Supplementary Material for PCCP

A Theoretical Study of the Copper(I)-Catalyzed 1,3-Dipolar Cycloaddition Reaction in Dabco-Based Ionic Liquids: the Anion Effect on Regioselectivity

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SUPPLEMENTAR INFORMATION

complex	ΔE Kcal/mol
Cu+C_4DABCO+Br	-114.39
Cu+C_4DABCO+2Br	-166.85
4Cu+4Br (cubic)	-722.39
4Cu+4Br(square)	-867.97
4Cu+6Br(chair)	-930.08
Cu+C_4DABCO+N(CN)2 (C)	33.32
Cu+C_4DABCO+N(CN)2 (T)	23.72
Cu+C_4DABCO+2N(CN)2 (T)	-65.26
Cu+C_4DABCO+2N(CN)2 (T+C)	-61.87

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
Cu+Br					
1	6	0	0.000000	0.000000	-3.253349
2	6	0	0.000000	0.000000	-2.007807
3	6	0	0.000000	0.000000	-4.730332
4	1	0	0.000000	1.024123	-5.136179
5	1	0	0.886917	-0.512062	-5.136179
6	1	0	-0.886917	-0.512062	-5.136179
7	29	0	0.000000	0.000000	-0.127018
8	35	0	0.000000	0.000000	2.258314
Cu+2N(CN)2C					
1	6	0	3.537162	-0.000209	-0.001353
2	6	0	2.287458	-0.000163	-0.001403
3	6	0	5.014827	-0.000232	-0.000150
4	1	0	5.421448	-0.016304	1.025540
5	1	0	5.426619	-0.879710	-0.524588
6	1	0	5.426755	0.895145	-0.496857
7	29	0	0.368178	-0.000051	-0.000808
8	7	0	-1.011441	-1.664283	-0.000159
9	6	0	-1.356269	-2.221723	-1.162250
10	6	0	-1.354200	-2.222312	1.162270
11	7	0	-1.620363	-2.659190	-2.245065
12	7	0	-1.616388	-2.660325	2.245324
13	7	0	-1.011186	1.664403	0.000550
14	6	0	-1.355187	2.223010	-1.161227
15	6	0	-1.354596	2.221375	1.163293
16	7	0	-1.618530	2.661557	-2.243788
17	7	0	-1.617400	2.658393	2.246600
Cu+2N(CN)2T					
1	6	0	0.214171	3.837493	0.008669
2	6	0	0.146568	2.589494	-0.027069
3	6	0	0.285056	5.312977	0.074717
4	1	0	0.304036	5.672549	1.118257
5	1	0	1.191816	5.706098	-0.416219
6	1	0	-0.580332	5.790419	-0.414962
7	29	0	0.034472	0.667368	-0.046181
8	7	0	-1.685546	-0.491221	-0.041353
9	6	0	-2.676184	-1.161956	-0.038079
10	7	0	-3.667692	-2.007426	-0.072077
11	6	0	-4.965887	-1.889579	0.055151
12	7	0	-6.163483	-1.926172	0.154356
13	7	0	1.511097	-0.744083	-0.067187
14	6	0	2.499307	-1.415492	-0.041989
15	7	0	3.490043	-2.262068	-0.038014
16	6	0	4.790852	-2.142886	0.055708
17	7	0	5.990080	-2.183749	0.139922
Cu+N(CN)2C					
1	6	0	3.309395	-0.000047	0.000159

2	6	0	2.065453	-0.000108	-0.000391
3	6	0	4.785537	0.000063	0.001077
4	1	0	5.188842	-0.054032	1.023935
5	1	0	5.189315	-0.858516	-0.557143
6	1	0	5.189031	0.912937	-0.463315
7	29	0	0.197203	-0.000080	-0.000718
8	7	0	-1.743371	0.000025	-0.000981
9	6	0	-2.411226	-1.166758	0.000228
10	6	0	-2.411070	1.166898	0.000220
11	7	0	-2.936651	-2.236748	0.001174
12	7	0	-2.936348	2.236960	0.001177

Cu+N(CN)2T

1	6	0	-3.910730	0.171320	0.001495
2	6	0	-2.671872	0.053706	0.000017
3	29	0	-0.811453	-0.122078	-0.002693
4	6	0	-5.380396	0.313707	0.004208
5	1	0	-5.876506	-0.605721	-0.345517
6	1	0	-5.763296	0.530009	1.014139
7	1	0	-5.707833	1.134023	-0.654219
8	7	0	1.049512	-0.293089	-0.005049
9	6	0	2.245879	-0.324959	-0.000175
10	7	0	3.514925	-0.508917	0.008575
11	6	0	4.602171	0.221398	0.002533
12	7	0	5.659773	0.783563	-0.001350

Cu+N(CN)2C+T

1	6	0	-2.897744	-2.446164	0.012411
2	6	0	-1.920499	-1.668146	-0.006687
3	6	0	-4.086838	-3.322741	0.039985
4	1	0	-4.255340	-3.814750	-0.932787
5	1	0	-3.991582	-4.121251	0.795349
6	1	0	-5.002476	-2.756686	0.279834
7	29	0	-0.409040	-0.512871	-0.025355
8	7	0	-1.193580	1.909242	0.014988
9	6	0	-1.400500	2.459709	1.197983
10	7	0	-1.546654	2.869163	2.339682
11	7	0	1.490930	-0.117237	-0.064728
12	6	0	2.678977	-0.070122	-0.051446
13	7	0	3.961524	0.113766	-0.062282
14	6	0	5.010635	-0.664694	0.013693
15	7	0	6.045979	-1.255280	0.073862
16	6	0	-1.464694	2.477558	-1.144223
17	7	0	-1.673122	2.905140	-2.269722

Cu+2Br

1	29	0	-0.288579	-0.000150	-0.000319
2	35	0	1.265198	2.191521	0.000132
3	35	0	1.265650	-2.191248	0.000131
4	6	0	-2.230973	-0.000184	-0.000635
5	6	0	-3.484770	-0.000214	-0.000687
6	6	0	-4.963315	-0.000333	0.000409
7	1	0	-5.380293	-0.913906	-0.462218
8	1	0	-5.380382	0.858756	-0.556840
9	1	0	-5.375884	0.054341	1.024558

2CuBr

1	6	0	0.006693	2.927933	0.001083

2	6	0	-0.000154	1.681484	0.001083
3	6	0	0.011448	4.399912	-0.001146
4	1	0	0.325125	4.803640	0.971596
5	1	0	0.693031	4.793502	-0.768215
6	1	0	-0.993133	4.789960	-0.217852
7	29	0	1.314247	0.243566	0.000836
8	29	0	-1.314496	0.244879	0.000832
9	35	0	3.191058	-1.182985	-0.000572
10	35	0	-3.194650	-1.177243	-0.000572

2CuN(CN)2C

1	29	0	-1.517784	0.253485	-0.092885
2	6	0	-0.024914	1.456765	-0.289158
3	6	0	-0.087360	2.699784	-0.429365
4	29	0	1.544948	0.370950	-0.068984
5	6	0	-0.161153	4.160701	-0.594356
6	1	0	-1.144907	4.453691	-0.984993
7	7	0	3.165775	-0.648335	0.190578
8	6	0	3.719337	-1.301095	-0.854169
9	6	0	3.601355	-0.892320	1.443252
10	7	0	4.175654	-1.813036	-1.824681
11	7	0	3.948494	-1.033820	2.575249
12	7	0	-3.012080	-0.962968	0.129221
13	6	0	-3.188502	-2.026496	-0.686487
14	6	0	-4.010880	-0.564384	0.939001
15	7	0	-3.343981	-2.963780	-1.405376
16	7	0	-4.836836	-0.143241	1.686047
17	1	0	0.595932	4.512670	-1.309092
18	1	0	-0.005253	4.683578	0.358705

2CuN(CN)2T

1	29	0	1.328240	0.725948	-0.064477
2	6	0	0.044441	2.173912	-0.009760
3	6	0	0.379909	3.362213	0.188089
4	6	0	0.761798	4.763141	0.430319
5	1	0	0.159672	5.199509	1.238681
6	29	0	-1.466608	1.015244	-0.130128
7	7	0	-2.936067	-0.111952	-0.242292
8	6	0	-3.844612	-0.893823	-0.248793
9	7	0	-4.855583	-1.655304	-0.385995
10	6	0	-5.420407	-2.665568	0.230539
11	7	0	-6.019600	-3.586343	0.701917
12	7	0	2.560828	-0.666199	-0.106368
13	6	0	3.394561	-1.526297	-0.083631
14	7	0	4.168494	-2.546048	-0.114574
15	6	0	5.462518	-2.715136	0.083756
16	7	0	6.615618	-2.990211	0.232496
17	1	0	1.815438	4.826690	0.733684
18	1	0	0.632478	5.380986	-0.468235

2CuN(CN)2T+C

1	29	0	-0.866673	0.695949	-0.049746
2	6	0	0.720236	1.782110	0.028470
3	6	0	1.069151	2.977778	0.068684
4	6	0	1.467498	4.393527	0.113547
5	1	0	2.331228	4.579576	-0.538714
6	29	0	1.677846	0.098107	0.014374
7	7	0	-2.529464	-0.124256	-0.144993

