610
1	4.589315558	-1.723713522	-0.633220767
1	5.127979315	-0.615089900	0.656802821
1	0.752272075	-2.346986493	-1.381372361
1	0.864619283	-4.150409931	0.388598998
1	0.114199821	-2.666544145	1.050283238
1	1.807329285	-3.070001013	1.459330197
1	2.459562512	-2.761950114	-0.992689322
1	-0.014596276	2.751825556	0.220349691
1	1.634848739	3.397765966	0.528073904
1	1.072224086	3.126410567	-1.161623856
29	-0.681776315	0.072848222	-0.747955084

53 -2.842143127 0.063321477 0.309198622

1c-CuBr

7 1.112808573 1.354892575 -0.057521059

6 0.310489062 0.181072033 -0.441534265

7 1.323405946 -0.870505253 -0.330595257

6 2.589354271 -0.360935458 0.105412451

6 2.473778542 1.002531008 0.225553409

29 -1.157574640 0.092069504 -0.684034970

35 -2.920845368 0.111927851 0.510909451

6 1.065940238 -2.298612247 -0.677430536

6 0.562034875 -3.155302523 0.528496185

6 3.790274624 -1.264697001 0.353037158

6 3.512236975 2.040961173 0.629051697

6 0.667776851 2.753037801 -0.316136784

1 4.469683780 1.543258095 0.842372656

1 3.201866189 2.591706020 1.534069488

1 3.680284926 2.776916829 -0.176265916

1 3.561216431 -2.042810515 1.101067945

1 4.114374088 -1.769900795 -0.573574432

1 4.633495461 -0.665788171 0.727517068

1 0.299551269 -2.299073774 -1.478272092

1 0.393099756 -4.192509574 0.199563136

1 -0.384896821 -2.749136103 0.915431576

1 1.302327292 -3.158384568 1.342366759

1 2.000412850 -2.732027178 -1.081926799

1	-0.402303307	2.846965646	-0.054859126
1	1.250055180	3.445231266	0.315800218
1	0.795271145	3.039022506	-1.379988901

1c-CuCl

7	-0.202005715	1.190894169	-0.407479941
6	-0.124455604	-0.304932553	-0.753522251
7	1.263760473	-0.647252219	-0.672257591
6	1.902660683	0.354943870	0.173762650
6	1.076170848	1.425043354	0.344309623
29	-1.550261254	-0.426353103	-0.443409142
17	-2.659145850	-0.184696432	1.244769747
6	1.700072481	-2.083544204	-0.713358682
6	1.316992863	-2.910826762	0.554609449
6	3.322851957	0.147481968	0.693018384
6	1.295601328	2.744417424	1.070666241
6	-0.321656835	2.134617074	-1.607660771
1	2.229019840	2.704419133	1.652035861
1	0.461182447	2.947034710	1.763608592
1	1.365570244	3.593092391	0.367551335
1	3.384115771	-0.727179823	1.361997345
1	4.021817637	-0.012602907	-0.145373209
1	3.649358278	1.036285023	1.252236845
1	1.221624174	-2.528552001	-1.606509345
1	1.672977796	-3.946056891	0.436857679
1	0.223773469	-2.925800859	0.681557817

1	1.772353913	-2.481190997	1.459163046
1	2.796415921	-2.096504860	-0.863453252
1	-1.205895068	1.845612402	-2.199658022
1	-0.453662331	3.164251064	-1.231817467
1	0.582694103	2.082578323	-2.243202880

1d-CuI

7	-2.007368218	0.956907002	-0.338889715
6	-2.759931176	-0.275868360	-0.161390073
6	-2.147629860	-1.496938957	0.051868279
16	-0.378052532	-1.851104060	0.187781514
6	-0.632120724	0.815122705	-0.259160349
6	-4.290488927	-0.131050234	-0.266647957
6	-2.996507163	-2.779958683	0.205326191
6	-2.651643291	2.315112993	-0.492478440
6	-2.921102363	3.005247514	0.879891101
1	-3.602810720	-2.975238508	-0.695198716
1	-3.679214152	-2.714694364	1.069496822
1	-2.337485787	-3.647208623	0.362414356
1	-4.663630973	0.639389254	0.426534806
1	-4.588385661	0.152561745	-1.290606323
1	-4.781184126	-1.080129840	-0.019133452
1	-1.942649877	2.923528603	-1.085329070
1	-3.356497253	4.001624641	0.706088532
1	-1.978209218	3.120781582	1.435040946
1	-3.621070828	2.414398573	1.489139641

