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SUPPLEMENTARY INFORMATION

Copper-catalysed electrophilic carboamination of cyclopropenes with arylboron reagents – A computational mechanistic probe

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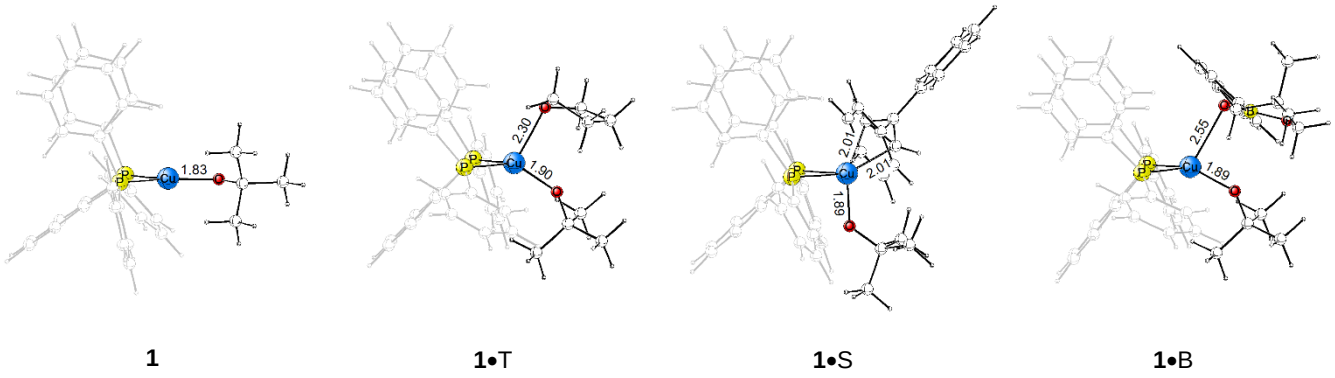


1 **1**•T **1**•S **1**•B

Fig. S1 Selected structural parameter (angstroms) of the optimised structures of various forms of {P^P}Cu^{I} butoxide **1**.

The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.

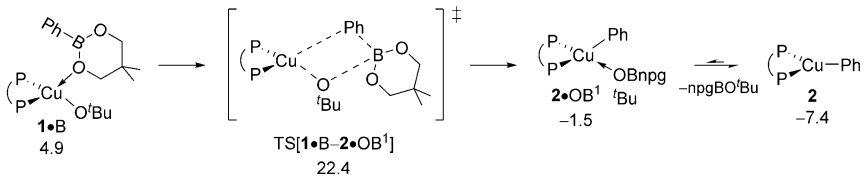
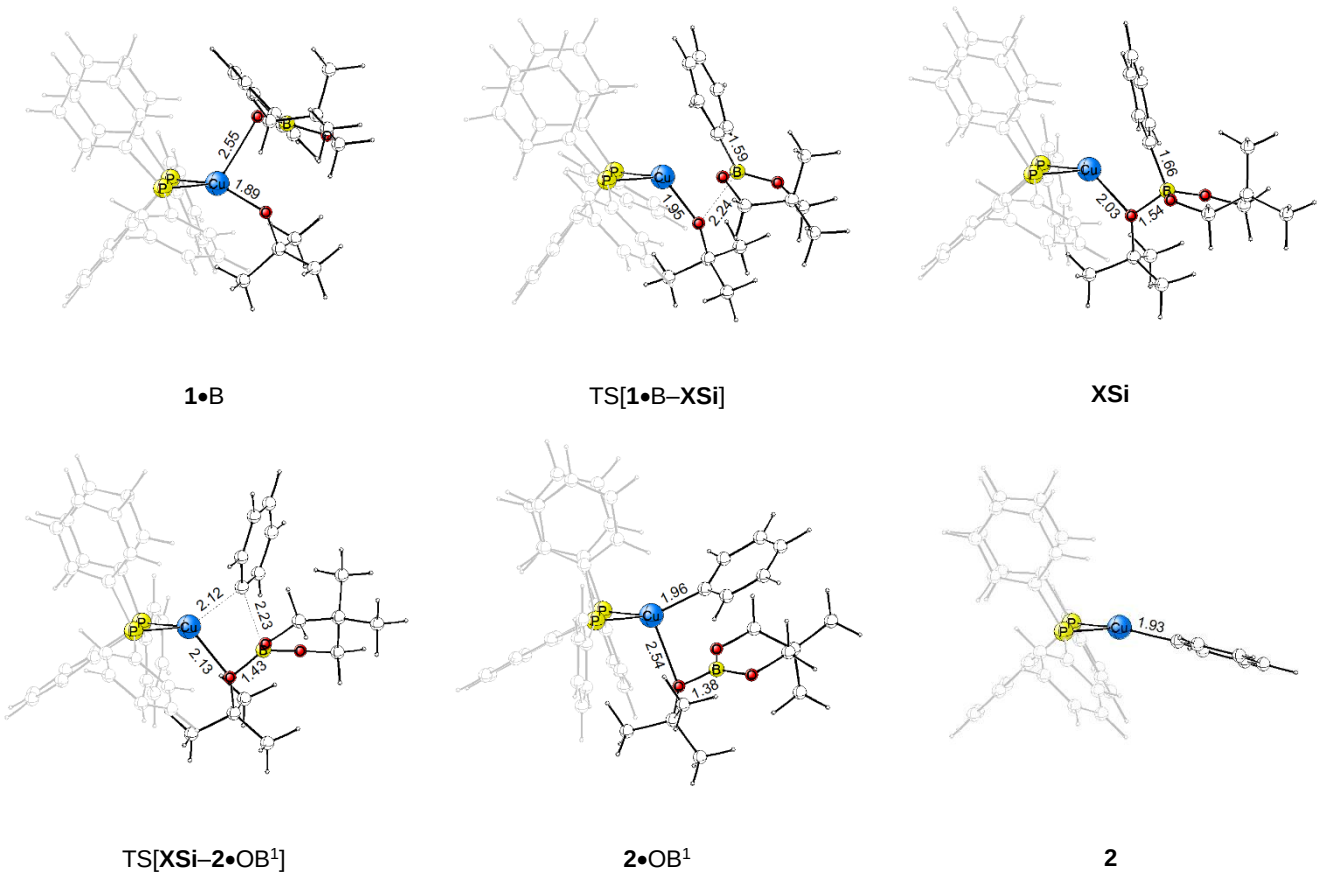