8	6	0	-3.620904	-0.620652	-0.142297
9	7	0	-4.721076	-1.254187	-0.194646
10	6	0	-5.995457	-1.079077	0.046386
11	7	0	-7.175495	-1.025196	0.232016
12	1	0	0.646279	5.035851	-0.232310
13	1	0	1.734732	4.704825	1.131983
14	7	0	2.873919	-1.412267	0.019597
15	6	0	3.236911	-1.976285	1.187476
16	6	0	3.379683	-1.864304	-1.143953
17	7	0	3.511329	-2.417114	2.258709
18	7	0	3.786651	-2.199331	-2.211405

Path 1,4

I3

CuBr

1	29	0	0.018213	-0.544269	-0.003477
2	35	0	2.461910	-0.746116	0.012483
3	7	0	-0.107177	1.731795	0.029057
4	7	0	-1.251028	2.288051	0.031497
5	6	0	1.091766	2.614894	-0.068772
6	7	0	-2.415007	2.475818	0.047022
7	6	0	-1.835776	-0.988171	-0.042120
8	6	0	-3.055391	-1.250083	-0.044070
9	6	0	-4.499095	-1.556085	0.008197
10	1	0	-4.802732	-1.902315	1.018712
11	1	0	-4.770572	-2.356355	-0.711962
12	1	0	-5.111562	-0.663568	-0.238233
13	1	0	1.944969	1.931769	-0.043462
14	1	0	1.148839	3.314434	0.778503
15	1	0	1.099475	3.180926	-1.012105

CuN(CN)2C

1	29	0	0.039987	-0.599685	0.084174
2	7	0	-1.940786	-0.662606	0.157681
3	6	0	-2.601924	-1.613045	-0.523951
4	6	0	-2.600083	0.180794	0.965758
5	7	0	-3.122460	-2.471146	-1.167636
6	7	0	-3.100376	0.990584	1.685472
7	7	0	0.109130	1.681427	-0.407034
8	7	0	1.207450	2.291860	-0.245554
9	6	0	-1.051662	2.464916	-0.925531
10	7	0	2.323001	2.588686	-0.023333
11	1	0	-0.787777	3.029329	-1.830907
12	6	0	1.881403	-1.018497	0.133921
13	6	0	3.104961	-1.248208	0.165196
14	6	0	4.553439	-1.534075	0.199983
15	1	0	5.128452	-0.655845	0.530575
16	1	0	4.931688	-1.819773	-0.793624
17	1	0	4.786029	-2.359869	0.889859
18	1	0	-1.819476	1.729131	-1.165830
19	1	0	-1.447077	3.144947	-0.160533

CuN(CN)2T

1	29	0	0.357131	-0.559388	-0.081379
2	7	0	0.920275	1.769025	0.003678
3	7	0	2.135486	2.116323	0.079893
4	6	0	-0.117074	2.838141	0.002030
5	7	0	3.310542	2.137106	0.138590
6	1	0	0.032790	3.556314	-0.816580
7	6	0	2.092421	-1.294635	-0.013652
8	6	0	3.252562	-1.745750	0.034684
9	6	0	4.630463	-2.282198	0.090038
10	1	0	5.360492	-1.554683	-0.294517
11	1	0	4.731326	-3.199528	-0.509554
12	1	0	4.925303	-2.529621	1.120971
13	1	0	-1.062753	2.315008	-0.137394
14	1	0	-0.140020	3.375912	0.960411
15	7	0	-1.511915	-0.201932	-0.159366
16	6	0	-2.707093	-0.136346	-0.126359
17	7	0	-3.972781	0.081478	-0.146633
18	6	0	-5.064068	-0.597636	0.100219
19	7	0	-6.128351	-1.106373	0.300252

2CuN(CN)2C

1	29	0	0.923540	-0.158715	-0.029154
2	6	0	0.006832	1.557800	0.107601
3	6	0	0.095883	2.799163	0.212490
4	29	0	-1.604346	0.465177	0.071299
5	7	0	2.983772	0.527797	-0.306316
6	7	0	3.224315	1.766516	-0.170010
7	6	0	4.141629	-0.381943	-0.571099
8	7	0	3.120684	2.924681	-0.011597
9	1	0	4.742723	-0.522734	0.335114
10	7	0	1.345681	-2.093643	-0.016726
11	6	0	0.925406	-2.909506	-1.000398
12	6	0	2.084589	-2.562673	1.002012
13	7	0	0.537835	-3.559074	-1.920084
14	7	0	2.772154	-2.866094	1.927376
15	7	0	-3.410215	-0.220023	0.067309
16	6	0	-4.189316	0.000510	-1.008329
17	6	0	-3.907816	-0.841646	1.153068
18	7	0	-4.814442	0.241276	-1.992912
19	7	0	-4.278953	-1.374111	2.151141
20	6	0	0.132850	4.266802	0.345446
21	1	0	0.704507	4.570235	1.231677
22	1	0	-0.885252	4.667073	0.444992
23	1	0	0.597720	4.735352	-0.531119
24	1	0	3.708771	-1.339473	-0.858141
25	1	0	4.768759	-0.000158	-1.386739

2CuN(CN)2T

1	29	0	1.013158	0.350661	-0.329037
2	6	0	-0.272779	1.746112	-0.876431
3	6	0	-0.167799	2.934731	-1.240468
4	29	0	-1.591284	0.390324	-0.532354
5	6	0	-0.058197	4.330452	-1.698520
6	7	0	1.857627	1.310652	1.479156
7	7	0	1.642799	2.536118	1.716879
8	6	0	2.672816	0.530471	2.458407
9	7	0	1.308102	3.660231	1.690799

10	1	0	2.166916	0.463523	3.430362
11	7	0	-3.045944	-0.723473	-0.210452
12	6	0	-4.027868	-1.372387	0.016255
13	7	0	-4.998985	-2.171221	0.210640
14	6	0	-6.231570	-2.154830	0.651100
15	7	0	-7.360830	-2.252406	1.032869
16	7	0	2.160893	-1.167729	-0.412501
17	6	0	2.965668	-2.047071	-0.542133
18	7	0	3.730776	-3.049331	-0.747785
19	6	0	4.944571	-3.413382	-0.406428
20	7	0	6.032648	-3.840754	-0.153252
21	1	0	-0.819680	4.552815	-2.458552
22	1	0	-0.184310	5.036680	-0.867856
23	1	0	0.925080	4.516441	-2.151971
24	1	0	2.767761	-0.465346	2.025237
25	1	0	3.671241	0.968139	2.587981

CuN(CN)2C+T

1	29	0	-0.782687	0.517733	0.185986
2	6	0	0.616009	1.923981	-0.131405
3	6	0	0.407920	3.138199	0.059544
4	7	0	-0.055797	-0.742228	1.863855
5	7	0	0.832990	-0.349757	2.674312
6	6	0	-0.493880	-2.176468	1.938017
7	7	0	1.636380	0.207268	3.322019
8	1	0	-0.835941	-2.429704	2.949967
9	7	0	-2.508360	-0.246361	-0.101435
10	6	0	-3.634719	-0.587485	-0.332101
11	7	0	-4.808170	-1.071792	-0.474509
12	6	0	-5.905869	-0.790685	-1.134456
13	7	0	-6.957274	-0.632862	-1.682645
14	29	0	1.729162	0.463978	-0.641877
15	7	0	2.907685	-1.019921	-1.011357
16	6	0	2.712610	-2.133032	-0.286397
17	6	0	3.889116	-0.938429	-1.927433
18	7	0	2.446442	-3.060725	0.412234
19	7	0	4.731404	-0.782713	-2.753814
20	6	0	0.161660	4.574933	0.266209
21	1	0	-0.782940	4.885881	-0.199883
22	1	0	-1.328210	-2.257397	1.240404
23	1	0	0.322960	-2.838939	1.628686
24	1	0	0.967262	5.170648	-0.184797
25	1	0	0.114910	4.827440	1.333979

CuN(CN)2T+C

1	29	0	-1.214855	-0.184206	0.081758
2	6	0	-0.410976	1.598102	0.153909
3	6	0	-0.612588	2.829602	0.210722
4	29	0	1.252029	0.598574	0.078121
5	7	0	-1.440745	-2.155042	0.099646
6	6	0	-1.712108	-2.783840	-1.055566
7	6	0	-1.332830	-2.834118	1.255001
8	7	0	-1.982356	-3.239690	-2.123306
9	7	0	-1.244533	-3.350463	2.324824
10	7	0	3.007504	-0.016540	-0.004809
11	6	0	4.169089	-0.304180	-0.069650
12	7	0	5.363361	-0.741421	-0.127164
13	6	0	6.584114	-0.283077	-0.243385

