

Supporting Information for:

Mechanistic understanding of the Cu(I)-catalyzed domino reaction constructing 1-aryl-1,2,3-triazole from electron-rich aryl bromide, alkyne, and sodium azide: a DFT study

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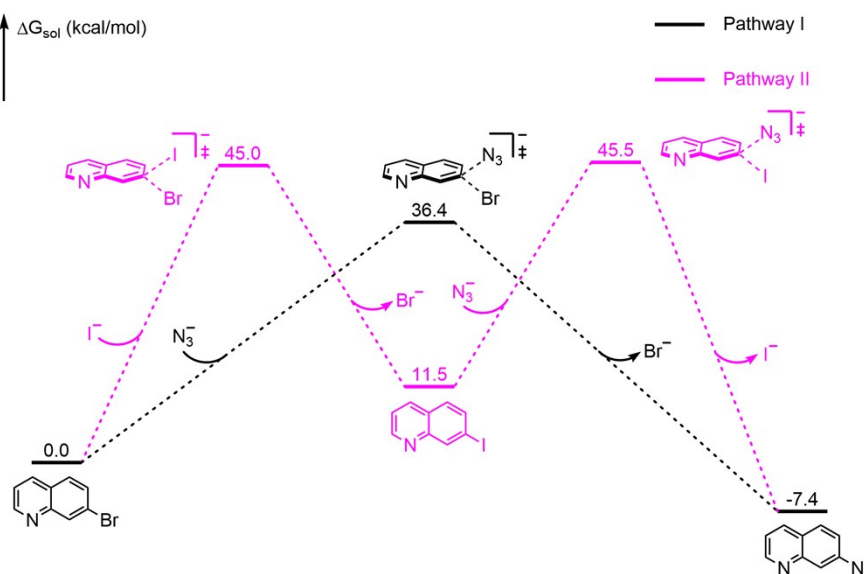
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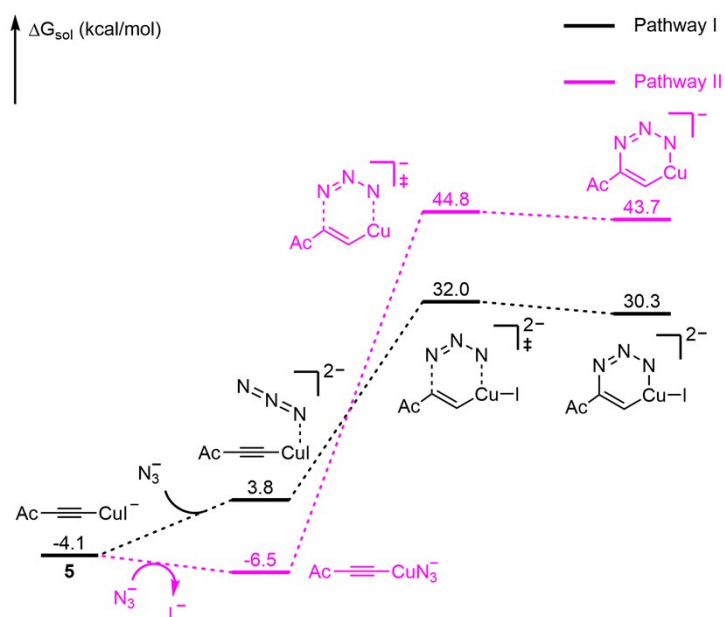
Section 1:

Fig. S1 Calculated free energy profile of the S_NAr reaction of 7-bromoquinoline. The values of free energy are in the units of kcal/mol. Pathway I is the S_NAr reaction of aryl bromide and N_3^- . Pathway II is that the aryl bromide first undergoes a nucleophilic substitution with I^- and subsequently the generated aryl iodide reacts with N_3^- . At the present theoretical level, they are likely to undergo concerted S_NAr reactions. The effects of surrounding counter-cation, Na^+ , are disregarded, which has been proven to give reliable mechanism of bimolecular S_NAr reaction.¹ Since the process of generating aryl iodide is both kinetically and thermodynamically unfavorable ($\Delta G^\ddagger = 45.0$ kcal/mol, $\Delta G = +11.5$ kcal/mol), pathway II could be safely ruled out, although the free energy barrier of the substitution reaction between aryl iodide and N_3^- (34.0 kcal/mol) is lower than that of aryl bromide (36.4 kcal/mol). However, the free energy barrier of the S_NAr reaction of aryl bromide and N_3^- corresponds to a very slow reaction rate. Under such a rate, it is impossible to reach a yield of 94% within 3 hours. We conclude that pathway I is thermodynamically favorable but kinetically unfavorable at the experimental conditions.



Section 2:

Fig. S2 Calculated free energy profile of mononuclear pathway for Cu-catalyzed cycloaddition with anionic copper acetylide and N_3^- . The values of free energy are in the units of kcal/mol.



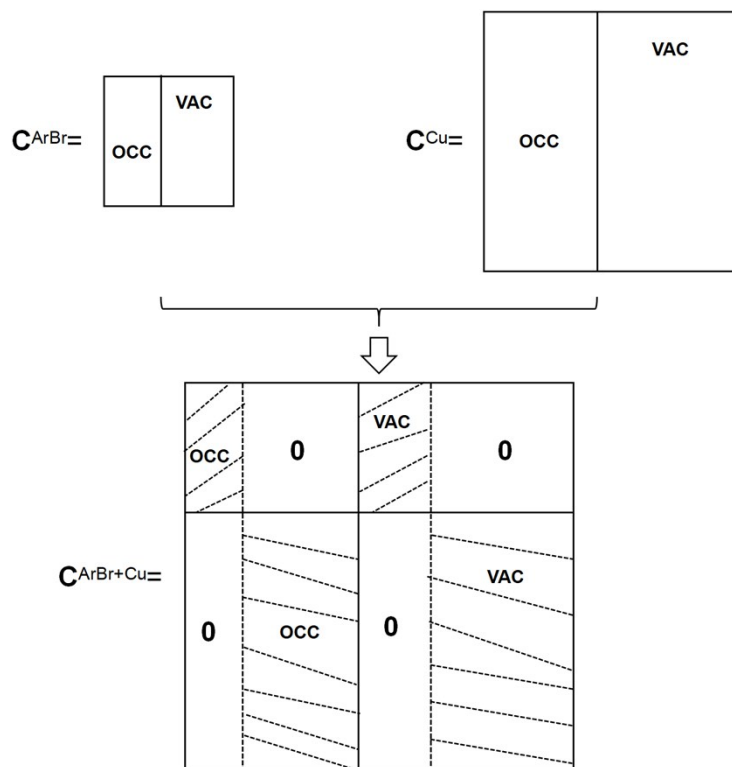
Section 3

Table S1 Calculated free energy changes ΔG_{sol} of deprotonation of the ring-protonated structure.

Reaction	ΔG_{sol} (kcal/mol)
	-9.0
	-11.0
	-0.3

Section 4

Scheme S1 Schematic construction of coefficient matrix of combined fragment wavefunction.



Section 5

Cartesian coordinates of intermediates and transition states.

Cartesian coordinates of **1**

Cu	1.094169	0.432717	-0.025393
N	-0.741296	0.981493	-0.107935
C	-1.737198	0.156858	-0.357207
C	-1.048443	2.408121	0.072214
C	-1.424058	-1.309630	-0.527205
N	-3.031503	0.539311	-0.431002
H	-1.064200	2.904087	-0.908306
H	-0.240420	2.860317	0.651284
C	-2.390133	2.591236	0.769730
C	-2.007809	-2.194874	0.593719
H	-1.780314	-1.658139	-1.503958
H	-0.334869	-1.399564	-0.536563
C	-4.108689	-0.395346	-0.787871
C	-3.466855	1.889855	-0.040950
H	-2.338085	2.159025	1.775721

H	-2.636177	3.651889	0.871014
C	-3.479227	-2.577138	0.399994
H	-1.869246	-1.688797	1.557917
H	-1.412634	-3.113699	0.635884
C	-4.451570	-1.396000	0.320905
H	-4.978808	0.222710	-1.018436
H	-3.847285	-0.923035	-1.710819
H	-3.712247	2.463183	-0.943865
H	-4.385696	1.786899	0.544373
H	-3.565503	-3.160472	-0.527218
H	-3.785605	-3.242806	1.215725
H	-4.489211	-0.860265	1.278160
H	-5.461098	-1.780518	0.132868
I	3.495547	-0.310448	0.006325

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2399.819591	0.202143	-670.748232	-670.787350	-0.039118

Cartesian coordinates of **2**

Cu	-0.692407	0.286152	0.299648
N	1.024509	-0.676697	0.287653
C	2.135710	-0.270066	-0.280777
C	1.068663	-1.884700	1.120714
C	2.090925	0.971448	-1.136523
N	3.331737	-0.882444	-0.118302
H	0.947202	-2.771563	0.483719
H	0.216157	-1.860382	1.803515
C	2.383934	-1.963939	1.884781
C	2.868719	2.156203	-0.526751
H	2.478028	0.747577	-2.137468
H	1.040442	1.238845	-1.260093
C	4.545661	-0.432994	-0.814405
C	3.532854	-1.935889	0.890154
H	2.457282	-1.108651	2.566707
H	2.436471	-2.877521	2.483460
C	4.375890	2.127872	-0.803991
H	2.682168	2.189192	0.554219
H	2.453970	3.080871	-0.943163
C	5.109292	0.888782	-0.279861
H	5.279270	-1.231662	-0.686175

H	4.349760	-0.359692	-1.888924
H	3.632240	-2.903611	0.382585
H	4.479194	-1.733104	1.401256
H	4.528873	2.188334	-1.890386
H	4.835510	3.026240	-0.374888
H	5.085746	0.861043	0.817284
H	6.164181	0.952878	-0.572259
C	-1.668016	1.964879	0.896449
C	-0.462321	2.069957	1.176713
H	0.472103	2.462474	1.533012
I	-2.603186	-1.381264	-0.670961
C	-3.107854	2.124119	0.712516
O	-3.883400	1.776573	1.595995
C	-3.541996	2.709012	-0.601003
H	-3.106994	3.707727	-0.722003
H	-3.166905	2.086787	-1.420379
H	-4.631302	2.766093	-0.640416