Fig. S2 Single-step transmetalation of {P^P}Cu^{I} alkoxide **1** with Ph-Bnpg. Free energies are given in kcal mol^{-1}, relative to {**1** + B}.

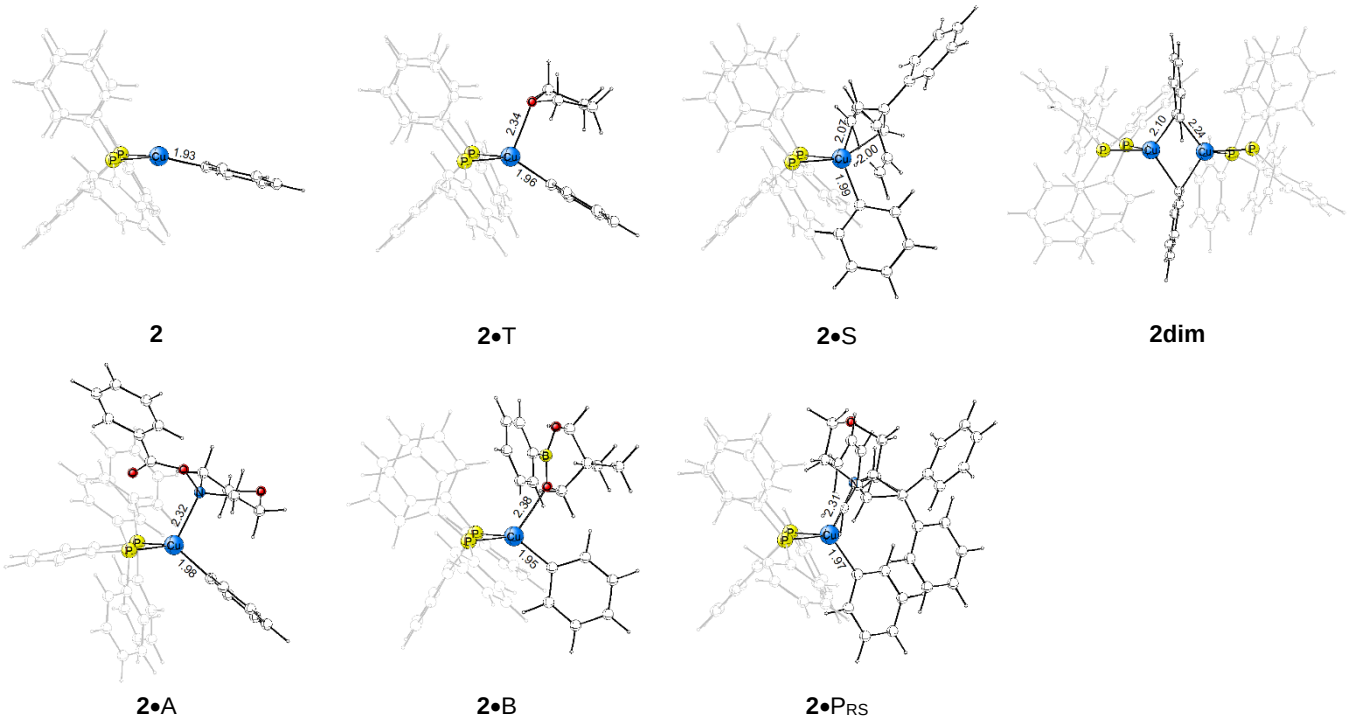


1•B TS[**1**•B–**XSi**] **XSi**

TS[**XSi**–**2**•OB[1]] **2**•OB[1] **2**

Fig. S3 Selected structural parameter (angstroms) of the optimised structures of key stationary points for stepwise transmetalation of {P^P}Cu[I] butoxide **1** with Ph-Bnpg via transient borate intermediate **XSi**.