1	-3.586749365	2.204527421	-1.070772177
29	0.471132789	-0.028682627	-0.079982030
53	2.923999926	0.188708863	0.011605184

1e-CuI

7	1.260251584	-1.432610371	0.070915251
7	2.577769258	-2.047023348	0.104681733
6	3.372832468	-0.957202860	-0.095938042
7	2.603770848	0.234571832	-0.251991098
6	1.235700903	-0.050773988	-0.142673704
6	4.893556169	-1.011761373	-0.171491361
6	3.149986641	1.629071452	-0.451902748
6	3.504373941	2.316848980	0.898854543
6	0.018661885	-2.238881036	0.244604605
1	4.037433779	1.555172532	-1.109228673
1	3.876573214	3.332642784	0.695859658
1	4.281936434	1.753156140	1.436185228
1	2.608817643	2.385055991	1.534867911
1	2.360748181	2.198961101	-0.978365917
1	-0.733624625	-1.418147544	0.154613631
1	-0.090882382	-2.998135536	-0.549621652
1	-0.013310531	-2.732685935	1.231683045
1	5.250960330	-0.646769451	-1.149605140
1	5.351594496	-0.395615210	0.620569245
1	5.213421834	-2.056857827	-0.041810865
29	-0.909488545	1.066280261	-0.214321971

53	-2.790787067	-0.137873178	0.060683580
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CuCl

29	0.000000000	0.000000000	0.714388212
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17	0.000000000	0.000000000	-1.218662242
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Cubr

29	0.000000000	0.000000000	-1.125821031
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35	0.000000000	0.000000000	0.932823140
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CuI

29	0.000000000	0.000000000	-1.540236028
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53	0.000000000	0.000000000	0.842770655
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1d_CuI_TS

6	2.900057740	-1.283845676	0.587120094
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16	2.728392048	-1.890598357	-1.071481369
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6	2.255463102	-0.315541608	-1.794790721
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7	2.269014485	0.546889489	-0.688018865
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6	2.622202801	0.051362739	0.643789347
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6	1.972727402	2.012909185	-0.925155398
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6	3.268084615	2.854462955	-1.130780554
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6	2.597228154	0.979103088	1.857574993
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6	3.299019968	-2.211015774	1.733051072
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29	-1.648312691	0.981432849	0.949029601
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53	-2.956160287	-0.461896094	-0.349361479
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1	3.376358556	-1.654354350	2.679320965
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1	4.274503822	-2.688410532	1.535606335
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1	2.556978884	-3.016907205	1.870013659
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1	3.281373790	1.834178839	1.729686023
1	1.580284331	1.374175672	2.030975582
1	2.906599329	0.423601877	2.754920629
1	1.353261015	2.054513392	-1.839738492
1	2.997188917	3.903599963	-1.326360258
1	3.834268695	2.467846174	-1.991505326
1	3.910963899	2.817644628	-0.238998848
1	1.379705225	2.399789751	-0.074639375

1d_CuBr_TS

16	2.512948062	-1.702773259	-1.188390028
6	1.971227423	-0.099345986	-1.791306645
7	1.851978515	0.648446562	-0.609992452
6	2.156844063	0.048685828	0.690466553
6	2.535418309	-1.252632140	0.527814109
6	1.463485943	2.107404816	-0.727975372
6	2.703590272	3.050390181	-0.764491333
6	1.987594716	0.848229828	1.981462769
6	2.929621338	-2.259350798	1.606299537
29	-2.179400111	0.677305698	0.781051496
35	-3.145212785	-0.616781606	-0.491413710
1	2.908199989	-1.794450217	2.603645893
1	3.947481108	-2.649166271	1.431799931
1	2.241198378	-3.122391778	1.616398212
1	2.613490278	1.755867941	1.982237379
1	0.935450589	1.155120898	2.120118803

1	2.280407359	0.229039158	2.841926704
1	0.900446075	2.197067149	-1.675004953
1	2.368768037	4.093053071	-0.878792248
1	3.348684311	2.789432294	-1.616931163
1	3.291246878	2.969307690	0.161789397
1	0.791966750	2.367566841	0.112368502