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2629.719869	0.256384	-900.617709	-900.6691171	-0.051408

Cartesian coordinates of **2-TS**

Cu	-1.474761	0.162456	0.356272
N	1.572775	-0.869113	1.118154
C	2.322651	-0.639895	0.078176
C	2.251834	-1.250177	2.355794
C	1.633407	-0.215487	-1.199654
N	3.688494	-0.711855	0.055331
H	2.410522	-2.339730	2.375531
H	1.592177	-1.016811	3.199030
C	3.595639	-0.540856	2.510208
C	1.952919	1.230943	-1.629526
H	1.879286	-0.905604	-2.016401
H	0.562394	-0.315269	-1.013733
C	4.472786	-0.507808	-1.165758
C	4.460107	-0.852880	1.297245
H	3.426297	0.540898	2.575893
H	4.112514	-0.852932	3.422973
C	3.266322	1.388112	-2.403543
H	1.958741	1.877188	-0.742217

H	1.131431	1.584385	-2.263876
C	4.522809	0.948655	-1.644781
H	5.483102	-0.858870	-0.941720
H	4.092383	-1.153505	-1.965146
H	4.864900	-1.872113	1.364457
H	5.313378	-0.167382	1.249034
H	3.195694	0.798729	-3.328536
H	3.378466	2.435021	-2.711130
H	4.695407	1.597475	-0.776042
H	5.391652	1.064741	-2.304345
C	-1.355640	2.186562	0.725851
C	-0.316641	1.652004	1.122667
H	0.626741	1.265680	1.468760
I	-2.787138	-1.857034	-0.453565
C	-2.430583	3.123889	0.382908
O	-3.489830	2.721562	-0.077383
C	-2.118283	4.570329	0.637845
H	-1.875782	4.714197	1.696741
H	-1.233734	4.861679	0.060133
H	-2.973389	5.187730	0.357731

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2629.684022	0.252078	-900.594015	-900.6470381	-0.053023

Cartesian coordinates of **3**

Cu	-2.094055	0.291205	0.044208
N	1.777616	-0.704290	0.469290
C	2.882578	-0.571263	-0.209988
C	1.764344	-1.627250	1.600363
C	2.883086	0.435501	-1.337934
N	4.037884	-1.239962	0.050664
H	1.493739	-2.636731	1.257121
H	0.974768	-1.307666	2.291021
C	3.120809	-1.668297	2.299764
C	3.821364	1.634981	-1.091135
H	3.149010	-0.054204	-2.282717
H	1.854234	0.786315	-1.443383
C	5.233791	-1.109829	-0.788574
C	4.191105	-2.032341	1.279912
H	3.335899	-0.681088	2.725413

H	3.128228	-2.395398	3.117155
C	5.293073	1.372625	-1.429982
H	3.722999	1.955973	-0.045914
H	3.468927	2.470406	-1.706707
C	5.952861	0.236412	-0.641833
H	5.901425	-1.923520	-0.496073
H	4.970777	-1.286197	-1.837324
H	4.142662	-3.101356	1.033320
H	5.188616	-1.835651	1.686095
H	5.364804	1.138596	-2.501385
H	5.864270	2.296164	-1.275801
H	6.010180	0.488686	0.425031
H	6.984279	0.115108	-0.994713
C	-1.131176	2.079487	0.492240
C	-0.304318	1.156226	0.474163
H	0.574063	0.408333	0.458515
I	-3.854228	-1.466302	-0.461196
C	-1.854028	3.345485	0.588680
O	-3.067268	3.392048	0.421229
C	-1.008645	4.548234	0.899812
H	-0.489549	4.397634	1.853046
H	-0.240143	4.667886	0.127812
H	-1.636943	5.439322	0.948451

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2629.689705	0.249978	-900.597927	-900.645299	-0.047372

Cartesian coordinates of **3-TS**

Cu	-2.056425	0.295110	0.042586
N	1.720216	-0.641928	0.501914
C	2.822967	-0.536553	-0.192478
C	1.663492	-1.571910	1.625014
C	2.847156	0.486347	-1.303715
N	3.943645	-1.254925	0.050236
H	1.329638	-2.559246	1.276384
H	0.903380	-1.206842	2.325628
C	3.026824	-1.692519	2.300039
C	3.843048	1.638114	-1.055311
H	3.076352	-0.004654	-2.257172
H	1.834441	0.885450	-1.390695

C	5.134817	-1.171545	-0.804365
C	4.062833	-2.089133	1.256887
H	3.297698	-0.726799	2.742042
H	3.008877	-2.436943	3.101058
C	5.295660	1.312475	-1.419917
H	3.774369	1.949652	-0.005100
H	3.519125	2.495568	-1.655662
C	5.914393	0.139265	-0.653131
H	5.766738	-2.017890	-0.527059
H	4.848276	-1.325241	-1.850168
H	3.950100	-3.145124	0.979452
H	5.074223	-1.959364	1.653974
H	5.340446	1.087039	-2.494512
H	5.910534	2.207181	-1.264787
H	5.998468	0.376481	0.415274
H	6.933727	-0.025370	-1.022597
C	-1.085683	2.093791	0.484076
C	-0.273099	1.150926	0.471576
H	0.670167	0.326697	0.454805
I	-3.820076	-1.460673	-0.463771
C	-1.784148	3.369117	0.570242
O	-2.997089	3.442382	0.395948
C	-0.920903	4.561347	0.880868
H	-0.410104	4.408631	1.838184
H	-0.145786	4.665834	0.113356
H	-1.534771	5.462995	0.921164

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2629.686613	0.248869	-900.595203	-900.644014	-0.048811

Cartesian coordinates of **4**

Cu	-2.043457	0.911424	-0.138403
N	0.927174	-0.466454	0.502930
C	2.013689	-0.843898	-0.155533
C	0.173425	-1.340076	1.401470
C	2.694597	0.177193	-1.022290
N	2.508662	-2.069199	-0.026162
H	-0.616633	-1.849730	0.839910
H	-0.301216	-0.710471	2.156395
C	1.139248	-2.340204	2.020010

C	4.110635	0.541044	-0.527400
H	2.740005	-0.201353	-2.049689
H	2.064390	1.068707	-1.037459
C	3.673146	-2.525606	-0.809647
C	1.926779	-3.041294	0.921805
H	1.826953	-1.817815	2.693192
H	0.591671	-3.084516	2.602622
C	5.197098	-0.468232	-0.911929
H	4.085859	0.681898	0.559899
H	4.366344	1.512442	-0.961986
C	4.991661	-1.885709	-0.368914
H	3.712318	-3.607674	-0.679225
H	3.486515	-2.338109	-1.871531
H	1.291285	-3.735866	0.360966
H	2.754868	-3.611008	1.349222
H	5.252577	-0.519618	-2.007731
H	6.166481	-0.089746	-0.567689
H	5.039592	-1.894004	0.727157
H	5.807346	-2.523719	-0.727578
C	0.107839	3.098430	0.196667
C	-0.751532	2.221775	0.061214
H	0.584094	0.482206	0.359262
I	-3.812564	-0.906172	-0.293104
C	1.098539	4.127422	0.360168
O	0.790215	5.322652	0.384155
C	2.532234	3.671339	0.483223
H	2.619847	2.857283	1.209144
H	2.868097	3.282268	-0.484739
H	3.169000	4.509871	0.774361

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2629.705344	0.256549	-900.607520	-900.674003	-0.066484

Cartesian coordinates of **5**

Cu	-0.088901	-0.172292	-0.000391
C	2.992460	-0.175232	0.000178
C	1.758522	-0.211646	0.000034
I	-2.625907	0.076941	0.000200
C	4.426603	-0.097322	-0.000011
O	5.137953	-1.107625	-0.000033

C	5.020070	1.292701	-0.000024
H	4.675197	1.845702	-0.881022
H	4.675413	1.845619	0.881114
H	6.111044	1.237234	-0.000156

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2167.330117	0.014296	-438.206059	-438.282578	-0.076519

Cartesian coordinates of **6**

C	-0.620710	1.527219	0.000185
C	0.721245	1.834136	0.000354
C	1.703621	0.811220	0.000289
C	1.288146	-0.556497	0.000044
C	-0.099560	-0.863054	-0.000130
C	-1.003436	0.168049	-0.000059
H	3.443588	2.105890	0.000663
H	-1.368149	2.311829	0.000238
H	1.040349	2.872266	0.000545
C	3.096454	1.076643	0.000456
H	-0.399625	-1.904210	-0.000327
C	3.463415	-1.297508	0.000099
C	3.978284	0.022092	0.000360
H	4.155514	-2.138424	0.000063
H	5.051382	0.179586	0.000490
N	2.176390	-1.595015	-0.000033
Br	-2.923501	-0.245590	-0.000315

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2974.914654	0.088279	-414.480815	-414.495718	-0.014903

Cartesian coordinates of **7**

C	0.810894	1.851661	0.000022
C	-0.558345	1.950132	0.000140
C	-1.370242	0.785135	-0.000012
C	-0.741055	-0.500728	-0.000110
C	0.672482	-0.583020	0.000025

C	1.428518	0.573282	-0.000154
H	-3.290160	1.790407	-0.000277
H	1.440345	2.735183	0.000376
H	-1.037348	2.924835	0.000326
C	-2.785515	0.828236	-0.000127
H	1.132309	-1.566193	0.000274
C	-2.777079	-1.572766	0.000177
C	-3.492925	-0.351596	-0.000133
H	-3.328236	-2.512008	0.000050
H	-4.577704	-0.363476	-0.000265
N	-1.458828	-1.665517	0.000140
N	2.848026	0.593159	0.000054
N	3.441897	-0.492242	-0.000045
N	4.103246	-1.419794	-0.000070

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-565.2915862	0.100455	-565.280200	-565.289718	-0.009517