The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.

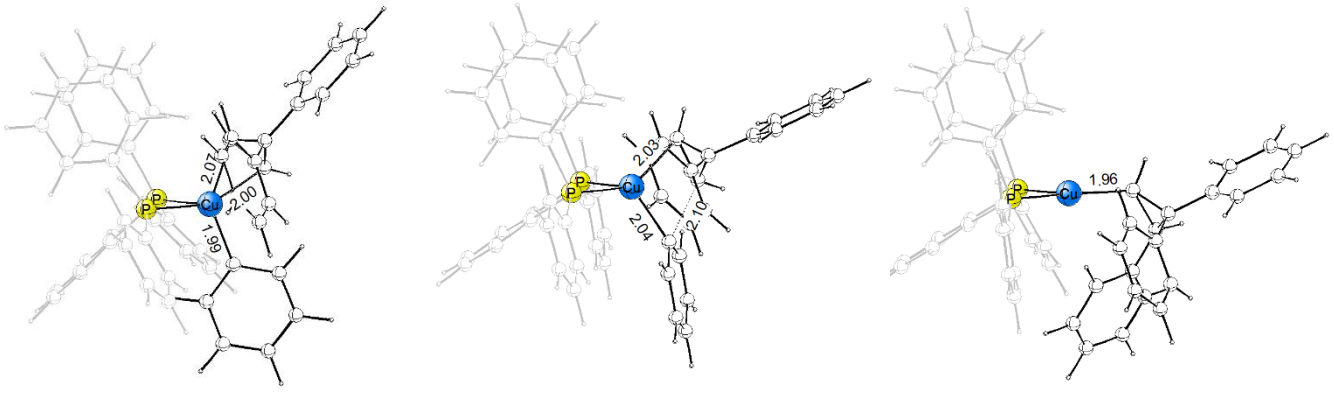


2 **2**•T **2**•S **2dim**

2•A **2**•B **2**•P[RS]

Fig. S4 Selected structural parameter (angstroms) of the optimised structures of various forms of the catalytically competent {P^P}Cu[I] phenyl **2**.

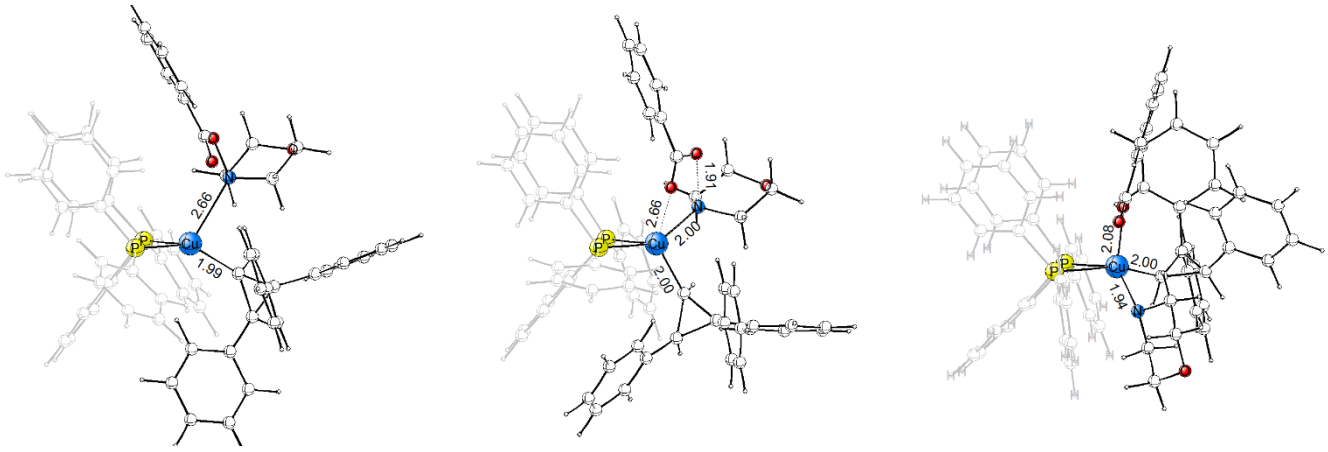
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



2•S TS[**2**•S–**3**] **3**

Fig. S5 Selected structural parameter (angstroms) of the optimised structures of key stationary points for cyclopropene S insertion into the Cu–C_{phenyl} linkage at cyclopropene adduct **2**•S of the {P^P}Cu^{I} phenyl.