14	7	0	7.735139	0.026411	-0.345111
15	6	0	-0.770283	4.293136	0.293371
16	1	0	-1.197215	4.701905	-0.631077
17	7	0	-3.314762	0.321179	-0.168014
18	7	0	-3.627612	1.548422	-0.269138
19	6	0	-4.416856	-0.685672	-0.257687
20	7	0	-3.585970	2.720486	-0.312674
21	1	0	-4.828529	-0.728148	-1.273672
22	1	0	-3.962614	-1.645853	-0.017505
23	1	0	-5.215523	-0.466286	0.462499
24	1	0	0.203156	4.773699	0.461489
25	1	0	-1.432883	4.574895	1.121713

2CuBr

1	29	0	-1.180693	0.218484	-0.036156
2	6	0	-0.064638	1.929688	-0.148190
3	6	0	-0.665949	3.008529	0.025941
4	6	0	-1.357695	4.295687	0.210745
5	29	0	1.410287	0.746661	-0.444374
6	35	0	3.282132	-0.682487	-0.677388
7	35	0	-3.035747	-1.143273	-0.816945
8	7	0	-0.348372	-1.018555	1.572398
9	7	0	0.138189	-0.557422	2.643299
10	6	0	-0.023211	-2.430655	1.189893
11	7	0	0.481192	0.067847	3.578017
12	1	0	-0.113955	-3.107455	2.049548
13	1	0	-0.755105	5.120378	-0.196049
14	1	0	-2.325272	4.301888	-0.310617
15	1	0	-1.544574	4.507196	1.272950
16	1	0	-0.759050	-2.695303	0.427851
17	1	0	0.988137	-2.476879	0.766998

TS 3-4

CuBr

1	29	0	0.167752	-0.530472	-0.000290
2	35	0	2.621426	-0.430161	0.000187
3	7	0	-0.460075	1.465197	-0.000100
4	7	0	-1.739351	1.751470	0.000032
5	6	0	0.455761	2.634331	-0.000010
6	7	0	-2.830367	1.237328	0.000119
7	6	0	-1.577546	-1.263681	-0.000387
8	6	0	-2.827368	-1.048337	-0.000048
9	6	0	-4.294822	-1.251393	0.000414
10	1	0	-4.543802	-2.322055	0.000697
11	1	0	-4.754763	-0.789797	-0.884235
12	1	0	-4.754236	-0.789469	0.885166
13	1	0	1.465837	2.216162	-0.000010
14	1	0	0.322324	3.260451	0.895441
15	1	0	0.322353	3.260553	-0.895388

CuN(CN)2C

1	29	0	0.169181	-0.442081	-0.067365
2	7	0	2.160329	-0.433396	-0.057664
3	6	0	2.793138	-1.568151	0.287815
4	6	0	2.864638	0.648753	-0.415433
5	7	0	3.288689	-2.603542	0.608959

6	7	0	3.402986	1.662994	-0.741453
7	7	0	-0.591475	1.518438	0.206097
8	7	0	-1.894393	1.675946	0.234767
9	6	0	0.177719	2.773243	0.432575
10	7	0	-2.932401	1.068651	0.143834
11	1	0	0.070706	3.132383	1.467308
12	6	0	-1.525332	-1.250752	-0.178259
13	6	0	-2.788204	-1.141283	-0.168879
14	6	0	-4.232272	-1.464835	-0.219243
15	1	0	-4.386546	-2.543393	-0.358791
16	1	0	-4.723264	-0.934681	-1.046484
17	1	0	-4.733550	-1.159931	0.709206
18	1	0	1.228113	2.548051	0.243152
19	1	0	-0.135953	3.572442	-0.254052

CuN(CN)2T

1	29	0	0.266833	-0.498782	0.000076
2	7	0	1.097898	1.440994	0.000050
3	7	0	2.399070	1.604553	-0.000079
4	6	0	0.298597	2.691902	0.000143
5	7	0	3.427156	0.971841	-0.000151
6	1	0	0.488888	3.303627	-0.894318
7	6	0	1.937687	-1.350057	0.000210
8	6	0	3.202585	-1.254552	-0.000029
9	6	0	4.638018	-1.620873	-0.000075
10	1	0	5.145144	-1.213605	-0.884995
11	1	0	4.763429	-2.712149	0.000090
12	1	0	5.145282	-1.213308	0.884625
13	1	0	-0.748486	2.380381	0.000083
14	1	0	0.488866	3.303475	0.894705
15	7	0	-1.623887	-0.185420	-0.000155
16	6	0	-2.813045	-0.050257	-0.000137
17	7	0	-4.060676	0.255400	-0.000196
18	6	0	-5.199588	-0.396118	-0.000062
19	7	0	-6.297676	-0.873655	0.000145

2CuN(CN)2C

1	29	0	-1.004057	-0.152395	-0.028017
2	6	0	-0.050295	1.523863	0.012864
3	6	0	-0.291057	2.768010	0.030095
4	29	0	1.525822	0.402932	0.025667
5	7	0	-2.886207	0.634823	-0.043572
6	7	0	-3.052541	1.923546	-0.017192
7	6	0	-4.123477	-0.190617	-0.068595
8	7	0	-2.467093	2.970738	0.009927
9	1	0	-4.742219	0.044603	-0.944357
10	7	0	-1.347634	-2.101909	-0.053449
11	6	0	-1.685261	-2.719970	1.091943
12	6	0	-1.308540	-2.774989	-1.217507
13	7	0	-1.995256	-3.173376	2.148994
14	7	0	-1.269026	-3.286128	-2.292386
15	7	0	3.333425	-0.261733	0.056779
16	6	0	3.911076	-0.594401	1.228062
17	6	0	4.044602	-0.312829	-1.086857
18	7	0	4.354033	-0.863429	2.299481
19	7	0	4.608966	-0.322834	-2.134753
20	6	0	-0.002678	4.222954	0.057367
21	1	0	1.080700	4.393207	0.074042

22	1	0	-0.447158	4.689879	0.944103
23	1	0	-0.424076	4.718554	-0.825079
24	1	0	-3.800807	-1.230482	-0.127454
25	1	0	-4.714510	-0.051369	0.845863

2CuN(CN)2T

1	29	0	-1.131844	-0.362262	-0.000601
2	6	0	0.073059	-1.866116	-0.041845
3	6	0	0.040130	-3.133716	-0.037967
4	29	0	1.437327	-0.498322	-0.087663
5	7	0	3.015362	0.483536	-0.134073
6	6	0	4.088614	1.018695	-0.144337
7	7	0	5.167175	1.683259	-0.231841
8	6	0	6.417644	1.633805	0.149456
9	7	0	7.575914	1.684144	0.442336
10	6	0	0.567198	-4.520459	-0.063864
11	1	0	0.263353	-5.068895	0.835562
12	7	0	-2.852507	-1.454996	0.099711
13	7	0	-2.815705	-2.754201	0.104565
14	6	0	-4.199521	-0.830007	0.167658
15	7	0	-2.068449	-3.693661	0.071397
16	1	0	-4.723252	-1.106273	1.092416
17	1	0	-4.037092	0.248371	0.156232
18	1	0	-4.816227	-1.110973	-0.696403
19	1	0	1.662797	-4.507263	-0.115974
20	1	0	0.179595	-5.067596	-0.931363
21	6	0	-2.153541	2.569379	-0.010768
22	7	0	-1.733518	1.446210	-0.001562
23	7	0	-2.480751	3.800535	-0.021910
24	6	0	-3.576691	4.519833	-0.016267
25	7	0	-4.511742	5.265330	-0.013364

CuN(CN)2T+C

1	29	0	1.284459	-0.200048	0.001378
2	6	0	0.464934	1.548775	-0.016582
3	6	0	0.816632	2.766852	-0.009767
4	29	0	-1.182289	0.543623	-0.046449
5	7	0	1.448668	-2.174092	0.001280
6	6	0	1.506460	-2.831452	1.172621
7	6	0	1.547497	-2.827677	-1.169443
8	7	0	1.567066	-3.322887	2.256005
9	7	0	1.645923	-3.315676	-2.251604
10	7	0	-2.948450	-0.034127	-0.079642
11	6	0	-4.118595	-0.296715	-0.092468
12	7	0	-5.321702	-0.697067	-0.152069
13	6	0	-6.541121	-0.280451	0.070607
14	7	0	-7.690982	0.001045	0.239984
15	6	0	0.651817	4.241410	-0.016217
16	1	0	1.102359	4.686748	0.878604
17	7	0	3.221999	0.423018	0.045704
18	7	0	3.497854	1.693641	0.052695
19	6	0	4.384362	-0.504802	0.069901
20	7	0	3.001095	2.786322	0.042187
21	1	0	4.984396	-0.369414	0.979189
22	1	0	3.974217	-1.515313	0.060736
23	1	0	5.022374	-0.368550	-0.813035
24	1	0	-0.413263	4.502335	-0.042192
25	1	0	1.144775	4.683650	-0.889964