Cartesian coordinates of **8**

Cu	-0.179386	-0.510492	-0.205164
N	-2.089943	-1.085781	-0.357066
C	-3.077616	-0.65514	0.390188
C	-2.406221	-2.006349	-1.454821
C	-2.761624	0.304388	1.511017
N	-4.37845	-0.987191	0.19352
H	-2.433676	-3.037134	-1.074138
H	-1.595615	-1.956606	-2.186334
C	-3.74337	-1.649785	-2.093094
C	-3.351254	1.712426	1.283634
H	-3.11922	-0.101198	2.464988
H	-1.674369	0.365542	1.580613
C	-5.448331	-0.550547	1.100182
C	-4.823265	-1.683382	-1.023572
H	-3.67846	-0.645208	-2.527578
H	-3.996793	-2.347978	-2.895942
C	-4.814079	1.85868	1.714545
H	-3.241394	1.978932	0.2258
H	-2.743111	2.43016	1.843795
C	-5.79584	0.93805	0.982137
H	-6.321214	-1.158188	0.851325

H	-5.181184	-0.798537	2.132702
H	-5.087537	-2.718426	-0.771132
H	-5.733098	-1.189163	-1.379312
H	-4.882025	1.654336	2.792208
H	-5.125971	2.900816	1.575286
H	-5.849459	1.20156	-0.082228
H	-6.800082	1.087903	1.39667
C	-0.354795	2.496285	-0.618264
C	0.192065	1.397809	-0.425311
I	1.382691	-2.732399	0.132236
C	-1.043237	3.732489	-0.81347
O	-1.432489	4.419207	0.143235
C	-1.288489	4.156023	-2.243632
H	-0.344066	4.199863	-2.796756
H	-1.921894	3.414823	-2.745137
H	-1.778946	5.131899	-2.26535
Cu	1.933415	0.652593	-0.066333
I	4.460257	0.927062	0.280512

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4567.169084	0.235519	-1108.966791	-1109.083649	-0.116858

Cartesian coordinates of **9**

C	-2.583182	2.136132	0.501683
C	-1.774864	1.198096	0.403862
N	-5.129828	1.179089	-0.991653
N	-4.447479	0.237670	-1.092320
N	-3.747175	-0.733242	-1.196219
Cu	-1.957752	-0.663533	-0.306334
Cu	-0.014077	0.548392	0.609917
I	-0.702859	-3.055365	-0.227833
N	1.849399	0.144527	0.890400
C	2.785176	0.364792	-0.008844
C	2.236996	-0.490193	2.156942
C	2.379122	0.999741	-1.316456
N	4.093286	0.085105	0.180713
H	2.229533	-1.581725	2.031518
H	1.481120	-0.245996	2.906913
C	3.617845	-0.022644	2.597556
C	2.947094	2.419883	-1.514022

H	2.680672	0.356441	-2.151592
H	1.286949	1.034990	-1.325534
C	5.101130	0.288313	-0.870566
C	4.617204	-0.326482	1.493605
H	3.591077	1.056008	2.791173
H	3.925258	-0.522884	3.520141
C	4.386701	2.457662	-2.037445
H	2.870337	2.971077	-0.567897
H	2.302242	2.940236	-2.230810
C	5.419921	1.762071	-1.145654
H	5.999306	-0.231347	-0.530957
H	4.780377	-0.211857	-1.790045
H	4.852979	-1.397706	1.464847
H	5.553804	0.213568	1.662670
H	4.406901	1.981892	-3.027645
H	4.685253	3.502025	-2.188035
H	5.517879	2.285174	-0.185740
H	6.399837	1.812102	-1.635221
C	-3.547664	3.189741	0.592418
O	-3.504888	4.178644	-0.153976
C	-4.577783	3.076132	1.694670
H	-4.929464	2.048293	1.807934
H	-4.116118	3.379388	2.643027
H	-5.417846	3.743088	1.485334

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4433.733028	0.247187	-1261.664448	-1261.794405	-0.129957

Cartesian coordinates of **9-TS**

C	3.116340	-1.746666	-0.283935
C	2.090121	-1.019117	-0.015737
N	4.744865	-0.874082	-0.686909
N	4.511225	0.300361	-0.620558
N	3.875593	1.304060	-0.453830
Cu	1.923762	0.895993	0.052655
Cu	0.257956	-1.028770	0.402746
I	0.445491	3.094980	0.389635
N	-1.617352	-1.091531	0.837804
C	-2.563745	-0.494803	0.144793
C	-2.002153	-1.807187	2.062572

C	-2.173721	0.230811	-1.119682
N	-3.874027	-0.526930	0.477648
H	-2.029952	-1.101250	2.904563
H	-1.226655	-2.544301	2.283804
C	-3.361553	-2.473648	1.898107
C	-2.737076	-0.421704	-2.399068
H	-2.490777	1.278409	-1.062234
H	-1.082318	0.237652	-1.158685
C	-4.895011	0.213953	-0.276557
C	-4.386816	-1.412475	1.535572
H	-3.302774	-3.225263	1.102169
H	-3.664197	-2.980511	2.818640
C	-4.182775	-0.032226	-2.726169
H	-2.645876	-1.512654	-2.316447
H	-2.098000	-0.118558	-3.235864
C	-5.210800	-0.391156	-1.648676
H	-5.790264	0.213539	0.348817
H	-4.587939	1.259441	-0.380945
H	-4.650425	-0.808763	2.413158
H	-5.306711	-1.875205	1.164940
H	-4.218768	1.053376	-2.892155
H	-4.474288	-0.501494	-3.673470
H	-5.294869	-1.480340	-1.541012
H	-6.196018	-0.026942	-1.963653
C	3.433415	-3.169675	-0.389603
O	4.540937	-3.622561	-0.680137
C	2.276031	-4.114915	-0.111831
H	1.889393	-3.951708	0.899152
H	1.453977	-3.919377	-0.807757
H	2.612466	-5.149283	-0.216998

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4433.711802	0.252152	-1261.637212	-1261.760988	-0.123776

Cartesian coordinates of **10**

C	-3.284034	-1.592482	0.317270
C	-2.153132	-0.925520	0.060626
N	-4.589555	-1.007288	0.567414
N	-4.614224	0.270562	0.529728
N	-3.775001	1.153721	0.328232

Cu	-1.918850	0.922068	-0.021092
Cu	-0.329560	-1.070541	-0.332253
I	-0.391894	3.109210	-0.346327
N	1.536931	-1.124690	-0.805187
C	2.498895	-0.529702	-0.132388
C	1.880594	-1.781452	-2.074350
C	2.150106	0.136115	1.176616
N	3.792773	-0.513645	-0.524916
H	1.844323	-1.043897	-2.888442
H	1.116795	-2.533823	-2.285380
C	3.265064	-2.411429	-2.004571
C	2.787121	-0.552403	2.401687
H	2.440067	1.192521	1.147451
H	1.061710	0.113935	1.264977
C	4.830030	0.222033	0.212340
C	4.276051	-1.335483	-1.646080
H	3.267758	-3.197163	-1.240127
H	3.536123	-2.869272	-2.959968
C	4.236892	-0.139933	2.678931
H	2.718027	-1.641081	2.278470
H	2.180563	-0.299199	3.278310
C	5.222360	-0.429740	1.542541
H	5.695199	0.268695	-0.452298
H	4.504562	1.254736	0.373224
H	4.476687	-0.685735	-2.507303
H	5.226897	-1.785177	-1.343468
H	4.255496	0.938745	2.887495
H	4.582350	-0.639275	3.592102
H	5.326444	-1.511262	1.386248
H	6.212262	-0.053902	1.827710
C	-3.353140	-3.083973	0.386846
O	-4.396947	-3.676460	0.659852
C	-2.093317	-3.878819	0.110147
H	-1.718035	-3.665072	-0.895490
H	-1.301754	-3.603051	0.813521
H	-2.313021	-4.945318	0.201920

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG_{sol}^* (a.u.)
-4433.718535	0.254538	-1261.630104	-1261.756898	-0.126793

Cartesian coordinates of **10-TS**

C	2.769828	2.137082	0.495704
C	1.848120	1.171787	0.307064
N	3.985717	1.946962	1.210151
N	4.054360	0.744347	1.686495
N	3.227629	-0.181746	1.546928
Cu	1.946820	-0.716460	0.205127
Cu	0.075294	0.966714	-0.285382
I	1.378710	-3.088570	-0.751421
N	-1.763538	0.847347	-0.846812
C	-2.674305	0.121683	-0.232136
C	-2.218006	1.785240	-1.883109
C	-2.214701	-0.857372	0.820027
N	-4.001488	0.225981	-0.466561
H	-2.331868	1.248317	-2.835404
H	-1.441429	2.539573	-2.027013
C	-3.541766	2.425585	-1.487207
C	-2.653047	-0.467889	2.246472
H	-2.579402	-1.862565	0.577691
H	-1.124632	-0.897627	0.763949
C	-4.987277	-0.628135	0.211686
C	-4.568174	1.327394	-1.263780
H	-3.401662	3.003041	-0.565931
H	-3.896860	3.109378	-2.263256
C	-4.087007	-0.877028	2.601399
H	-2.521128	0.614083	2.377937
H	-1.968103	-0.952535	2.951134
C	-5.175071	-0.290751	1.695513
H	-5.927000	-0.488951	-0.326862
H	-4.709909	-1.679799	0.089660
H	-4.925703	0.927244	-2.220662
H	-5.436976	1.716380	-0.723746
H	-4.154113	-1.972901	2.558324
H	-4.292836	-0.593633	3.640557
H	-5.222289	0.800695	1.803682
H	-6.148577	-0.682363	2.013835
C	2.617194	3.524737	-0.029350
O	3.530340	4.347933	0.051019
C	1.319034	3.915677	-0.704901
H	1.220344	3.382249	-1.656377
H	0.455588	3.643004	-0.091690
H	1.323243	4.991469	-0.896984

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4433.710524	0.253725	-1261.633573	-1261.763388	-0.129815