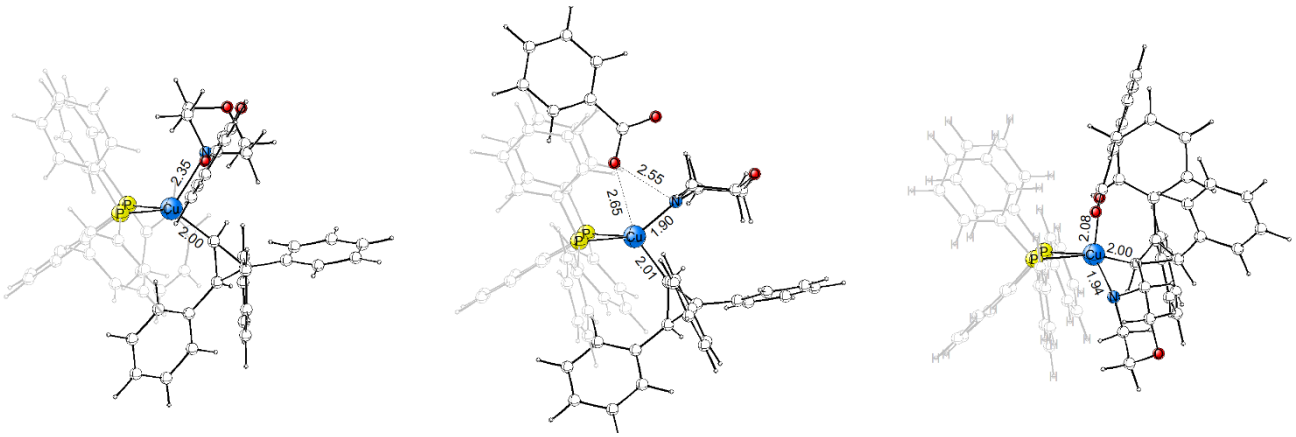
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



$\mathbf{3}_1$•A TS[$\mathbf{3}_1$•A–**4**] **4**

Fig. S6 Selected structural parameter (angstrom) of the optimised structures of key stationary points for S_N2-type displacement of the O-benzoylhydroxylamine's benzoate leaving group evolving through a multi-centre TS structure at amine adduct **2**•A of the phenylcopper.

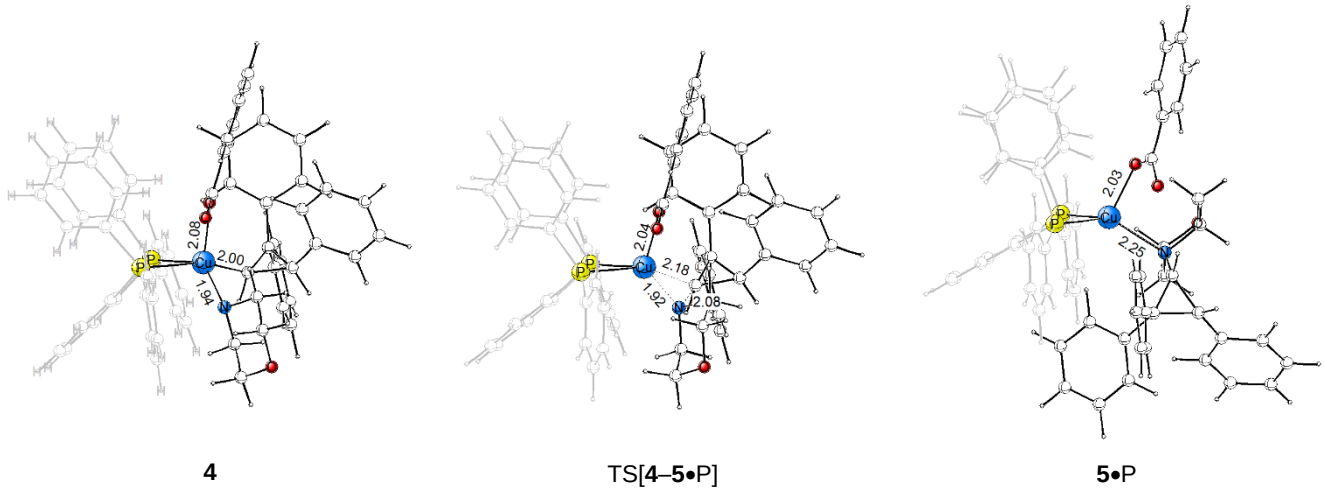
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



$\mathbf{3}_2$•A TS_{OA}[$\mathbf{3}_2$•A–**4**] **4**

Fig. S7 Selected structural parameter (angstrom) of the optimised structures of key stationary points for three-centred cyclic oxidative addition of O-benzoylhydroxylamine at amine adduct **2**•A of the phenylcopper.