CuN(CN)2C+T

1	29	0	-0.649937	0.605566	-0.000395
2	6	0	1.082230	1.446997	0.000051
3	6	0	1.605882	2.601337	0.000536
4	29	0	1.732272	-0.377191	-0.000114
5	7	0	-1.731457	2.338374	-0.000134
6	7	0	-1.136351	3.493468	0.000375
7	6	0	-3.217886	2.357548	-0.000434
8	7	0	-0.056222	4.017895	0.000750
9	1	0	-3.612068	2.855862	-0.895999
10	7	0	2.813033	-1.971756	0.000167
11	6	0	3.213943	-2.508050	1.169230
12	6	0	3.215582	-2.507468	-1.168595
13	7	0	3.530156	-2.916760	2.241550
14	7	0	3.533315	-2.915593	-2.240689
15	6	0	2.681222	3.623365	0.000837
16	1	0	3.664679	3.137697	0.001391
17	1	0	2.605087	4.266734	0.885310
18	1	0	2.605896	4.266338	-0.884002
19	1	0	-3.536822	1.314673	-0.000942
20	1	0	-3.612439	2.855092	0.895396
21	7	0	-1.974819	-0.763127	-0.000919
22	6	0	-2.846693	-1.586520	-0.001111
23	7	0	-3.683477	-2.546660	-0.001845
24	6	0	-4.984016	-2.710105	0.000216
25	7	0	-6.151839	-2.967542	0.002066

I4

N(CN)2C

1	29	0	-0.203835	-0.422452	0.104969
2	7	0	-2.188115	-0.336650	0.095025
3	6	0	-2.881017	-1.362465	-0.429736
4	6	0	-2.830508	0.710418	0.636308
5	7	0	-3.422244	-2.306102	-0.916164
6	7	0	-3.310032	1.682544	1.133075
7	7	0	0.794105	1.279783	-0.337769
8	7	0	2.100397	1.563946	-0.398948
9	6	0	-0.068634	2.438581	-0.697604
10	7	0	3.044564	0.720034	-0.168005
11	1	0	-0.550252	2.270634	-1.671517
12	6	0	1.479015	-1.130523	0.281113
13	6	0	2.735575	-0.691624	0.180899
14	6	0	4.006307	-1.487242	0.388946
15	1	0	3.787728	-2.529577	0.643205
16	1	0	4.597607	-1.036119	1.196904
17	1	0	4.614515	-1.459552	-0.525012
18	1	0	-0.854299	2.570015	0.054149
19	1	0	0.540752	3.347946	-0.751891

N(CN)2T

1	29	0	-0.214135	-0.396313	0.004104
2	7	0	-1.350150	1.281029	-0.003340
3	7	0	-2.672099	1.487197	-0.006645
4	6	0	-0.581984	2.556127	0.000985
5	7	0	-3.552649	0.549481	-0.006865

6	1	0	-0.794273	3.141951	0.906860
7	6	0	-1.844672	-1.230347	0.002305
8	6	0	-3.132167	-0.877542	-0.001864
9	6	0	-4.336653	-1.794336	-0.002454
10	1	0	-4.955441	-1.594338	0.882458
11	1	0	-4.037050	-2.847482	0.000199
12	1	0	-4.951889	-1.597784	-0.890600
13	1	0	0.482026	2.309133	-0.023192
14	1	0	-0.830356	3.168721	-0.877269
15	7	0	1.675544	-0.080152	0.007611
16	6	0	2.867731	0.030832	0.005813
17	7	0	4.118358	0.305735	0.007056
18	6	0	5.252404	-0.352271	-0.005119
19	7	0	6.345132	-0.840704	-0.014314

Br

1	29	0	-0.239153	-0.426262	0.001621
2	35	0	-2.684447	-0.347876	-0.001215
3	7	0	0.755689	1.326119	0.000555
4	7	0	2.058507	1.632244	-0.002351
5	6	0	-0.108742	2.537773	0.001962
6	7	0	3.010484	0.764244	-0.002790
7	6	0	1.454631	-1.164891	0.002948
8	6	0	2.704521	-0.689574	0.000009
9	6	0	3.980978	-1.505718	-0.000905
10	1	0	3.767497	-2.579933	0.002025
11	1	0	4.582156	-1.256266	0.884060
12	1	0	4.578335	-1.260435	-0.889621
13	1	0	-1.149793	2.204720	-0.000864
14	1	0	0.077767	3.154997	-0.889122
15	1	0	0.074039	3.150376	0.897061

2CuN(CN)2C

1	29	0	-1.089029	-0.161255	-0.016930
2	6	0	-0.082118	1.421974	0.010344
3	6	0	-0.458748	2.696739	0.014431
4	29	0	1.479723	0.326262	0.014001
5	7	0	-2.697937	0.942079	-0.048686
6	7	0	-2.826502	2.260565	-0.033340
7	6	0	-3.998351	0.213621	-0.038150
8	7	0	-1.882491	3.120030	-0.010976
9	1	0	-4.668114	0.624547	-0.802472
10	7	0	-1.492857	-2.090328	-0.024267
11	6	0	-1.789564	-2.708191	1.135177
12	6	0	-1.540092	-2.762634	-1.190629
13	7	0	-2.050335	-3.165789	2.202568
14	7	0	-1.570709	-3.273499	-2.265147
15	7	0	3.274183	-0.347829	0.034260
16	6	0	3.883431	-0.614936	1.208386
17	6	0	3.956328	-0.483302	-1.122258
18	7	0	4.354838	-0.823642	2.280338
19	7	0	4.494460	-0.570596	-2.179460
20	6	0	0.438574	3.917031	0.042619
21	1	0	1.496468	3.639912	0.064540
22	1	0	0.204582	4.521770	0.927774
23	1	0	0.244533	4.533167	-0.844301
24	1	0	-3.803618	-0.838485	-0.252438
25	1	0	-4.479286	0.295148	0.945285

2CuN(CN)2T

1	29	0	-1.214285	-0.340137	0.037575
2	6	0	-0.065919	-1.819460	-0.058724
3	6	0	-0.309289	-3.126606	-0.055752
4	29	0	1.364242	-0.562043	-0.136512
5	7	0	2.978461	0.341025	-0.230251
6	6	0	4.065254	0.851197	-0.249703
7	7	0	5.185476	1.419040	-0.401373
8	6	0	6.293321	1.707470	0.229591
9	7	0	7.342212	2.014889	0.712815
10	6	0	0.708918	-4.243906	-0.159545
11	1	0	0.641662	-4.884265	0.729082
12	7	0	-2.692315	-1.611766	0.171464
13	7	0	-2.696857	-2.936835	0.153199
14	6	0	-4.051001	-1.012132	0.288538
15	7	0	-1.674797	-3.697905	0.055820
16	1	0	-4.554464	-1.377723	1.192242
17	1	0	-3.938357	0.071391	0.348961
18	1	0	-4.661654	-1.264443	-0.588086
19	1	0	1.727521	-3.854584	-0.246753
20	1	0	0.482810	-4.864749	-1.035666
21	6	0	-2.147267	2.618478	0.059485
22	7	0	-1.767551	1.479846	0.068582
23	7	0	-2.431821	3.853832	0.084653
24	6	0	-3.440356	4.668063	-0.091795
25	7	0	-4.295412	5.492008	-0.229650

CuN(CN)2C+T

1	29	0	0.702440	0.660212	-0.014916
2	6	0	-1.039068	1.350793	0.000954
3	6	0	-1.497911	2.598408	0.003980
4	29	0	-1.645315	-0.460609	-0.001309
5	7	0	1.334510	2.507768	0.004837
6	7	0	0.663039	3.650564	0.011394
7	6	0	2.813082	2.683202	0.049846
8	7	0	-0.607610	3.785501	0.005608
9	1	0	3.126782	3.072778	1.027298
10	7	0	-2.670863	-2.080732	0.012844
11	6	0	-3.094472	-2.619494	-1.149088
12	6	0	-3.015347	-2.649206	1.186791
13	7	0	-3.433232	-3.028525	-2.213598
14	7	0	-3.282484	-3.086297	2.260447
15	6	0	-2.946709	3.041433	0.005667
16	1	0	-3.630059	2.187253	-0.004434
17	1	0	-3.138292	3.668108	-0.874337
18	1	0	-3.141846	3.649443	0.898058
19	1	0	3.275946	1.708567	-0.112017
20	1	0	3.138293	3.378313	-0.733619
21	7	0	2.100607	-0.626876	-0.043245
22	6	0	3.027315	-1.389829	-0.053980
23	7	0	3.923290	-2.285469	-0.078607
24	6	0	5.219595	-2.437955	-0.006637
25	7	0	6.388980	-2.681226	0.046660

CuN(CN)2T+C

1	29	0	-1.340019	-0.270782	-0.008056
2	6	0	-0.603596	1.457561	0.027139

3	6	0	-1.190893	2.649532	-0.017256
4	29	0	1.099753	0.613531	0.129842
5	7	0	-1.395878	-2.242733	0.008317
6	6	0	-1.379715	-2.918687	-1.156164
7	6	0	-1.491922	-2.895216	1.182293
8	7	0	-1.372647	-3.428749	-2.231657
9	7	0	-1.587932	-3.383794	2.263496
10	7	0	2.891139	0.159293	0.233629
11	6	0	4.073281	-0.049842	0.261451
12	7	0	5.301825	-0.301106	0.423054
13	6	0	6.452541	-0.311445	-0.195555
14	7	0	7.550305	-0.350818	-0.666393
15	6	0	-0.510269	4.002734	0.022656
16	1	0	-0.756776	4.563349	-0.887905
17	7	0	-3.105247	0.546606	-0.128770
18	7	0	-3.450009	1.826293	-0.159981
19	6	0	-4.266807	-0.385004	-0.189327
20	7	0	-2.661696	2.829970	-0.116780
21	1	0	-4.828407	-0.238675	-1.120425
22	1	0	-3.885852	-1.407020	-0.156081
23	1	0	-4.935980	-0.220785	0.664504
24	1	0	0.576299	3.905078	0.102766
25	1	0	-0.886319	4.575805	0.879527