Cartesian coordinates of **11**

C	-3.869556	-0.718934	0.249331
C	-2.499949	-0.414341	0.074885
N	-4.573584	0.442114	0.472090
N	-3.726844	1.435105	0.444556
N	-2.463291	0.943644	0.206075
Cu	-0.966148	2.082197	0.008863
Cu	-0.926911	-1.412831	-0.229151
I	0.949031	3.686990	-0.309756
N	0.724579	-2.360199	-0.491292
C	1.903490	-1.787388	-0.364816
C	0.684954	-3.806180	-0.749596
C	1.949125	-0.303011	-0.097762
N	3.077259	-2.456117	-0.423237
H	0.783799	-3.987262	-1.829244
H	-0.295771	-4.180330	-0.447200
C	1.800734	-4.521791	0.000766
C	2.478625	0.047963	1.306666
H	2.553763	0.198960	-0.862034
H	0.929510	0.076287	-0.208534
C	4.374959	-1.771478	-0.332049
C	3.135011	-3.927070	-0.418655
H	1.653749	-4.389491	1.079027
H	1.792201	-5.594566	-0.211366
C	4.006713	0.070336	1.416533
H	2.052921	-0.653748	2.035822
H	2.095107	1.040681	1.565684
C	4.702106	-1.251260	1.072589
H	5.123505	-2.502504	-0.644878
H	4.412758	-0.955197	-1.060381
H	3.421438	-4.277788	-1.418203
H	3.926083	-4.227776	0.275294
H	4.389414	0.849462	0.742653
H	4.289041	0.371853	2.432403
H	4.440485	-2.027447	1.803421
H	5.787263	-1.107627	1.138079
C	-4.542511	-2.009392	0.217036
O	-5.767515	-2.122314	0.372520

C	-3.696714	-3.248263	-0.012130
H	-3.130205	-3.167901	-0.945276
H	-2.967871	-3.369724	0.796297
H	-4.345730	-4.126420	-0.050448

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4433.798899	0.257375	-1261.759563	-1261.882561	-0.122997

Cartesian coordinates of **12**

Cu	-0.488898	-0.036446	-0.318168
N	-2.362342	-0.694522	-0.462077
C	-3.345534	-0.395783	0.352632
C	-2.630147	-1.625452	-1.563823
C	-3.073008	0.579644	1.472408
N	-4.607622	-0.877092	0.227823
H	-2.489048	-2.657882	-1.21521
H	-1.887381	-1.448415	-2.346346
C	-4.044595	-1.443539	-2.100708
C	-3.867378	1.897651	1.35084
H	-3.283493	0.1072	2.439568
H	-2.002548	0.792557	1.451502
C	-5.655307	-0.617394	1.223881
C	-5.031519	-1.632094	-0.960315
H	-4.146713	-0.435642	-2.519824
H	-4.25844	-2.162242	-2.896924
C	-5.298339	1.829553	1.89339
H	-3.876525	2.2176	0.302358
H	-3.319766	2.66874	1.903305
C	-6.204581	0.812801	1.193071
H	-6.455939	-1.329321	1.011407
H	-5.281518	-0.859489	2.22453
H	-5.125277	-2.694533	-0.700235
H	-6.025604	-1.275014	-1.247754
H	-5.254133	1.579205	2.962495
H	-5.753543	2.825015	1.825698
H	-6.37295	1.101667	0.147459
H	-7.185159	0.812912	1.684212
C	-0.169196	1.933944	-0.722087
C	0.976088	1.473949	-0.484237
I	0.984861	-2.345234	0.26073

C	-1.287072	2.814911	-1.012538
O	-1.513746	3.797636	-0.304324
C	-2.155735	2.453734	-2.189276
H	-1.541021	2.299325	-3.08259
H	-2.664286	1.506637	-1.979353
H	-2.89229	3.239856	-2.367654
Cu	2.723317	0.942824	-0.150083
I	5.178067	0.450055	0.292809

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4567.169700	0.236907	-1108.970835	-1109.087069	-0.116233

Cartesian coordinates of **13**

Cu	0.718753	1.309445	-0.288631
N	2.16374	0.09278	0.068332
C	2.000146	-1.211055	0.136617
C	3.495691	0.645373	0.344971
C	0.622787	-1.769496	-0.122479
N	3.000413	-2.081368	0.397143
H	3.609101	0.79124	1.428111
H	3.560703	1.630782	-0.121628
C	4.583757	-0.281919	-0.18018
C	0.525495	-2.62873	-1.397384
H	0.285413	-2.346082	0.74681
H	-0.05983	-0.919462	-0.208906
C	2.766498	-3.525366	0.542736
C	4.408382	-1.655153	0.447245
H	4.499808	-0.3554	-1.270839
H	5.578419	0.106629	0.05556
C	0.992218	-4.077613	-1.223921
H	1.088411	-2.139734	-2.203313
H	-0.525165	-2.635276	-1.708764
C	2.448272	-4.238979	-0.776088
H	3.67957	-3.935451	0.979058
H	1.967685	-3.696394	1.271614
H	4.744871	-1.651977	1.491625
H	5.002029	-2.402218	-0.088643
H	0.344747	-4.5622	-0.48002
H	0.842162	-4.617979	-2.166267
H	3.134606	-3.870669	-1.549575

H	2.662044	-5.306465	-0.644815
C	-0.216117	3.15411	-0.780358
C	-1.042275	2.225518	-0.625226
C	0.457771	4.418789	-0.998585
O	-0.195685	5.42977	-1.2586
C	1.958945	4.422715	-0.888262
H	2.255847	4.077818	0.108302
H	2.386292	3.722932	-1.615367
H	2.34528	5.428253	-1.067244
N	-0.574782	0.711438	2.774555
N	0.189753	1.617315	2.721317
N	0.957457	2.519392	2.674785
Cu	-2.05118	0.706229	-0.267134
I	-3.497389	-1.360323	0.111374

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4433.718799	0.248269	-1261.653318	-1261.785866	-0.132548

Cartesian coordinates of **13-TS**

Cu	0.19823	1.30922	-0.278231
N	-1.68939	1.377528	-0.641534
C	-2.488211	0.338562	-0.509871
C	-2.300225	2.684489	-0.920888
C	-1.864845	-1.006551	-0.234772
N	-3.835754	0.414397	-0.575214
H	-2.476684	2.781436	-2.00146
H	-1.58887	3.462925	-0.636811
C	-3.613145	2.836332	-0.164035
C	-2.187865	-1.55498	1.168574
H	-2.176706	-1.727702	-0.999682
H	-0.782468	-0.88851	-0.340618
C	-4.69332	-0.776049	-0.480644
C	-4.544698	1.705298	-0.567361
H	-3.414907	2.794305	0.913344
H	-4.084998	3.798268	-0.382927
C	-3.547172	-2.254319	1.275539
H	-2.120452	-0.736353	1.897071
H	-1.402814	-2.272583	1.430905
C	-4.756865	-1.380661	0.926704
H	-5.688238	-0.456031	-0.797258

H	-4.361705	-1.526508	-1.205159
H	-4.968967	1.885577	-1.562957
H	-5.378594	1.622562	0.136604
H	-3.541885	-3.123584	0.603276
H	-3.668695	-2.648039	2.291763
H	-4.867984	-0.565771	1.653795
H	-5.665413	-1.990962	0.993855
C	1.91153	1.915415	0.663046
C	2.226097	0.991869	-0.231752
C	2.106378	2.983746	1.554206
O	3.11078	3.064149	2.317786
C	0.992372	4.0101	1.706604
H	0.218266	3.908596	0.941175
H	0.52623	3.902881	2.694121
H	1.422388	5.016384	1.656412
N	3.054665	1.445709	-1.538041
N	3.18866	2.684216	-1.460762
N	2.994009	3.714191	-0.939477
Cu	1.856405	-0.879812	-0.196291
I	1.511818	-3.407825	-0.020632

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4433.686573	0.251454	-1261.619936	-1261.744862	-0.124926

Cartesian coordinates of **14**

Cu	0.108967	-1.306654	-0.761693
N	2.034689	-1.217414	-0.903036
C	2.723119	-0.148854	-0.560489
C	2.772965	-2.469303	-1.120659
C	1.969851	1.138302	-0.337676
N	4.060952	-0.144945	-0.36547
H	3.161025	-2.490624	-2.148889
H	2.07201	-3.301336	-1.02137
C	3.922901	-2.596455	-0.129511
C	1.960164	1.590388	1.135348
H	2.385259	1.931228	-0.970966
H	0.943516	0.964927	-0.672846
C	4.795611	1.078536	-0.012977
C	4.83851	-1.393262	-0.285025
H	3.518335	-2.631408	0.888797

H	4.490133	-3.515924	-0.29921
C	3.221081	2.344227	1.57131
H	1.795254	0.714447	1.776183
H	1.09288	2.244857	1.275474
C	4.531864	1.565009	1.417262
H	5.853926	0.840935	-0.13941
H	4.564488	1.86795	-0.735004
H	5.457236	-1.487767	-1.186164
H	5.514347	-1.310282	0.571722
H	3.294554	3.265993	0.977485
H	3.109008	2.656439	2.616555
H	4.547419	0.697973	2.090397
H	5.365087	2.212429	1.715784
C	-2.37344	-2.188492	0.593949
C	-1.799293	-1.596564	-0.567624
C	-1.98249	-2.03774	1.988433
O	-1.006146	-1.349594	2.332992
C	-2.814542	-2.745577	3.035658
H	-3.839687	-2.359653	3.024601
H	-2.876981	-3.816528	2.819173
H	-2.375701	-2.589667	4.023302
N	-2.561859	-2.064886	-1.609759
N	-3.517463	-2.88332	-1.107501
N	-3.422008	-2.968233	0.216499
Cu	-1.602976	0.383196	-0.489379
I	-1.951975	2.894214	-0.207011

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4433.784937	0.254386	-1261.744944	-1261.876467	-0.131523

Cartesian coordinates of **14-TS**

C	-1.266776	0.017688	-1.873175
C	-1.277932	-1.270311	-2.443620
C	-0.087833	-1.744121	-2.946391
C	1.092130	-0.947594	-2.928719
C	1.040828	0.379558	-2.398396
C	-0.195815	0.871043	-1.882955
H	-2.170941	-1.882527	-2.429972
H	-0.037127	-2.750564	-3.352602
H	-0.243892	1.887657	-1.511741