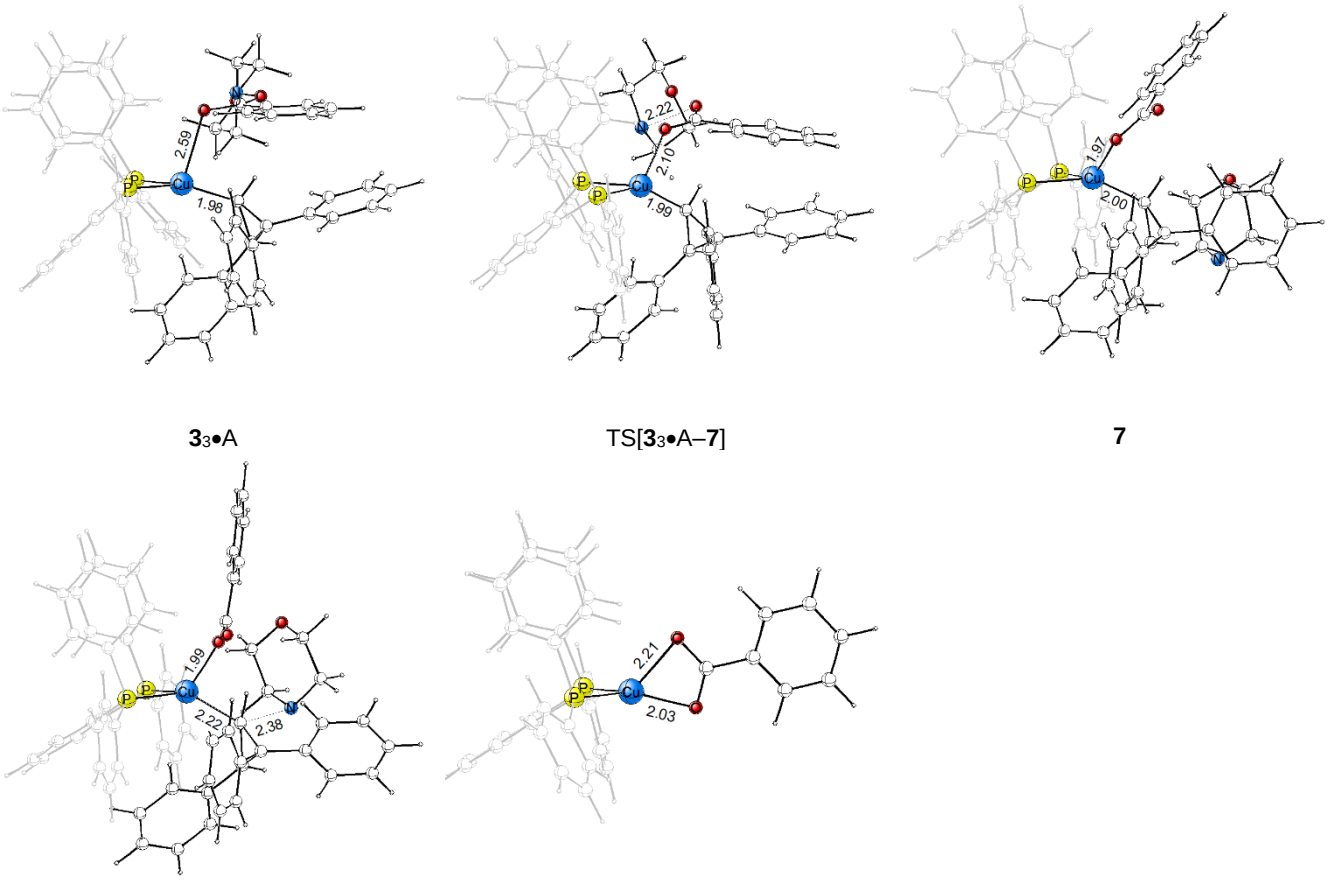
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



4 TS[**4**–**5**•P] **5**•P

Fig. S8 Selected structural parameter (angstrom) of the optimised structures of key stationary points for N–C bond forming reductive elimination at formal {P^P}Cu^{III} intermediate **4**.

The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.

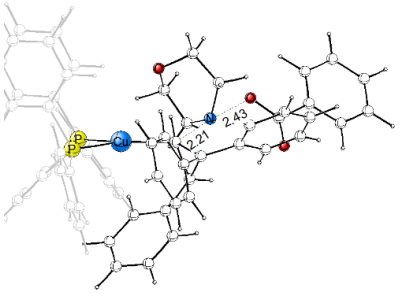


3$_3$•A TS[**3**$_3$•A–**7**] **7**

TS[**7**–**5**] **5**

Fig. S9 Selected structural parameter (angstrom) of the optimised structures of key stationary points for backside S_N2-attack of aminating agent A at {P^P}Cu^{I} cyclopropyl **3** to deliver 2-arylcyclopropylamine product P through N–O bond cleavage and subsequent N–C generation via *anti* morpholido approach.

The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



TS[**3**+A–**5**+P]

Fig. S10 Selected structural parameter (angstrom) of the optimised structures of key stationary points for backside S_N2-attack of aminating agent A at {P^P}Cu^I cyclopropyl **3** where morpholido displacement and N–C bond formation take place concurrently.

The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.