TS 4-P

CuBr

1	29	0	0.690780	-0.465652	0.000050
2	6	0	-1.098276	-0.955504	0.000040
3	6	0	-2.416366	-1.142901	0.000015
4	6	0	-3.052516	-2.525456	0.000156
5	1	0	-3.691329	-2.629092	0.887053
6	7	0	-1.939646	1.596453	-0.000318
7	7	0	-3.176686	1.156261	-0.000225
8	6	0	-1.763462	3.060174	0.000306
9	7	0	-3.488200	-0.111400	-0.000189
10	1	0	-1.187198	3.366141	-0.884664
11	1	0	-2.733701	3.578539	-0.003746
12	1	0	-1.194485	3.366800	0.889831
13	1	0	-2.301272	-3.322677	0.000358
14	1	0	-3.691134	-2.629368	-0.886849
15	35	0	2.999484	0.076185	-0.000041

CuN(CN)2C

1	29	0	0.641732	-0.447519	0.017386
2	6	0	-1.158692	-0.874508	0.005663
3	6	0	-2.465386	-1.152653	-0.019000
4	7	0	2.525388	-0.019152	-0.004494
5	6	0	3.448900	-0.996799	0.030993
6	6	0	2.894692	1.272704	-0.070070
7	7	0	4.208033	-1.913660	0.070650
8	7	0	3.137862	2.437637	-0.128888
9	6	0	-3.011838	-2.570379	-0.043017
10	1	0	-3.674197	-2.719086	0.819137
11	7	0	-1.983459	1.471951	0.014170
12	7	0	-3.245526	1.100157	-0.015228
13	6	0	-1.685901	2.910671	0.098335

14	7	0	-3.565598	-0.170477	-0.041619
15	1	0	-2.263443	3.492913	-0.635358
16	1	0	-1.898186	3.306470	1.105339
17	1	0	-0.618942	3.049341	-0.103650
18	1	0	-2.213381	-3.319793	-0.017066
19	1	0	-3.609643	-2.711200	-0.952164

CuN(CN)2T

1	29	0	0.146797	-0.579949	-0.122848
2	6	0	-1.668581	-0.887677	0.011868
3	6	0	-2.994263	-0.994000	0.106801
4	6	0	-3.714960	-2.331968	0.172244
5	1	0	-4.288929	-2.388662	1.106131
6	7	0	-2.264676	1.630566	0.030496
7	7	0	-3.542278	1.341261	0.120527
8	6	0	-1.901336	3.057620	-0.025426
9	7	0	-3.977441	0.110164	0.165508
10	1	0	-2.790101	3.693692	0.091883
11	1	0	-1.183767	3.289040	0.773628
12	1	0	-1.419734	3.288310	-0.986638
13	1	0	-3.018515	-3.175878	0.125048
14	1	0	-4.425008	-2.401371	-0.661885
15	6	0	3.167059	-0.124822	-0.300795
16	7	0	4.414267	0.066435	-0.493443
17	7	0	1.981502	-0.287988	-0.258528
18	6	0	5.521372	0.126658	0.203783
19	7	0	6.590509	0.202208	0.735952

2CuN(CN)2C

1	29	0	-1.540697	0.236917	-0.057977
2	6	0	-0.017830	1.319958	-0.420958
3	6	0	0.300596	2.595057	-0.711877
4	29	0	1.132336	-0.163825	-0.205484
5	7	0	-3.240816	-0.590822	0.258306
6	6	0	-3.882752	-0.355062	1.420982
7	6	0	-3.822680	-1.351796	-0.691403
8	7	0	-4.385274	-0.097238	2.468198
9	7	0	-4.276154	-2.004308	-1.576644
10	7	0	1.962647	-1.934503	-0.252507
11	6	0	-0.547548	3.513003	-1.569745
12	1	0	-0.845054	4.388215	-0.978580
13	7	0	2.066923	1.324762	0.875939
14	7	0	2.294782	2.591314	0.554360
15	6	0	3.045504	0.734940	1.834630
16	7	0	1.490564	3.266402	-0.214918
17	1	0	3.435750	1.523973	2.485167
18	1	0	2.539094	-0.020945	2.441387
19	1	0	3.877360	0.256232	1.301684
20	1	0	-1.442771	3.008833	-1.944477
21	1	0	0.048335	3.869052	-2.418906
22	6	0	2.222480	-2.585468	0.895907
23	7	0	2.421722	-3.071491	1.964376
24	6	0	2.316354	-2.464177	-1.439606
25	7	0	2.600607	-2.853225	-2.527609

2CuN(CN)2T

1	29	0	-1.382234	0.138171	-0.368285
2	6	0	0.000377	1.436272	-0.549229

3	6	0	-0.000842	2.770306	-0.888824
4	29	0	1.383757	0.139069	-0.368624
5	7	0	2.794310	-1.052352	-0.190119
6	6	0	3.755744	-1.761986	-0.082363
7	7	0	4.684732	-2.618755	0.021475
8	6	0	5.981576	-2.700841	0.173581
9	7	0	7.154422	-2.886551	0.310413
10	6	0	0.000706	3.220161	-2.337844
11	1	0	-0.884922	3.838900	-2.524847
12	7	0	-0.003595	2.230842	1.615069
13	7	0	-0.005071	3.501267	1.330925
14	6	0	-0.005433	1.790321	3.018942
15	7	0	-0.003529	3.845244	0.031773
16	1	0	-0.007008	2.661629	3.684752
17	1	0	-0.894418	1.178663	3.211450
18	1	0	0.883767	1.179814	3.214038
19	1	0	0.002218	2.373073	-3.029776
20	1	0	0.885949	3.840145	-2.522570
21	6	0	-3.753227	-1.764280	-0.082802
22	7	0	-4.681836	-2.621503	0.020666
23	7	0	-2.792100	-1.054153	-0.190044
24	6	0	-5.978796	-2.704273	0.171371
25	7	0	-7.151673	-2.890650	0.307030

CuN(CN)2C+T

1	29	0	1.384694	-0.285056	0.177588
2	6	0	0.538542	1.401653	0.291172
3	6	0	1.098760	2.617399	0.427907
4	29	0	-1.159350	0.555760	0.181446
5	7	0	1.855318	-2.173825	0.383537
6	6	0	1.978120	-2.958705	-0.701970
7	6	0	2.082305	-2.662829	1.617825
8	7	0	2.073391	-3.562523	-1.723744
9	7	0	2.269563	-3.008160	2.741146
10	7	0	-2.913865	-0.029234	0.114209
11	6	0	-4.074748	-0.328125	0.052805
12	7	0	-5.274136	-0.730884	0.087458
13	6	0	-6.442787	-0.540200	-0.466243
14	7	0	-7.550608	-0.441382	-0.903871
15	6	0	0.486405	3.753176	1.223823
16	1	0	1.188173	4.068482	2.005641
17	7	0	2.505272	0.894068	-1.088492
18	7	0	2.974422	2.124357	-0.919263
19	6	0	3.310080	0.042923	-2.012317
20	7	0	2.352561	3.008716	-0.195044
21	1	0	4.076563	-0.518329	-1.461932
22	1	0	2.647517	-0.670403	-2.510320
23	1	0	3.792885	0.677693	-2.762097
24	1	0	-0.460719	3.461785	1.686667
25	1	0	0.317114	4.610686	0.560494

P

CuBr

1	29	0	0.583118	0.025220	0.000024
2	6	0	-1.336279	0.029528	-0.000033
3	6	0	-2.277393	1.087642	0.000022

4	6	0	-2.018957	2.569099	0.000202
5	1	0	-2.455140	3.054490	-0.884904
6	7	0	-2.166184	-1.081887	-0.000229
7	7	0	-3.534656	-0.750455	-0.000253
8	6	0	-1.794895	-2.490642	0.000303
9	7	0	-3.578539	0.590157	-0.000127
10	1	0	-2.715863	-3.081535	-0.004384
11	1	0	-1.197500	-2.734687	-0.886471
12	1	0	-1.205640	-2.736557	0.892063
13	1	0	-0.939077	2.756484	-0.001381
14	1	0	-2.452328	3.053863	0.887049
15	35	0	2.959312	0.013660	-0.000039