Cu	-2.285957	0.387234	-0.223473
C	2.335465	-1.402920	-3.428120
H	2.412487	-2.407299	-3.834514
C	3.425163	-0.561551	-3.386587
H	4.396160	-0.874887	-3.754554
C	3.263352	0.738274	-2.854212
H	4.115278	1.414302	-2.823236
N	2.121523	1.208620	-2.379364
N	-2.127691	-1.394545	0.555483
C	-1.034127	-2.126257	0.888202
N	-3.278745	-2.120531	0.723310
C	-1.594903	-3.362317	1.288091
Cu	0.727727	-1.467260	0.753321
N	-2.965613	-3.308083	1.168507
C	-0.931003	-4.573440	1.752490
N	2.532824	-0.831728	0.599684
O	-1.562014	-5.583068	2.097219
C	0.585328	-4.587213	1.783896
C	2.871642	0.438857	0.638625
C	3.554474	-1.828148	0.246267
H	0.976160	-4.605116	0.759809
H	0.984819	-3.688329	2.262643
H	0.928913	-5.480548	2.310962
C	1.813251	1.446025	1.016100
N	4.120379	0.898017	0.397404
H	3.550345	-1.980116	-0.840317
H	3.271786	-2.779093	0.705590
C	4.939255	-1.395334	0.708229
C	2.101107	2.197304	2.330753
H	1.683600	2.159474	0.195517
H	0.872686	0.898958	1.106695
C	4.422650	2.332123	0.297724
C	5.239333	-0.016789	0.143380
H	4.967655	-1.361466	1.803669
H	5.700085	-2.106320	0.373784
C	3.042771	3.396375	2.179090
H	2.497143	1.491946	3.072958
H	1.141863	2.555072	2.721243
C	4.438546	3.058293	1.647042
H	5.406197	2.400585	-0.171563
H	3.714407	2.809859	-0.387441
H	5.424936	-0.072613	-0.937602
H	6.132065	0.408384	0.611571
H	2.574782	4.117419	1.494465

H	3.138743	3.903259	3.146847
H	4.988804	2.442217	2.369800
H	5.006519	3.988566	1.525487
I	-2.363836	2.309606	1.671032
Br	-3.369873	1.301939	-2.207057

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-7408.706759	0.369608	-1676.207508	-1676.343027	-0.135520

Cartesian coordinates of **15**

C	-0.866244	-0.329720	1.777056
C	-0.859362	0.637826	2.797247
C	0.320732	0.847229	3.480858
C	1.490113	0.102214	3.168528
C	1.435281	-0.898913	2.148052
C	0.211433	-1.102755	1.445737
H	-1.742473	1.227796	3.014932
H	0.369887	1.602207	4.261132
H	0.183651	-1.860295	0.670928
Cu	-2.29994	-0.509729	0.495219
C	2.730655	0.297654	3.825149
H	2.809541	1.051968	4.603159
C	3.812001	-0.473461	3.464303
H	4.778506	-0.352663	3.941772
C	3.646542	-1.448125	2.451565
H	4.491468	-2.071353	2.165221
N	2.510354	-1.667510	1.812037
N	-2.037307	1.332545	0.091719
C	-0.982224	2.084748	-0.304123
N	-3.167608	2.081137	0.289821
C	-1.554882	3.376365	-0.363943
Cu	0.781422	1.450014	-0.527748
N	-2.879672	3.321628	0.009300
C	-0.93727	4.650715	-0.719306
N	2.614683	0.880032	-0.607384
O	-1.589012	5.702391	-0.757586
C	0.548508	4.669744	-1.013149
C	3.014495	-0.303489	-1.018700
C	3.578672	1.739369	0.094574
H	1.105842	4.548938	-0.076444

H	0.842557	3.844697	-1.668338
H	0.817541	5.628209	-1.463351
C	2.013893	-1.193904	-1.714847
N	4.280853	-0.760387	-0.893497
H	3.555054	1.506361	1.167470
H	3.253438	2.776819	-0.017622
C	4.988413	1.550579	-0.449269
C	2.364461	-1.501378	-3.185025
H	1.907166	-2.128458	-1.152697
H	1.047473	-0.687362	-1.666188
C	4.650243	-2.145451	-1.213296
C	5.357496	0.079802	-0.355351
H	5.024788	1.878938	-1.494535
H	5.707985	2.149019	0.116703
C	3.358813	-2.652490	-3.369435
H	2.742867	-0.589488	-3.664960
H	1.433543	-1.760971	-3.701255
C	4.726654	-2.435509	-2.715938
H	5.627150	-2.310056	-0.754216
H	3.954205	-2.834335	-0.723173
H	5.550609	-0.204586	0.687398
H	6.264885	-0.130950	-0.929694
H	2.912440	-3.564100	-2.948443
H	3.496683	-2.839922	-4.441115
H	5.261830	-1.611133	-3.204471
H	5.334523	-3.337148	-2.858169
I	-3.436873	-1.114883	-1.876707
Br	-3.010497	-2.381404	1.780211

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-7408.709572	0.370307	-1676.205347	-1676.339494	-0.134147

Cartesian coordinates of **15-TS**

C	2.199671	0.777739	-0.123545
C	3.576030	0.929981	-0.387614
C	4.130773	2.177675	-0.203565
C	3.348566	3.265138	0.271993
C	1.964840	3.055270	0.575704
C	1.403777	1.763423	0.389719
H	4.170383	0.099281	-0.748360

H	5.182025	2.341517	-0.424079
H	0.365062	1.596065	0.652748
Cu	1.296890	-0.694597	-1.066964
C	3.874566	4.563682	0.476648
H	4.920801	4.756617	0.256250
C	3.047896	5.556722	0.950313
H	3.411473	6.564975	1.117564
C	1.694717	5.245301	1.223194
H	1.033851	6.023795	1.600556
N	1.156632	4.049937	1.050090
N	1.765374	-1.083308	0.741288
C	0.856945	-1.197264	1.746491
N	2.908886	-1.811186	0.960806
C	1.518083	-2.090521	2.609989
Cu	-0.822513	-0.345410	1.679574
N	2.753547	-2.428627	2.092491
C	1.066730	-2.646559	3.884731
N	-2.521195	0.530399	1.541748
O	1.769366	-3.429484	4.533040
C	-0.299097	-2.236142	4.391066
C	-2.980836	1.035207	0.414990
C	-3.327981	0.698973	2.758130
H	-0.355061	-1.149061	4.510055
H	-1.075350	-2.521254	3.673114
H	-0.490654	-2.721305	5.350609
C	-2.154261	0.856273	-0.835844
N	-4.166365	1.674729	0.306316
H	-3.092401	1.667507	3.221492
H	-3.039077	-0.078834	3.468827
C	-4.814972	0.623172	2.437801
C	-2.823401	-0.026483	-1.906577
H	-1.897065	1.833735	-1.260598
H	-1.213488	0.392975	-0.530801
C	-4.606781	2.309180	-0.944459
C	-5.149064	1.683500	1.401828
H	-5.050135	-0.372396	2.043829
H	-5.418379	0.781668	3.335928
C	-3.846894	0.699132	-2.785146
H	-3.285478	-0.893929	-1.417827
H	-2.025948	-0.415688	-2.547081
C	-5.029155	1.313880	-2.030325
H	-5.448631	2.950672	-0.675603
H	-3.817527	2.969551	-1.318172
H	-5.169949	2.681571	1.857535

H	-6.135641	1.499495	0.965170
H	-3.328995	1.500818	-3.330311
H	-4.224882	0.002268	-3.542911
H	-5.643696	0.530027	-1.568985
H	-5.672133	1.841790	-2.744783
I	0.068861	-3.111228	-1.628942
Br	1.158867	0.398344	-3.210930

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-7408.704857	0.370165	-1676.209906	-1676.346256	-0.136350

Cartesian coordinates of **16**

C	-2.269762	-1.985181	-0.666281
C	-3.054035	-2.669595	0.296480
C	-4.266860	-2.148199	0.678779
C	-4.736496	-0.922090	0.137498
C	-3.942453	-0.245422	-0.840846
C	-2.711661	-0.815315	-1.245905
H	-2.671474	-3.582894	0.732746
H	-4.872789	-2.660175	1.420683
H	-2.125944	-0.311737	-2.006327
Cu	1.048402	-1.138443	0.666987
C	-5.960589	-0.320780	0.521496
H	-6.585873	-0.809477	1.263559
C	-6.330243	0.873418	-0.051873
H	-7.257676	1.368280	0.216286
C	-5.473898	1.463032	-1.013150
H	-5.758279	2.408520	-1.471916
N	-4.325841	0.939924	-1.406390
N	-1.002614	-2.513036	-1.019639
C	0.161354	-1.821127	-1.262826
N	-0.835592	-3.869318	-1.089607
C	1.052227	-2.881692	-1.525468
Cu	0.300092	0.076639	-1.419957
N	0.405939	-4.089105	-1.388138
C	2.476740	-2.830628	-1.885843
N	0.490099	1.985418	-1.540013
O	3.195494	-3.827413	-1.773465
C	3.015917	-1.544588	-2.463296
C	-0.118808	2.811496	-0.714935

C	1.541223	2.523626	-2.414290
H	2.642866	-1.437272	-3.489655
H	2.672061	-0.674983	-1.898637
H	4.107223	-1.576696	-2.480522
C	-1.178856	2.250200	0.200677
N	0.177464	4.125606	-0.611819
H	1.085234	2.920831	-3.332162
H	2.194978	1.698853	-2.707282
C	2.327448	3.618333	-1.705017
C	-0.781147	2.283078	1.690031
H	-2.125335	2.782543	0.051062
H	-1.345578	1.216619	-0.105135
C	-0.564978	5.029250	0.278856
C	1.364915	4.706569	-1.259633
H	2.834774	3.186856	-0.834913
H	3.087754	4.045755	-2.364760
C	-1.021770	3.629706	2.379306
H	0.270526	1.985973	1.784620
H	-1.365463	1.513407	2.206462
C	-0.266090	4.813643	1.766943
H	-0.283858	6.042021	-0.017506
H	-1.638457	4.933975	0.086501
H	1.044886	5.319174	-2.111986
H	1.845160	5.372468	-0.536198
H	-2.098037	3.849771	2.346014
H	-0.754949	3.541940	3.439350
H	0.816930	4.686916	1.892470
H	-0.543030	5.727752	2.305677
I	3.280079	0.316939	1.071050
Br	-0.046554	-2.225641	2.538709

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-7408.787698	0.373084	-1676.334239	-1676.466868	-0.132630