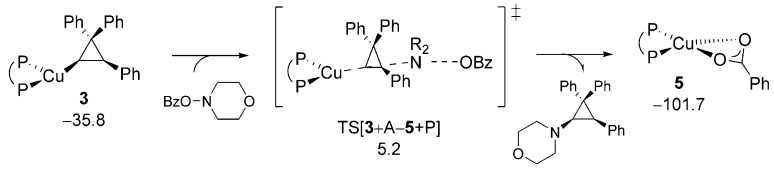
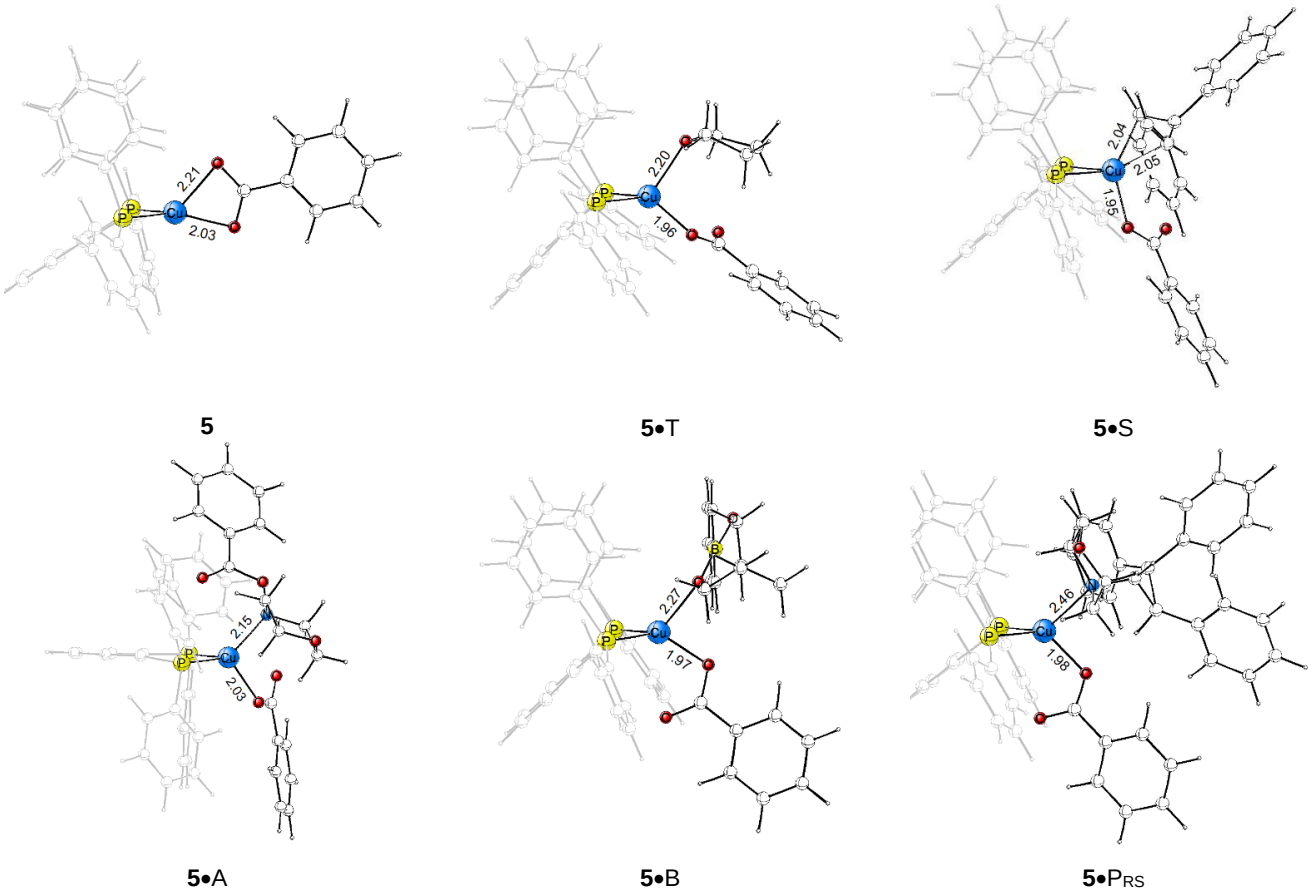