1d_CuCl_TS

6	-1.773159590	0.138997946	1.756088343
7	-1.490997291	0.732007052	0.515948600
6	-1.663825914	-0.017846787	-0.729542308
6	-2.103866346	-1.281100173	-0.457711072
16	-2.296904692	-1.515294073	1.290443056
6	-1.064252845	2.184784511	0.503416036
6	-2.264963527	3.153741292	0.284691458
6	-1.324215921	0.613742303	-2.078687113
6	-2.405860335	-2.405319188	-1.446172549
29	2.753392249	0.355924663	-0.444836886
1	-2.248694300	-2.069921731	-2.482575537
1	-3.451469086	-2.746133006	-1.351388098
1	-1.754909828	-3.278755019	-1.266667789
1	-1.919633509	1.523317421	-2.262702236
1	-0.255356176	0.886866842	-2.130347624
1	-1.534118045	-0.102349072	-2.886624306
1	-0.606462914	2.376737023	1.491112260
1	-1.906905536	4.194597676	0.311909243

1	-3.009902713	3.013920375	1.082405604
1	-2.748686191	2.973380587	-0.686630817
1	-0.295122690	2.324924670	-0.279566988
17	3.686541690	-0.859984977	0.712360008

PhC≡CH

6	1.214567797	-0.118684802	0.000000000
6	0.000000000	0.594794566	0.000000000
6	-1.213817624	-0.120744625	0.000000000
6	-1.208459890	-1.515087048	0.000000000
6	0.002058632	-2.215792382	0.000000000
6	1.211261730	-1.513253237	0.000000000
6	-0.001906509	2.025814649	0.000000000
6	-0.003931195	3.237971540	0.000000000
1	-2.151984856	0.426340647	0.000000000
1	-2.151226958	-2.056045307	0.000000000
1	0.002824299	-3.302670217	0.000000000
1	2.155030176	-2.052456231	0.000000000
1	2.152160247	0.429437346	0.000000000
1	-0.005440547	4.305281808	0.000000000

Benzaldehyde

6	0.282912169	2.027650735	0.000000000
1	-0.618933479	2.678200052	0.000000000
8	1.395671074	2.523786723	0.000000000
6	0.000000000	0.574375003	0.000000000
6	1.047405233	-0.362511812	0.000000000

6	0.759420735	-1.724850756	0.000000000
6	-0.572981960	-2.160803770	0.000000000
6	-1.619085576	-1.233116433	0.000000000
6	-1.331422558	0.132767241	0.000000000
1	2.072112007	-0.002272440	0.000000000
1	1.567775576	-2.451333811	0.000000000
1	-0.793822178	-3.225225301	0.000000000
1	-2.651069743	-1.573456976	0.000000000
1	-2.138919052	0.862733465	0.000000000

1c-CuI-C≡CPh

7	1.534567608	0.983732653	0.037900039
6	1.338237975	-0.354299304	-0.447165587
7	2.611621664	-0.948235914	-0.149852741
6	3.489618569	-0.042108746	0.526070423
6	2.833010829	1.163931466	0.613228578
29	-0.040488775	-1.135423042	-0.709741501
6	2.950631586	-2.363537776	-0.477778063
6	4.870245192	-0.458050152	1.013182155
6	3.285044291	2.486626161	1.217185806
6	0.544557537	2.089829697	-0.175104276
6	0.712166419	2.773068234	-1.566309713
6	-1.514574789	-0.996019614	-0.062822984
6	-0.702334401	-2.055503837	0.253085564
6	-2.850509197	-0.415174824	0.154115180
6	-3.357848010	0.583070951	-0.723039763

6	-4.632378182	1.139284427	-0.517237503
6	-5.420672924	0.717694839	0.573789992
6	-4.931046928	-0.268825213	1.454973227
6	-3.661206541	-0.835292090	1.246859674
1	5.338686752	0.376955902	1.554760181
1	5.528271169	-0.735138697	0.171187604
1	4.806659973	-1.322573593	1.695986354
1	3.274061079	3.295495637	0.466904268
1	2.633812246	2.788410749	2.055773214
1	4.311772712	2.384608249	1.598459490
1	-0.464733620	1.643786215	-0.089922769
1	-0.046973755	3.562288459	-1.680100644
1	0.577392334	2.028944854	-2.365485339
1	1.711157104	3.224109763	-1.662499690
1	0.677198254	2.822802910	0.642100896
1	-3.278797925	-1.607843782	1.928091894
1	-5.545258817	-0.599827423	2.303304583
1	-6.415300775	1.154754691	0.735387362
1	-5.014737336	1.904164388	-1.206620946
1	-2.741333226	0.904340709	-1.573987529
1	2.331591102	-2.662369809	-1.343299740
1	4.022630226	-2.433473296	-0.732723156
1	2.727103380	-3.038810195	0.370660191