Cartesian coordinates of **16-TS**

C	1.867208	0.969965	-0.426320
C	2.348055	0.611755	-1.707706
C	3.603636	0.061207	-1.789729
C	4.410901	-0.106034	-0.629284
C	3.918698	0.326962	0.642779

C	2.628943	0.922590	0.718305
H	1.723606	0.722152	-2.586244
H	3.990236	-0.267558	-2.750386
H	2.274532	1.286034	1.676594
Br	0.411723	2.841197	-0.501856
Cu	0.021944	0.467514	0.064761
I	0.253077	-2.236451	-0.326486
N	-1.746676	0.429519	0.954081
C	-2.898988	0.484180	0.331287
C	-1.729541	0.228217	2.406350
C	-2.887273	0.622684	-1.172143
N	-4.096570	0.376711	0.951298
H	-1.767787	1.203011	2.912562
H	-0.776247	-0.237663	2.671312
C	-2.899935	-0.640963	2.848257
C	-3.458635	-0.607270	-1.907591
H	-3.431642	1.526031	-1.471964
H	-1.847824	0.770387	-1.472459
C	-5.371647	0.533673	0.238197
C	-4.195523	-0.007329	2.368024
H	-2.790058	-1.640801	2.412912
H	-2.921406	-0.746233	3.936497
C	-4.987251	-0.633999	-2.009161
H	-3.091583	-1.518022	-1.419021
H	-3.042774	-0.609120	-2.921270
C	-5.725162	-0.650813	-0.667190
H	-6.134776	0.657226	1.009486
H	-5.358205	1.464167	-0.338898
H	-4.441582	0.878798	2.967169
H	-5.026804	-0.712212	2.464720
H	-5.313362	0.250123	-2.574466
H	-5.289538	-1.508361	-2.597818
H	-5.519112	-1.582093	-0.124128
H	-6.805099	-0.625528	-0.855963
C	5.704682	-0.677269	-0.670990
H	6.109266	-1.014699	-1.620873
C	6.423358	-0.796903	0.496962
H	7.416464	-1.232915	0.508458
C	5.845063	-0.338421	1.703837
H	6.405525	-0.429263	2.632542
N	4.643086	0.205950	1.792988

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-5374.718855	0.310520	-1085.192298	-1085.240122	-0.047824

Cartesian coordinates of **17**

C	-1.893885	0.083494	0.286493
C	-2.207532	-0.329790	1.600930
C	-3.529149	-0.512052	1.949162
C	-4.565256	-0.294413	1.003775
C	-4.226298	0.119766	-0.324329
C	-2.855907	0.299474	-0.664780
H	-1.421580	-0.503170	2.328736
H	-3.790966	-0.829592	2.955226
H	-2.616104	0.609760	-1.676560
Br	-0.398408	2.703177	0.485464
Cu	-0.036252	0.389506	-0.125256
I	0.032443	-2.108388	-0.811159
N	1.836574	0.717703	-0.588181
C	2.857230	0.511047	0.205858
C	2.052021	1.265525	-1.928081
C	2.594993	-0.077283	1.569882
N	4.137884	0.761116	-0.146141
H	2.023795	2.361910	-1.880854
H	1.221186	0.945893	-2.564022
C	3.383277	0.786210	-2.492616
C	3.176687	-1.496142	1.745726
H	2.991585	0.589904	2.344118
H	1.512817	-0.106606	1.711146
C	5.259641	0.584407	0.787234
C	4.495209	1.146723	-1.520329
H	3.346767	-0.300095	-2.631687
H	3.580726	1.246438	-3.464674
C	4.665302	-1.530837	2.106819
H	2.993294	-2.072562	0.831690
H	2.611707	-1.990445	2.543663
C	5.596418	-0.881859	1.078087
H	6.115326	1.081671	0.326438
H	5.051853	1.120887	1.718938
H	4.703874	2.223749	-1.549703
H	5.418993	0.623360	-1.783146
H	4.802718	-1.021482	3.070622
H	4.968916	-2.573356	2.259803

H	5.578768	-1.440115	0.133252
H	6.625456	-0.926854	1.454119
C	-5.937767	-0.471333	1.307081
H	-6.226710	-0.787326	2.305850
C	-6.878034	-0.239025	0.330236
H	-7.938589	-0.362667	0.522470
C	-6.439633	0.170650	-0.951495
H	-7.175909	0.358273	-1.731648
N	-5.172419	0.347285	-1.284121

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-5374.733313	0.311388	-1085.194752	-1085.239054	-0.044302

Cartesian coordinates of **17-TS**

C	1.863368	-0.658215	-0.191423
C	2.539398	-0.866876	-1.421245
C	3.854813	-0.490509	-1.519213
C	4.543014	0.076499	-0.408405
C	3.855168	0.241632	0.834933
C	2.500376	-0.179845	0.935387
H	2.011057	-1.283123	-2.270173
H	4.387756	-0.611937	-2.458462
H	2.002959	-0.111077	1.896305
Cu	0.046105	0.128691	-0.159758
N	-1.653941	0.790126	0.640039
C	-2.843298	0.666299	0.105193
C	-1.490625	1.679535	1.793381
C	-2.997516	-0.252587	-1.08201
N	-3.953505	1.283249	0.576993
H	-1.299626	2.70276	1.440789
H	-0.605131	1.35952	2.349575
C	-2.727688	1.650401	2.682428
C	-3.869976	-1.491406	-0.792987
H	-3.405262	0.303591	-1.934409
H	-1.995699	-0.575065	-1.368992
C	-5.256848	1.18341	-0.09326
C	-3.944705	2.020299	1.849991
H	-2.851675	0.643137	3.09683
H	-2.626204	2.348124	3.518486
C	-5.378694	-1.245504	-0.900671

H	-3.618059	-1.88288	0.200675
H	-3.591837	-2.269208	-1.513078
C	-5.930998	-0.184622	0.056216
H	-5.883602	1.959415	0.351095
H	-5.147992	1.440213	-1.152283
H	-3.961452	3.09823	1.643585
H	-4.866293	1.773539	2.386417
H	-5.606974	-0.93705	-1.930402
H	-5.907897	-2.191577	-0.735096
H	-5.830797	-0.513791	1.098561
H	-7.003479	-0.058924	-0.135181
C	6.492406	1.001578	0.660984
H	7.529176	1.32055	0.658099
C	5.724606	1.123184	1.842142
H	6.184411	1.537265	2.737841
Br	0.4342	1.96252	-1.846282
N	4.456012	0.762313	1.944807
C	5.898892	0.475385	-0.464866
H	6.451077	0.361182	-1.393466
I	0.191913	-2.437262	0.326676

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-5374.725450	0.309191	-1085.200061	-1085.245896	-0.045835

Cartesian coordinates of **18**

C	-0.05423	1.583232	0.000232
C	1.294929	1.856844	0.000403
C	2.25081	0.80891	0.000336
C	1.798383	-0.547069	0.000087
C	0.402967	-0.815087	-0.000088
C	-0.48345	0.234544	-0.000012
H	4.024792	2.056613	0.000706
H	-0.77986	2.38827	0.000285
H	1.641079	2.886536	0.000595
C	3.649963	1.036979	0.000507
H	0.077741	-1.848812	-0.000279
C	3.95374	-1.346079	0.00016
C	4.503339	-0.040658	0.000422
H	4.622733	-2.205234	0.000107
H	5.5804	0.088857	0.000551

N	2.659131	-1.609176	0.000004
I	-2.597727	-0.164749	-0.000269

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-698.6826904	0.087137	-412.5175102	-412.5301178	-0.012608

Cartesian coordinates of **18-TS**

C	1.881051	0.713082	-0.256828
C	2.383035	0.534857	-1.569553
C	3.636253	-0.006253	-1.721407
C	4.425957	-0.356974	-0.589973
C	3.915927	-0.12225	0.726093
C	2.628844	0.467527	0.871763
H	1.773195	0.78627	-2.429075
H	4.036122	-0.185787	-2.715731
H	2.262717	0.682514	1.870019
Cu	0.019306	0.328775	0.164327
I	0.057099	-2.329268	-0.798313
N	-1.73119	0.079225	1.075593
C	-2.916457	0.272376	0.548286
C	-1.638391	-0.59449	2.375899
C	-2.995186	0.911076	-0.81598
N	-4.072835	-0.109533	1.138574
H	-1.717613	0.148999	3.181349
H	-0.647674	-1.05056	2.450618
C	-2.731802	-1.645353	2.52049
C	-3.54269	-0.035347	-1.904641
H	-3.606506	1.820261	-0.769576
H	-1.985724	1.226854	-1.077386
C	-5.389372	0.199632	0.563628
C	-4.08345	-0.978511	2.325836
H	-2.58442	-2.421871	1.76145
H	-2.692443	-2.120666	3.504553
C	-5.071371	-0.123527	-1.958149
H	-3.106659	-1.032136	-1.764346
H	-3.181168	0.328784	-2.872892
C	-5.735113	-0.633439	-0.675344
H	-6.116217	0.012016	1.356796
H	-5.448369	1.26835	0.333489
H	-4.355158	-0.38329	3.206963

H	-4.866084	-1.72972	2.18132
H	-5.468895	0.876474	-2.181123
H	-5.363228	-0.767885	-2.796062
H	-5.457086	-1.678076	-0.485182
H	-6.823596	-0.613779	-0.807253
C	5.71678	-0.926283	-0.700456
H	6.135107	-1.114323	-1.68522
C	6.415472	-1.233636	0.445132
H	7.405523	-1.674893	0.403378
C	5.820338	-0.964147	1.699759
H	6.364613	-1.204705	2.61139
N	4.621016	-0.428407	1.854155
I	0.449426	2.888393	-0.104112

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-3098.495812	0.310471	-1083.233475	-1083.286136	-0.052660

Cartesian coordinates of **19**

C	-1.889336	-0.056573	0.250636
C	-2.247393	-0.132572	1.616982
C	-3.577009	-0.246983	1.959596
C	-4.582612	-0.293084	0.957975
C	-4.201922	-0.224746	-0.420471
C	-2.821742	-0.104037	-0.752542
H	-1.484937	-0.093172	2.387829
H	-3.871519	-0.300568	3.004572
H	-2.551508	-0.049809	-1.802393
Cu	-0.022039	0.145236	-0.201481
I	0.114578	-2.445662	-0.226171
N	1.830528	0.351832	-0.815638
C	2.887906	0.404522	-0.044762
C	1.987824	0.331642	-2.270589
C	2.682061	0.398069	1.449792
N	4.151963	0.430557	-0.521515
H	2.021908	1.361814	-2.650798
H	1.10255	-0.145699	-2.699755
C	3.254451	-0.42321	-2.654857
C	3.256631	-0.854352	2.143856
H	3.120225	1.303312	1.886636
H	1.607183	0.456812	1.628741