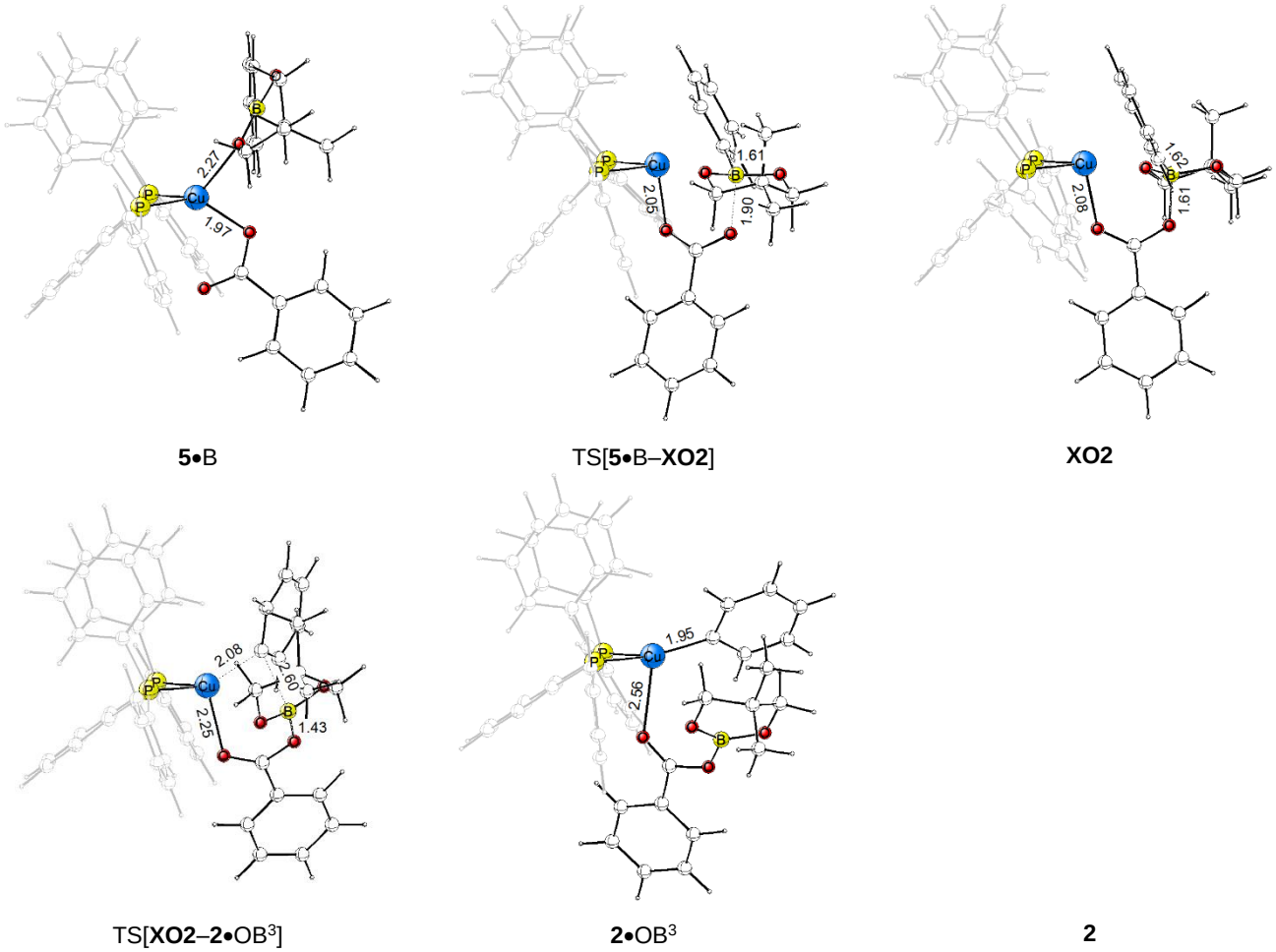
Fig. S11 Rival stereoinvertive pathway through *anti*-S_N2-attack of the hydroxylamine ester at {P^P}Cu^I cyclopropyl **3** to afford 2-arylcyclopropylamine product P in a single step. Free energies are given in kcal mol^{-1}, relative to {½×**2dim** + reactants}.



5 **5•T** **5•S**

5•A **5•B** **5•P$_{RS}$**

Fig. S12 Selected structural parameter (angstrom) of the optimised structures of various forms of {P^P}Cu^I benzoate **5**. The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



5•B TS[**5**•B–**XO2**] **XO2**

TS[**XO2**–**2**•OB^3] **2**•OB^3 **2**

Fig. S13 Selected structural parameter (angstrom) of the optimised structures of key stationary points for transmetalation of {P^P}Cu^I benzoate **5** with phenylboronate B.

The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.

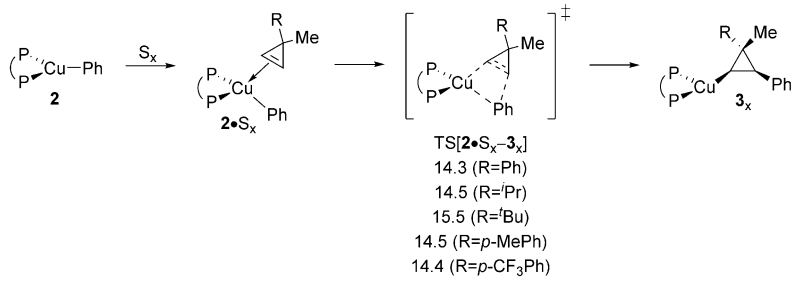


Fig. S14 Insertion of 3,3-Me,R-substituted cyclopropenes S_x into the Cu–C_{aryl} linkage at adduct **2**•S_x of the {P^P}Cu^{I} phenyl. Free energies are given in kcal mol^{-1}, relative to {½×**2dim** + S_x}.