CuN(CN)2C

1	29	0	0.540945	0.023920	-0.000071
2	6	0	-1.365744	0.031785	-0.000052
3	6	0	-2.298648	1.095534	0.000210
4	7	0	2.479292	0.015927	-0.000080
5	6	0	3.159079	1.175785	-0.001526
6	6	0	3.126958	-1.161927	0.001837
7	7	0	3.686719	2.244200	-0.003541
8	7	0	3.622407	-2.245913	0.003554
9	6	0	-2.037560	2.576595	0.002686
10	1	0	-2.496373	3.065414	-0.868210
11	7	0	-2.198320	-1.077788	-0.000138
12	7	0	-3.562356	-0.737727	-0.000381
13	6	0	-1.836200	-2.490168	-0.002406
14	7	0	-3.601328	0.602185	-0.000001
15	1	0	-2.761610	-3.073237	0.006696
16	1	0	-1.254938	-2.742193	-0.897540
17	1	0	-1.238266	-2.739951	0.882185
18	1	0	-0.958832	2.768945	-0.023776
19	1	0	-2.449592	3.055523	0.902311

CuN(CN)2T

1	29	0	0.084837	-0.089749	-0.113582
2	6	0	-1.816740	-0.011876	0.013851
3	6	0	-2.793034	-1.033077	0.101098
4	6	0	-2.595714	-2.523874	0.119650
5	1	0	-3.027649	-2.973605	1.024707
6	7	0	-2.602768	1.131698	0.039607
7	7	0	-3.977136	0.851478	0.136419
8	6	0	-2.184333	2.526681	-0.015775
9	7	0	-4.071582	-0.484911	0.172645
10	1	0	-3.083979	3.148161	0.015886
11	1	0	-1.539725	2.774323	0.836389
12	1	0	-1.631787	2.730195	-0.940911
13	1	0	-1.525773	-2.760816	0.093985
14	1	0	-3.074935	-3.003980	-0.745499
15	6	0	3.142610	-0.190504	-0.273862
16	7	0	4.406086	-0.288824	-0.440664
17	7	0	1.945777	-0.165955	-0.238288
18	6	0	5.504116	0.066839	0.179269
19	7	0	6.568499	0.339844	0.653698

2CuN(CN)2C

1	29	0	-1.266913	-0.126095	-0.032551
2	6	0	0.000107	1.399748	-0.036631

3	6	0	0.001358	2.310053	-1.129272
4	29	0	1.266697	-0.126450	-0.030778
5	7	0	-2.763317	-1.331524	0.008421
6	6	0	-3.285057	-1.680296	1.200171
7	6	0	-3.311729	-1.771378	-1.140591
8	7	0	-3.683961	-1.932331	2.292941
9	7	0	-3.737487	-2.111499	-2.198469
10	7	0	2.762954	-1.331997	0.011667
11	6	0	0.003117	2.025330	-2.604336
12	1	0	-0.877836	2.466548	-3.087148
13	7	0	-0.000760	2.271077	1.065848
14	7	0	-0.000162	3.598149	0.682774
15	6	0	-0.002468	1.948893	2.495656
16	7	0	0.001152	3.616950	-0.662631
17	1	0	-0.002426	2.892514	3.045962
18	1	0	-0.894843	1.371826	2.759973
19	1	0	0.888590	1.370646	2.761814
20	1	0	-0.002630	0.947130	-2.796399
21	1	0	0.891368	2.456132	-3.083272
22	6	0	3.280274	-1.685248	1.204026
23	7	0	3.675154	-1.941476	2.297279
24	6	0	3.315926	-1.767160	-1.136948
25	7	0	3.745697	-2.103154	-2.194523

2CuN(CN)2T

1	29	0	1.259158	0.149963	0.012135
2	6	0	0.001785	1.678782	0.027357
3	6	0	-0.026644	2.558336	1.144634
4	29	0	-1.263591	0.157930	-0.049709
5	7	0	-2.677092	-1.039231	-0.123840
6	6	0	-3.639541	-1.756190	-0.132976
7	7	0	-4.573575	-2.610385	-0.196974
8	6	0	-5.848840	-2.753746	0.054969
9	7	0	-7.004966	-2.988150	0.247778
10	6	0	-0.067771	2.230324	2.609917
11	1	0	0.801941	2.652976	3.128732
12	7	0	0.033836	2.584695	-1.046819
13	7	0	0.025790	3.900696	-0.625628
14	6	0	0.071499	2.306495	-2.483718
15	7	0	-0.011481	3.878948	0.718819
16	1	0	0.105777	3.265907	-3.005225
17	1	0	0.959984	1.718915	-2.737991
18	1	0	-0.822188	1.753683	-2.792665
19	1	0	-0.070909	1.146300	2.766074
20	1	0	-0.966661	2.650509	3.078682
21	6	0	3.627246	-1.776331	-0.010259
22	7	0	4.551570	-2.643132	-0.026520
23	7	0	2.669077	-1.053614	-0.009360
24	6	0	5.853133	-2.752919	0.038025
25	7	0	7.029046	-2.962070	0.086022

CuN(CN)2T+C

1	29	0	1.461988	-0.450868	0.043228
2	6	0	0.715990	1.389140	0.027733
3	6	0	0.980084	2.255010	1.124514
4	29	0	-0.944333	0.316101	-0.015049
5	7	0	2.506375	-2.064793	0.017967

6	6	0	2.890862	-2.569117	-1.169912
7	6	0	2.876923	-2.650720	1.172518
8	7	0	3.188136	-2.940744	-2.261051
9	7	0	3.162302	-3.102627	2.235820
10	7	0	-2.655317	-0.392936	-0.071176
11	6	0	-3.792009	-0.777643	-0.091295
12	7	0	-4.942430	-1.305058	-0.150502
13	6	0	-6.209129	-1.024733	0.012586
14	7	0	-7.388464	-0.872753	0.134508
15	6	0	0.855209	1.987637	2.597418
16	1	0	1.824449	2.103026	3.098928
17	7	0	1.020893	2.213916	-1.068631
18	7	0	1.429906	3.474460	-0.678588
19	6	0	0.952950	1.906307	-2.499290
20	7	0	1.403297	3.494632	0.666352
21	1	0	1.255770	2.803318	-3.044341
22	1	0	1.628200	1.081285	-2.749848
23	1	0	-0.067812	1.631003	-2.784759
24	1	0	0.491750	0.970915	2.780907
25	1	0	0.157477	2.694741	3.063378

Path 1,5 (CuBr)

I3

1	29	0	0.614093	0.519222	0.026484
2	35	0	2.861710	-0.390075	-0.044241
3	7	0	-0.686811	-1.355447	0.292687
4	7	0	-1.825188	-1.607965	0.110983
5	7	0	-3.073601	-1.542631	-0.157703
6	6	0	-0.862949	1.709008	0.001021
7	6	0	-1.832948	2.488982	-0.012567
8	6	0	-2.983776	3.414317	-0.018709
9	1	0	-3.965091	2.820489	-0.132081
10	1	0	-2.895819	4.159088	-0.896120
11	1	0	-3.024995	4.012637	0.968009
12	6	0	-3.808865	-2.841731	-0.081967
13	1	0	-4.846941	-2.612280	-0.336538
14	1	0	-3.424456	-3.584361	-0.798682
15	1	0	-3.780802	-3.281533	0.927369

TS34

1	29	0	-0.647385	0.299547	0.000009
2	35	0	-3.053754	-0.092756	0.000005
3	7	0	0.533958	-1.381526	-0.000038
4	7	0	1.745829	-1.552682	-0.000053
5	7	0	2.798346	-0.766550	-0.000092
6	6	0	0.943944	1.307053	0.000015
7	6	0	2.227967	1.233716	-0.000004
8	6	0	3.530841	1.963340	-0.000015
9	1	0	3.351582	3.045738	0.000004
10	1	0	4.132352	1.722292	-0.889323
11	1	0	4.132385	1.722268	0.889263
12	6	0	4.133372	-1.402580	0.000089
13	1	0	4.305002	-2.022776	-0.893288
14	1	0	4.865679	-0.589257	0.000027
15	1	0	4.304887	-2.022539	0.893654

I4

1	29	0	-0.872424	0.125302	-0.015484
2	35	0	-3.265501	-0.033082	0.015258
3	7	0	1.187903	-1.182331	-0.031710
4	7	0	2.452881	-1.606836	-0.022112
5	7	0	3.216060	-0.467003	0.026660
6	6	0	1.091741	0.252607	-0.036376
7	6	0	2.416213	0.680803	0.000430
8	6	0	3.000567	2.069243	-0.005700
9	1	0	2.261789	2.759556	-0.424949
10	1	0	3.918702	2.143834	-0.606835
11	1	0	3.240101	2.423806	1.013084
12	6	0	4.665908	-0.547633	0.040831
13	1	0	5.104675	0.021332	-0.790710
14	1	0	5.080347	-0.160377	0.982400
15	1	0	4.942732	-1.600964	-0.062941

TS4P

1	29	0	0.976777	-0.041481	-0.008059
2	35	0	3.345577	0.035516	0.025894
3	7	0	-2.228638	2.266997	-0.048696
4	7	0	-3.303671	1.676322	-0.052114
5	7	0	-3.356678	0.174964	-0.115077
6	6	0	-0.874367	-0.204191	-0.025391
7	6	0	-2.145685	-0.617136	-0.053100
8	6	0	-2.411189	-2.130374	-0.099981
9	1	0	-1.465085	-2.675430	-0.068880
10	1	0	-2.936574	-2.402763	-1.026934
11	1	0	-3.024909	-2.458900	0.750710
12	6	0	-4.678779	-0.362106	0.223542
13	1	0	-5.396753	0.445756	0.053797
14	1	0	-4.951881	-1.210967	-0.417593
15	1	0	-4.763507	-0.682940	1.277143