C	5.320735	0.601505	0.352713
C	4.442003	0.209443	-1.946865
H	3.152882	-1.471588	-2.352882
H	3.413377	-0.39562	-3.736316
C	4.760437	-0.788777	2.430426
H	3.021025	-1.738231	1.53909
H	2.726666	-0.977547	3.09481
C	5.650561	-0.6361	1.193464
H	6.157088	0.841158	-0.307248
H	5.172521	1.473506	0.997956
H	4.706994	1.167009	-2.412602
H	5.31818	-0.44281	-2.010321
H	4.94995	0.060177	3.10187
H	5.057481	-1.690831	2.978514
H	5.580995	-1.525171	0.553625
H	6.6955	-0.558569	1.516741
C	-5.963178	-0.402739	1.254565
H	-6.283434	-0.454364	2.2917
C	-6.872033	-0.441527	0.222382
H	-7.937768	-0.52428	0.407738
C	-6.393338	-0.371088	-1.107126
H	-7.103944	-0.401955	-1.93179
N	-5.116424	-0.266227	-1.434818
I	-0.38173	2.718588	0.074284

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-3098.506918	0.310759	-1083.234399	-1083.282399	-0.048000

Cartesian coordinates of **19-TS**

Cu	-0.022787	0.087615	0.060232
N	-1.918586	0.509056	0.403439
C	-2.908403	0.155496	-0.377698
C	-2.191456	1.243034	1.641572
C	-2.600323	-0.642294	-1.621906
N	-4.205737	0.433066	-0.109095
H	-2.176228	2.321221	1.434547
H	-1.375749	1.037654	2.337342
C	-3.534502	0.828263	2.226715
C	-3.164553	-2.078495	-1.581832
H	-2.981497	-0.114506	-2.503915

H	-1.516099	-0.681528	-1.732646
C	-5.293057	0.097674	-1.038783
C	-4.617674	1.015223	1.177537
H	-3.487443	-0.223892	2.53031
H	-3.771389	1.424408	3.112475
C	-4.638957	-2.192638	-1.982967
H	-3.00799	-2.496577	-0.58028
H	-2.568368	-2.688216	-2.26982
C	-5.611586	-1.399737	-1.104756
H	-6.16709	0.651694	-0.690543
H	-5.05831	0.48269	-2.036608
H	-4.842743	2.080226	1.036946
H	-5.543038	0.519567	1.486015
H	-4.744894	-1.845113	-3.020033
H	-4.928763	-3.250224	-1.978193
H	-5.625588	-1.800645	-0.083094
H	-6.625866	-1.515569	-1.505231
I	-0.145311	-2.143378	1.397017
N	0.432864	3.806103	2.163998
N	0.725941	2.699913	2.460543
N	1.014547	1.589318	2.772719
C	1.815182	-0.368747	-0.344758
C	2.032118	-1.159613	-1.497912
C	2.843266	0.074233	0.444742
C	3.32101	-1.500306	-1.847686
H	1.195461	-1.494857	-2.102311
C	4.182171	-0.267041	0.099769
H	2.659286	0.682438	1.326547
C	4.422958	-1.065601	-1.064628
H	3.507698	-2.106602	-2.730513
N	5.196696	0.186231	0.896269
C	5.766957	-1.382819	-1.379743
C	6.434115	-0.136255	0.560422
H	5.981113	-1.986551	-2.257663
C	6.776108	-0.91875	-0.567811
H	7.225166	0.236592	1.209576
H	7.818072	-1.13892	-0.77503
I	0.329741	2.199799	-1.444402

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-3262.718966	0.315554	-1247.406946	-1247.537549	-0.130604

Cartesian coordinates of **20**

C	-1.851452	0.079628	0.245197
C	-2.170504	-0.277315	1.575561
C	-3.494854	-0.417743	1.932646
C	-4.52811	-0.216821	0.98059
C	-4.185072	0.134003	-0.364432
C	-2.812472	0.275308	-0.713317
H	-1.38561	-0.43724	2.307758
H	-3.7619	-0.688794	2.950835
H	-2.567951	0.545649	-1.735687
Cu	-0.018548	0.502851	-0.126598
N	1.861702	0.937063	-0.556634
C	2.892884	0.77636	0.233442
C	2.062749	1.422663	-1.922667
C	2.654567	0.25266	1.628346
N	4.168025	1.021736	-0.145606
H	2.042125	2.521046	-1.928334
H	1.222516	1.078981	-2.532692
C	3.385677	0.9126	-2.481273
C	3.267827	-1.142267	1.873405
H	3.047251	0.966417	2.36231
H	1.574677	0.212395	1.781539
C	5.300453	0.922927	0.785677
C	4.510604	1.322861	-1.544325
H	3.344672	-0.179591	-2.560468
H	3.570989	1.318609	-3.479544
C	4.758639	-1.126237	2.227004
H	3.092249	-1.769556	0.991747
H	2.718	-1.606341	2.699704
C	5.671006	-0.516597	1.158168
H	6.141655	1.410311	0.288727
H	5.088913	1.508172	1.686691
H	4.724413	2.395067	-1.639996
H	5.429023	0.779946	-1.786851
H	4.889646	-0.560978	3.160143
H	5.085082	-2.151944	2.43636
H	5.661475	-1.128185	0.246783
H	6.702523	-0.517632	1.530233
C	-5.903378	-0.344638	1.296367
H	-6.195442	-0.610076	2.308794
C	-6.841726	-0.128158	0.314289
H	-7.904267	-0.21428	0.515709
C	-6.39882	0.214753	-0.985437
H	-7.133741	0.388575	-1.770031

N	-5.129046	0.343589	-1.329959
N	-0.37807	2.375675	0.273781
N	-1.46355	2.754584	0.661164
N	-2.473861	3.173265	1.031065
I	0.210322	-1.980161	-0.776123

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2965.085250	0.322092	-1235.952505	-1235.998489	-0.045984

Cartesian coordinates of **20-TS**

C	-1.905907	0.578981	0.769902
C	-2.198697	-0.215951	1.90104
C	-3.461977	-0.750427	2.007203
C	-4.458824	-0.468683	1.032796
C	-4.145112	0.392017	-0.069638
C	-2.83765	0.939106	-0.171099
H	-1.43691	-0.41532	2.646885
H	-3.713685	-1.391472	2.847635
H	-2.60545	1.587042	-1.010359
Cu	0.002586	0.505783	0.228978
N	1.913883	0.999214	-0.133136
C	2.974252	0.499011	0.450294
C	2.089447	1.994453	-1.194844
C	2.769215	-0.540252	1.525979
N	4.244141	0.834301	0.121643
H	2.145163	2.999526	-0.753478
H	1.200678	1.97104	-1.832569
C	3.348265	1.704715	-2.0037
C	3.330575	-1.930258	1.161321
H	3.214123	-0.193633	2.466715
H	1.693312	-0.616479	1.695137
C	5.409778	0.342326	0.868035
C	4.540693	1.656578	-1.061361
H	3.235157	0.740508	-2.512325
H	3.511447	2.471569	-2.766082
C	4.833398	-2.094655	1.411027
H	3.091839	-2.148939	0.113557
H	2.794291	-2.672534	1.762993
C	5.728614	-1.135871	0.620472
H	6.251669	0.963681	0.55537

H	5.266309	0.527043	1.938012
H	4.820995	2.667371	-0.737845
H	5.409231	1.21857	-1.562917
H	5.026404	-1.947237	2.482823
H	5.121511	-3.127751	1.182578
H	5.653482	-1.33586	-0.456126
H	6.773402	-1.311183	0.903887
C	-6.679757	-0.667553	0.121363
H	-7.694145	-1.051409	0.137275
C	-6.269087	0.187867	-0.927969
H	-6.979425	0.450787	-1.710175
N	-0.623077	2.031822	1.29891
N	-0.93842	3.022412	0.654469
N	-1.267928	3.982812	0.114635
N	-5.057632	0.706455	-1.036647
C	-5.77142	-0.993291	1.102848
H	-6.041496	-1.646108	1.928238
I	-0.160085	-1.706315	-1.252089

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-2965.066565	0.321552	-1235.947908	-1235.996615	-0.048707

Cartesian coordinates of **21-TS**

Cu	0.013769	-0.097187	0.413817
N	1.907331	0.246281	0.846877
C	2.895383	-0.484732	0.397162
C	2.204974	1.383963	1.718756
C	2.579523	-1.657388	-0.499197
N	4.195892	-0.223354	0.670708
H	2.301680	1.028014	2.754588
H	1.351574	2.063502	1.690783
C	3.493934	2.062785	1.272484
C	3.159291	-1.530645	-1.923177
H	2.932564	-2.583738	-0.030442
H	1.492566	-1.738078	-0.557087
C	5.282113	-1.133070	0.283826
C	4.619674	1.041702	1.292326
H	3.359556	2.457607	0.258983
H	3.744476	2.899946	1.930178
C	4.629018	-1.942947	-2.054045

H	3.020753	-0.502298	-2.276674
H	2.558514	-2.168683	-2.580958
C	5.606048	-1.116463	-1.213305
H	6.155412	-0.819337	0.859971
H	5.042791	-2.150655	0.610147
H	4.944914	0.843522	2.321491
H	5.488417	1.411141	0.737539
H	4.723404	-2.998020	-1.761459
H	4.922123	-1.885225	-3.109153
H	5.626661	-0.074420	-1.557512
H	6.618464	-1.515749	-1.348309
I	0.116367	1.244174	-1.800483
N	-1.124582	4.294322	0.297657
N	-1.050577	3.402379	1.069181
N	-0.977772	2.509720	1.852761
C	-1.808538	-0.520606	-0.075785
C	-2.015678	-1.645804	-0.907585
C	-2.841688	0.224890	0.424625
C	-3.304006	-2.022877	-1.218019
H	-1.173465	-2.210375	-1.293884
C	-4.180833	-0.150235	0.115691
H	-2.660908	1.088600	1.057950
C	-4.413777	-1.292092	-0.716767
H	-3.484240	-2.887500	-1.851870
N	-5.202440	0.597951	0.630600
C	-5.757650	-1.637370	-1.000521
C	-6.439810	0.235585	0.337254
H	-5.966044	-2.499550	-1.628503
C	-6.774381	-0.874521	-0.473508
H	-7.236554	0.846664	0.759103
H	-7.816572	-1.106617	-0.666175
Br	-0.238553	-1.715821	2.199155

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-5538.946291	0.318587	-1249.369253	-1249.492435	-0.123182

Cartesian coordinates of **22**

C	1.801769	-0.020331	-0.222030
C	2.129645	-0.828458	-1.333146
C	3.441467	-1.213909	-1.511386

C	4.449389	-0.801227	-0.601384
C	4.094741	0.023395	0.513845
C	2.734288	0.406117	0.686002
H	1.364541	-1.146457	-2.034102
H	3.718077	-1.838232	-2.357051
H	2.479633	1.029599	1.537180
Br	0.304968	2.348690	-1.190030
Cu	-0.052823	0.345482	0.077287
N	-1.959623	0.753928	0.387032
C	-2.964973	0.120640	-0.163569
C	-2.213692	1.758310	1.421789
C	-2.676502	-0.924620	-1.213612
N	-4.257443	0.330334	0.177928
H	-2.358728	2.739128	0.950717
H	-1.322662	1.833013	2.052497
C	-3.433396	1.378023	2.251499
C	-3.008545	-2.359190	-0.750870
H	-3.234515	-0.689899	-2.127580
H	-1.619694	-0.857195	-1.476238
C	-5.369788	-0.367342	-0.482926
C	-4.621433	1.177621	1.324578
H	-3.225771	0.450517	2.797116
H	-3.664074	2.157118	2.983325
C	-4.485535	-2.740479	-0.897166
H	-2.680471	-2.483125	0.287590
H	-2.408229	-3.051365	-1.351778
C	-5.466050	-1.854198	-0.121965
H	-6.277843	0.152840	-0.172035
H	-5.295065	-0.240637	-1.567932
H	-4.994283	2.141823	0.956138
H	-5.442696	0.686686	1.854649
H	-4.750560	-2.701113	-1.962809
H	-4.617202	-3.782650	-0.582411
H	-5.313357	-1.962248	0.959637
H	-6.488252	-2.190378	-0.332902
C	5.811191	-1.167886	-0.740371
H	6.112248	-1.794305	-1.575631
C	6.725388	-0.721896	0.185271
H	7.776862	-0.979306	0.113957
C	6.272558	0.091877	1.251028
H	6.988668	0.451532	1.988376
N	5.014692	0.459221	1.425018
N	-0.192066	-1.291538	1.095052
N	0.755822	-2.029559	1.274413

N 1.608369 -2.777696 1.482772

E_{elec} (a.u.)	G_{corr} (a.u.)	E_g (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-5241.311410	0.324601	-1237.913559	-1237.954556	-0.040997

Cartesian coordinates of **22-TS**

C	-1.830705	0.563388	0.314447
C	-2.171411	1.455719	-0.727428
C	-3.498041	1.575961	-1.071707
C	-4.503199	0.852727	-0.373989
C	-4.129222	-0.003551	0.713075
C	-2.759719	-0.111078	1.069996
H	-1.405456	2.001157	-1.269444
H	-3.790198	2.226287	-1.891723
H	-2.479336	-0.736020	1.910968
Cu	-0.048205	-0.286985	0.179003
N	1.865110	-0.813714	0.491984
C	2.903709	-0.268274	-0.088616
C	2.069687	-1.972907	1.362854
C	2.673934	0.929149	-0.979191
N	4.178780	-0.690557	0.090224
H	2.048569	-2.891096	0.759911
H	1.229167	-2.027668	2.061414
C	3.392368	-1.862873	2.111289
C	3.298040	2.232436	-0.438328
H	3.054364	0.722315	-1.986676
H	1.593419	1.056317	-1.076899
C	5.313962	-0.108358	-0.637817
C	4.519386	-1.701612	1.103373
H	3.360187	-0.992503	2.776997
H	3.571457	-2.749798	2.725629
C	4.790478	2.397084	-0.743962
H	3.120833	2.292457	0.642898
H	2.756385	3.071751	-0.887019
C	5.694674	1.301101	-0.172404
H	6.151702	-0.791786	-0.484513
H	5.103761	-0.110377	-1.712739
H	4.733638	-2.655319	0.604044
H	5.437627	-1.378330	1.603535

H	4.920332	2.420436	-1.834935
H	5.124832	3.372347	-0.370351
H	5.684519	1.323686	0.925003
H	6.727782	1.495941	-0.484304
C	-6.790706	0.221682	0.038568
H	-7.853093	0.263981	-0.176430
C	-6.319589	-0.594094	1.094515
H	-7.033412	-1.170721	1.680799
N	-0.334987	1.168658	1.467148
N	-0.020485	2.288739	1.086974
N	0.244671	3.370176	0.799920
Br	-0.608982	-1.868154	-1.601993
N	-5.047712	-0.714921	1.433910
C	-5.878556	0.946578	-0.693970
H	-6.192972	1.587754	-1.512851

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-5241.296050	0.323588	-1237.911657	-1237.955211	-0.043554

Cartesian coordinates of **Product**

C	0.314402	-0.5503	-0.00138
C	0.963991	-1.7754	-0.294184
C	2.335354	-1.807277	-0.369629
C	3.103427	-0.630996	-0.168323
C	2.433589	0.598494	0.122038
C	1.019803	0.613211	0.211089
H	0.371425	-2.666352	-0.461519
H	2.847714	-2.737628	-0.595577
H	0.524592	1.545219	0.459176
C	4.518759	-0.609344	-0.241989
H	5.056105	-1.527288	-0.462865
C	5.181021	0.576493	-0.031134
H	6.26307	0.637829	-0.0778
C	4.424446	1.739847	0.253442
H	4.942082	2.682671	0.422646
N	3.106289	1.770395	0.331499
N	-1.106918	-0.538398	0.069865
C	-1.965957	0.470665	-0.194496
N	-1.791704	-1.656975	0.463209
C	-3.218272	-0.064592	0.050524

N	-3.054583	-1.368142	0.448627
C	-4.54848	0.561281	-0.071414
O	-5.564773	-0.077282	0.186133
C	-4.587711	1.998784	-0.519698
H	-4.029889	2.628837	0.182306
H	-4.110314	2.103151	-1.500427
H	-5.622687	2.339332	-0.57611
H	-1.641723	1.439134	-0.540365

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-795.275805	0.166018	-795.270340	-795.299103	-0.028763

Cartesian coordinates of (DBU)CuBr

Cu	1.577112	0.240876	-0.060592
N	-0.215554	0.885875	-0.130748
C	-1.277229	0.141576	-0.365619
C	-0.405972	2.333182	0.053561
C	-1.087147	-1.344616	-0.546194
N	-2.536229	0.628105	-0.415644
H	-0.405145	2.827974	-0.927527
H	0.447618	2.720573	0.61376
C	-1.71302	2.618084	0.780594
C	-1.729229	-2.186287	0.576648
H	-1.482374	-1.656171	-1.520502
H	-0.010227	-1.52792	-0.570287
C	-3.692782	-0.210873	-0.764592
C	-2.857241	2.006146	-0.008931
H	-1.673058	2.179677	1.784418
H	-1.873031	3.694355	0.888752
C	-3.228598	-2.446589	0.397348
H	-1.539717	-1.69914	1.541938
H	-1.209985	-3.150456	0.606899
C	-4.101955	-1.189727	0.340609
H	-4.511032	0.480605	-0.975393
H	-3.489959	-0.747536	-1.696911
H	-3.07755	2.601415	-0.903885
H	-3.76817	1.969784	0.596292
H	-3.372648	-3.012317	-0.533564
H	-3.578396	-3.092712	1.211281
H	-4.083262	-0.661099	1.302314

H	-5.141971	-1.488168	0.162883
Br	3.795834	-0.4385	0.034883

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-4676.050010	0.202939	-672.711129	-672.7472571	-0.036128

Cartesian coordinates of **DBUH⁺**

N	-1.463167	1.339337	-0.138634
C	-0.327982	0.691035	-0.373529
C	-2.747143	0.68312	0.112677
C	0.918063	1.50952	-0.557274
N	-0.287537	-0.633708	-0.409612
H	-3.293073	0.576077	-0.831253
H	-3.328062	1.32907	0.773155
C	-2.477445	-0.6747	0.744989
C	1.95931	1.282734	0.559749
H	1.356514	1.276941	-1.534126
H	0.622107	2.560577	-0.584745
C	0.952963	-1.366293	-0.735019
C	-1.479747	-1.451048	-0.102472
H	-2.075764	-0.535399	1.753913
H	-3.405765	-1.244926	0.823187
C	2.801224	0.014669	0.387727
H	1.448923	1.276865	1.530477
H	2.626708	2.150526	0.561341
C	2.008819	-1.296299	0.370851
H	0.649682	-2.399739	-0.905836
H	1.352889	-0.990324	-1.681704
H	-1.929314	-1.777708	-1.046779
H	-1.13349	-2.338141	0.432018
H	3.363067	0.094696	-0.55264
H	3.543973	-0.027074	1.192602
H	1.519328	-1.46782	1.337622
H	2.705449	-2.127923	0.215904
H	-1.416614	2.348475	-0.091609

E_{elec} (a.u.)	G_{corr} (a.u.)	E_{g} (a.u.)	E_{sol} (a.u.)	ΔG^*_{solv} (a.u.)
-462.262745	0.223324	-462.289738	-462.3785298	-0.088792

Section 6

References

- [1] Rohrbach, S.; Murphy, J. A.; Tuttle, T. Computational Study on the Boundary Between the Concerted and Stepwise Mechanism of Bimolecular S_NAr Reactions. *J. Am. Chem. Soc.* **2020**, *142*, 14871-14876.