P

1	29	0	-0.834307	-0.251077	-0.000025
2	35	0	-3.192174	0.134456	0.000021
3	7	0	1.787050	-1.675562	-0.000001
4	7	0	3.114706	-1.466694	-0.000012
5	7	0	3.288792	-0.071987	-0.000037
6	6	0	1.074305	-0.449659	-0.000003
7	6	0	2.058471	0.561391	-0.000017
8	6	0	1.911756	2.055210	-0.000039
9	1	0	0.843668	2.294166	0.000026
10	1	0	2.364192	2.523116	-0.888941
11	1	0	2.364313	2.523156	0.888782
12	6	0	4.631668	0.481914	0.000081
13	1	0	5.333482	-0.356872	-0.000053
14	1	0	4.812161	1.099289	-0.891065
15	1	0	4.812141	1.098979	0.891448

Cu+C4DABCO+Br

1	29	0	-1.585356	0.011395	-0.244379
2	35	0	0.007427	2.003064	-0.137753

3	35	0	-0.007438	-1.996487	-0.150321
4	29	0	1.585346	-0.003890	-0.244373
5	7	0	-3.627507	0.007631	-0.264488
6	6	0	-4.154390	-1.229438	0.430554
7	6	0	-4.146968	0.013051	-1.686134
8	6	0	-4.160567	1.235230	0.442543
9	6	0	-5.701358	-1.249316	0.460131
10	1	0	-3.763663	-2.098358	-0.113810
11	1	0	-3.752607	-1.227266	1.451845
12	1	0	-3.753490	0.914919	-2.174282
13	1	0	-3.748292	-0.881567	-2.183225
14	6	0	-5.686548	0.008783	-1.709194
15	6	0	-5.707566	1.248214	0.470574
16	1	0	-3.773134	2.111402	-0.092642
17	1	0	-3.759792	1.224412	1.464193
18	1	0	-6.112398	-2.114630	-0.080091
19	1	0	-6.078471	-1.205005	1.489429
20	7	0	-6.256679	0.001040	-0.259275
21	1	0	-6.090104	0.920384	-2.174577
22	1	0	-6.085139	-0.900795	-2.182583
23	1	0	-6.121662	2.115848	-0.063611
24	1	0	-6.085738	1.194491	1.499014
25	6	0	-7.815167	-0.002685	-0.351119
26	6	0	-8.590815	-0.009352	0.974915
27	1	0	-8.058218	-0.894044	-0.943847
28	1	0	-8.062810	0.891703	-0.937386
29	6	0	-10.118229	-0.012812	0.703858
30	1	0	-8.337117	-0.893599	1.573236
31	1	0	-8.342067	0.872387	1.578960
32	6	0	-10.944127	-0.018889	2.006862
33	1	0	-10.384533	0.870905	0.104387
34	1	0	-10.379642	-0.894437	0.099192
35	1	0	-12.020121	-0.020886	1.792443
36	1	0	-10.720901	-0.907591	2.612323
37	1	0	-10.725234	0.867155	2.617753
38	7	0	3.627500	-0.003278	-0.264468
39	6	0	4.156847	1.225944	0.442501
40	6	0	4.146931	0.004044	-1.686117
41	6	0	4.158128	-1.238733	0.430624
42	6	0	5.703893	1.242946	0.471499
43	1	0	3.767389	2.100886	-0.093056
44	1	0	3.755559	1.214342	1.463935
45	1	0	3.751354	-0.892021	-2.183166
46	1	0	3.750332	0.904472	-2.174305
47	6	0	5.686517	0.004996	-1.709187
48	6	0	5.705059	-1.254587	0.459203
49	1	0	3.769399	-2.108885	-0.113368
50	1	0	3.756901	-1.237354	1.452141
51	1	0	6.116102	2.112343	-0.061203
52	1	0	6.081497	1.188927	1.500149
53	7	0	6.256680	-0.001903	-0.259278
54	1	0	6.088077	-0.903064	-2.183098
55	1	0	6.087088	0.918118	-2.174050
56	1	0	6.117964	-2.118130	-0.082501
57	1	0	6.082783	-1.210568	1.488272
58	6	0	7.815171	-0.000861	-0.351134
59	6	0	8.590841	-0.006338	0.974892
60	1	0	8.060221	0.894667	-0.936720

61	1	0	8.060796	-0.891080	-0.944542
62	6	0	10.118258	-0.005240	0.703834
63	1	0	8.339601	0.874199	1.579672
64	1	0	8.339648	-0.891788	1.572479
65	6	0	10.944171	-0.010322	2.006832
66	1	0	10.382135	-0.885528	0.098291
67	1	0	10.382090	0.879815	0.105245
68	1	0	12.020167	-0.009306	1.792413
69	1	0	10.722965	0.874586	2.618539
70	1	0	10.723268	-0.900159	2.611475

Cu+C4DABCO+2Br

1	29	0	-2.572097	0.010242	-0.207221
2	7	0	-0.041063	0.018488	-0.181637
3	6	0	0.576110	1.304366	-0.572863
4	6	0	0.577258	-1.102632	-0.921917
5	6	0	0.087618	-0.194282	1.279825
6	6	0	2.070311	1.338110	-0.099712
7	1	0	0.511603	1.403196	-1.660543
8	1	0	-0.010137	2.119497	-0.137076
9	1	0	0.101398	-2.030856	-0.592399
10	1	0	0.365475	-0.986648	-1.988596
11	6	0	2.128473	-1.108132	-0.678842
12	6	0	1.594196	-0.381052	1.652324
13	1	0	-0.496367	-1.078289	1.552830
14	1	0	-0.344930	0.671312	1.789500
15	1	0	2.758071	1.601525	-0.906298
16	1	0	2.227836	2.021427	0.741639
17	7	0	2.462065	-0.066841	0.409684
18	1	0	2.499583	-2.074079	-0.320203
19	1	0	2.686687	-0.820847	-1.573178
20	1	0	1.829498	-1.411839	1.937018
21	1	0	1.923242	0.293361	2.449405
22	6	0	3.938978	-0.123913	0.823020
23	6	0	4.973700	0.026574	-0.304129
24	1	0	4.074634	-1.086412	1.330829
25	1	0	4.073278	0.672167	1.565467
26	6	0	6.405694	0.043385	0.287187
27	1	0	4.897123	-0.803184	-1.018243
28	1	0	4.815623	0.957464	-0.864046
29	6	0	7.484377	0.181703	-0.806179
30	1	0	6.498025	0.876714	0.999787
31	1	0	6.578769	-0.881129	0.858144
32	1	0	8.488199	0.194428	-0.365249
33	1	0	7.441264	-0.655089	-1.515724
34	1	0	7.356653	1.112779	-1.373960
35	35	0	-2.762168	2.397494	0.008577
36	35	0	-2.656461	-2.396317	-0.021385

4Cu+4Br(cubic)

1	29	0	-0.927411	0.950336	1.064836
2	35	0	0.667012	-0.561983	2.473122
3	35	0	0.453171	2.540584	-0.471712
4	35	0	-2.548780	-0.515274	-0.357358

5	29	0	-0.431534	0.363887	-1.605210
6	29	0	-0.294193	-1.648473	0.307054
7	29	0	1.654177	0.333565	0.233122
8	35	0	1.427736	-1.462759	-1.643888

4Cu+4Br(square)

1	29	0	1.540201	1.776547	-0.017796
2	29	0	1.778933	-1.538614	0.003480
3	29	0	-1.539897	-1.778806	-0.000483
4	29	0	-1.779023	1.539183	0.001886
5	35	0	0.242036	-3.346281	-0.208331
6	35	0	3.347472	0.242077	0.213034
7	35	0	-0.241859	3.347276	-0.200544
8	35	0	-3.347827	-0.241672	0.206540

4Cu+6Br(chair)

1	29	0	-1.460710	0.464929	0.040236
2	35	0	0.649832	1.923032	-0.140299
3	35	0	-0.650198	-1.921741	0.142981
4	35	0	-3.742662	1.574817	0.121526
5	29	0	-5.732526	0.248700	0.004567
6	29	0	1.460177	-0.463729	-0.038601
7	35	0	3.741929	-1.574012	-0.121848
8	29	0	5.732826	-0.249398	-0.005692
9	35	0	-7.833500	-0.816557	-0.080471
10	35	0	7.834794	0.814045	0.077688

Cu+C4DABCO+N(CN)2(C)

1	29	0	2.389136	0.016209	-0.032546
2	7	0	4.241322	0.198880	-0.195360
3	6	0	4.789978	1.418265	0.001165
4	6	0	4.985047	-0.885966	-0.505806
5	7	0	5.170962	2.526755	0.193111
6	7	0	5.547362	-1.895423	-0.780165
7	7	0	0.424376	-0.154219	0.150431
8	6	0	-0.189969	-0.600036	-1.158295
9	6	0	-0.172445	1.181027	0.539716
10	6	0	0.081472	-1.168413	1.218883
11	6	0	-1.703120	-0.917953	-0.962560
12	1	0	-0.041029	0.198252	-1.890022
13	1	0	0.339382	-1.485640	-1.517282
14	1	0	0.184227	1.431983	1.542097
15	1	0	0.194139	1.948104	-0.146411
16	6	0	-1.728786	1.111905	0.487319
17	6	0	-1.449629	-1.144860	1.501987
18	1	0	0.639055	-0.931214	2.127766
19	1	0	0.409716	-2.151556	0.871778
20	1	0	-2.313072	-0.464215	-1.745119
21	1	0	-1.901410	-1.993376	-0.944075
22	7	0	-2.164630	-0.356841	0.390006
23	1	0	-2.187031	1.536977	1.384358
24	1	0	-2.130349	1.628238	-0.386410
25	1	0	-1.687814	-0.647216	2.446246

26	1	0	-1.875634	-2.151441	1.522777
27	6	0	-3.697934	-0.514555	0.574241
28	6	0	-4.581132	0.350975	-0.337233
29	1	0	-3.894306	-0.282834	1.627643
30	1	0	-3.905161	-1.578866	0.411620
31	6	0	-6.076747	0.012877	-0.091520
32	1	0	-4.429010	1.419180	-0.136502
33	1	0	-4.357584	0.175272	-1.398262
34	6	0	-7.011344	0.868009	-0.971031
35	1	0	-6.251072	-1.053026	-0.299243
36	1	0	-6.321120	0.175522	0.968502
37	1	0	-8.059516	0.614453	-0.778186
38	1	0	-6.885350	1.938890	-0.765851
39	1	0	-6.820098	0.700749	-2.038937

Cu+C4DABCO+N(CN)2(T)

1	29	0	2.033867	0.069968	0.010313
2	7	0	0.071738	0.260956	0.006009
3	6	0	-0.523827	-0.411514	1.221948
4	6	0	-0.506127	-0.378701	-1.236150
5	6	0	-0.313240	1.722258	0.022604
6	6	0	-2.047884	-0.097771	1.320315
7	1	0	-0.342264	-1.485850	1.135766
8	1	0	-0.004932	-0.055670	2.114762
9	1	0	-0.163302	0.193562	-2.102086
10	1	0	-0.109708	-1.392288	-1.329376
11	6	0	-2.062765	-0.414343	-1.153031
12	6	0	-1.849219	1.871413	-0.188903
13	1	0	0.231636	2.242401	-0.768287
14	1	0	0.002739	2.144863	0.979775
15	1	0	-2.631602	-0.998301	1.517598
16	1	0	-2.270019	0.639700	2.097114
17	7	0	-2.526179	0.500708	-0.010864
18	1	0	-2.530771	-0.059919	-2.075480
19	1	0	-2.435668	-1.416967	-0.936038
20	1	0	-2.095759	2.217296	-1.196632
21	1	0	-2.296352	2.558930	0.533922
22	6	0	-4.065198	0.698406	-0.019340
23	6	0	-4.909946	-0.584628	-0.038152
24	1	0	-4.280393	1.309315	-0.903875
25	1	0	-4.289648	1.293872	0.873550
26	6	0	-6.418047	-0.222645	0.037899
27	1	0	-4.735758	-1.157102	-0.958071
28	1	0	-4.668400	-1.236862	0.812002
29	6	0	-7.312343	-1.478734	0.006155
30	1	0	-6.613676	0.343713	0.960265
31	1	0	-6.681303	0.435973	-0.802678
32	1	0	-8.370212	-1.199609	0.062542
33	1	0	-7.167992	-2.049405	-0.920180
34	1	0	-7.098420	-2.143431	0.853078
35	7	0	3.820425	-0.109673	0.004093
36	6	0	5.026038	-0.231187	0.001467
37	7	0	6.247195	-0.355883	-0.002734
38	6	0	7.528370	-0.483697	-0.004242
39	7	0	8.714648	-0.602740	-0.006528

Cu+C4DABCO+2N(CN)2(T)

1	6	0	0.449116	4.807273	-0.151044
2	6	0	-1.574864	3.618039	-0.239937
3	29	0	-2.886775	0.931347	-0.106696
4	7	0	-3.450457	-0.817286	0.082976
5	6	0	-3.773650	-1.966028	0.185076
6	7	0	-4.019510	-3.210877	0.320790
7	6	0	-5.000355	-3.970929	-0.127640
8	7	0	-5.853885	-4.716768	-0.508278
9	7	0	-0.082936	0.210186	-0.008849
10	6	0	0.803680	0.902412	-0.972060
11	6	0	0.034230	-1.257878	-0.157647
12	6	0	0.276075	0.610604	1.370996
13	6	0	2.261924	0.339247	-0.858269
14	1	0	0.423013	0.772624	-1.988540
15	1	0	0.808573	1.968336	-0.736846
16	1	0	-0.741006	-1.745810	0.437247
17	1	0	-0.142095	-1.519129	-1.205126
18	6	0	1.458085	-1.729693	0.301746
19	6	0	1.806555	0.379730	1.601328
20	1	0	-0.322866	0.021835	2.071824
21	1	0	0.028416	1.664609	1.519914
22	1	0	2.512892	-0.334549	-1.680626
23	1	0	3.012324	1.133519	-0.802561
24	7	0	2.358934	-0.484615	0.440405
25	1	0	1.442215	-2.212403	1.283972
26	1	0	1.925249	-2.405850	-0.416940
27	1	0	2.023034	-0.155027	2.530973
28	1	0	2.372503	1.316152	1.585527
29	6	0	3.811640	-0.866474	0.768069
30	6	0	4.596404	-1.577467	-0.345834
31	1	0	3.760972	-1.501840	1.660470
32	1	0	4.313259	0.068380	1.044867
33	6	0	6.016394	-1.943970	0.154333
34	1	0	4.088231	-2.497430	-0.663948
35	1	0	4.692424	-0.931798	-1.227764
36	6	0	6.848319	-2.652083	-0.933820
37	1	0	6.538219	-1.031504	0.479232
38	1	0	5.938492	-2.595239	1.037629
39	1	0	7.848256	-2.901330	-0.559868
40	1	0	6.369188	-3.586042	-1.255230
41	1	0	6.972017	-2.013479	-1.818243
42	7	0	-2.321710	2.684287	-0.296801
43	7	0	1.632362	4.977597	-0.157798
44	7	0	-0.866819	4.688936	-0.125809

Cu+C4DABCO+2N(CN)2(T+C)

1	6	0	1.653362	2.741052	0.187443
2	6	0	0.033408	4.491854	-0.221545
3	29	0	3.468071	0.369984	0.086924
4	7	0	-0.546062	5.467955	-0.588817
5	7	0	2.594272	2.000459	0.228675
6	7	0	0.532189	3.361292	0.239222
7	7	0	-0.022069	-0.653109	0.633833
8	6	0	-0.753019	0.358799	1.429316

9	6	0	-0.649359	-1.985958	0.782645
10	6	0	-0.008909	-0.278638	-0.800941
11	6	0	-2.277251	0.348257	1.050293
12	1	0	-0.635439	0.136093	2.494068
13	1	0	-0.328435	1.345743	1.234687
14	1	0	-0.009246	-2.729578	0.299933
15	1	0	-0.716945	-2.224411	1.848837
16	6	0	-2.079819	-1.976656	0.129947
17	6	0	-1.469681	-0.006119	-1.287345
18	1	0	0.447750	-1.101161	-1.357378
19	1	0	0.599420	0.615061	-0.944420
20	1	0	-2.897878	-0.097230	1.831527
21	1	0	-2.655267	1.347869	0.815055
22	7	0	-2.455990	-0.519486	-0.210714
23	1	0	-2.106769	-2.529758	-0.814617
24	1	0	-2.849448	-2.371252	0.796975
25	1	0	-1.711906	-0.524390	-2.220378
26	1	0	-1.673032	1.062837	-1.404675
27	6	0	-3.879888	-0.417546	-0.775849
28	6	0	-5.028423	-0.740534	0.193458
29	1	0	-3.910752	-1.096764	-1.636490
30	1	0	-3.982061	0.608130	-1.149780
31	6	0	-6.386611	-0.652576	-0.547002
32	1	0	-4.921729	-1.750060	0.611988
33	1	0	-5.041047	-0.035163	1.033936
34	6	0	-7.576987	-0.966037	0.381672
35	1	0	-6.508253	0.355216	-0.970995
36	1	0	-6.389063	-1.354323	-1.394572
37	1	0	-8.525689	-0.897650	-0.163707
38	1	0	-7.501679	-1.980173	0.796017
39	1	0	-7.623081	-0.260356	1.221568
40	7	0	4.027864	-1.440925	-0.161028
41	6	0	5.310364	-1.837772	-0.034788
42	6	0	3.047694	-2.299239	-0.472529
43	7	0	6.460496	-2.107282	0.094381
44	7	0	2.088899	-2.954840	-0.740839