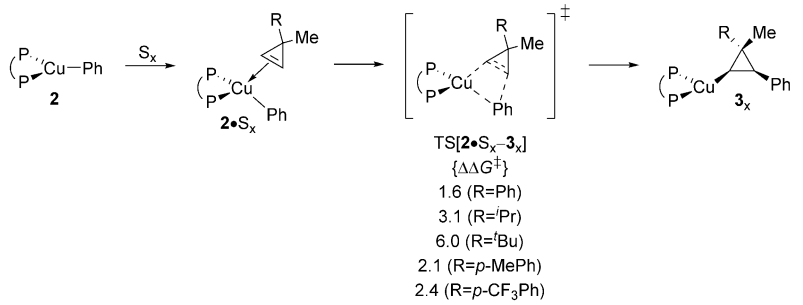


Fig. S15 Kinetic gap ($\Delta\Delta G^{‡}$) between diastereoisomeric pathways for insertion of 3,3-Me,R-substituted cyclopropenes into the Cu–C_{aryl} linkage at adduct **2**•S of the {P^P}Cu^{I} phenyl. Free energies are given in kcal mol^{-1}.

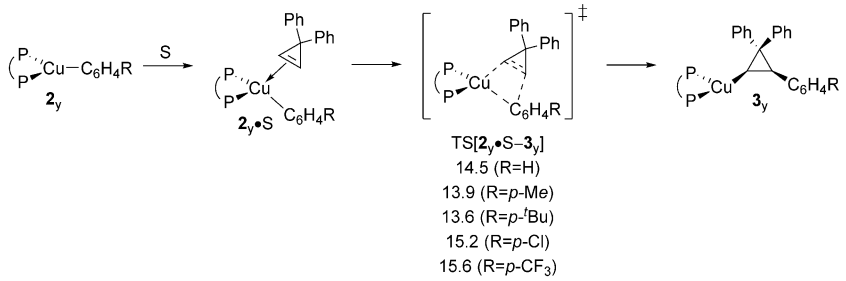


Fig. S16 Cyclopropene S insertion into the Cu–C_{aryl} linkage at the cyclopropene adduct **2**$_y$•S of the {P^P}Cu^{I} aryl. Free energies are given in kcal mol^{-1}, relative to {½×**2**$_y$**dim** + S}.

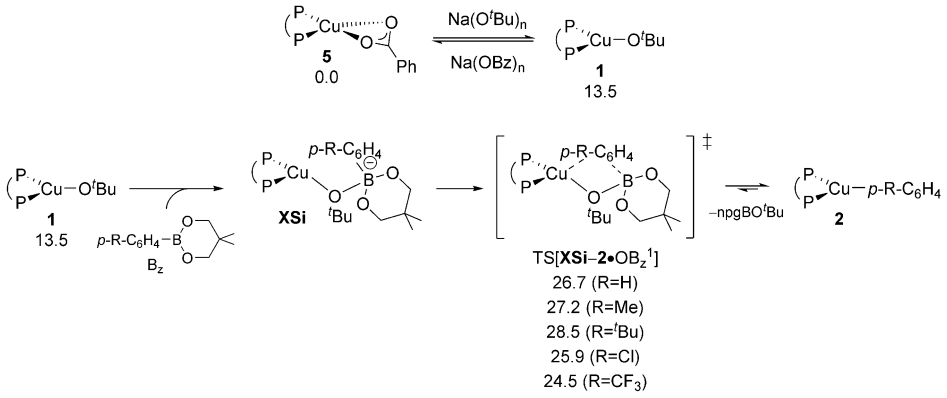


Fig. S17 Salt metathesis of {P^P}Cu^{I} benzoate **5** with Na(O^{t}Bu) base with consecutive transmetalation of the thus generated {P^P}Cu^{I} butoxide **1** with various arylboronates B_z. Free energies are given in kcal mol^{-1} relative to {**5** + reactants}.

Cartesian coordinates (in Å) of located key structures

1
E_t = -3713.522555 a.u.

Cu	1.393518	-0.249566	-0.132493
P	-0.320927	-0.381222	1.281896
P	-0.125152	-0.116672	-1.775656
C	-1.619971	-1.233457	0.286597
C	-1.531558	-1.103586	-1.115248
C	-2.469968	-1.742534	-1.927353
C	-3.489118	-2.500588	-1.361409
C	-3.579030	-2.626424	0.022542
C	-2.648847	-1.996419	0.842158
H	-2.392660	-1.655744	-3.007902
H	-4.210064	-2.999886	-2.002424
H	-4.371075	-3.223583	0.465476
H	-2.708544	-2.113433	1.921131
C	-1.055183	1.270378	1.606084
C	-0.373577	-1.245383	2.893718
C	-0.796327	1.580781	-1.949542
C	0.059625	-0.692054	-3.505651
C	-2.392310	1.432855	1.979477
C	-2.918100	2.707247	2.154360
C	-2.115094	3.827582	1.952058
C	-0.784360	3.671879	1.579459
C	-0.254943	2.397284	1.405687
H	-3.025481	0.561140	2.124531
H	-3.958742	2.827509	2.442294
H	-2.530724	4.823208	2.079867
H	-0.157968	4.542643	1.410558
H	0.781010	2.270823	1.096819
C	-0.590295	-0.577414	4.101464
C	-0.508158	-1.268376	5.307384
C	-0.211098	-2.626615	5.320263
C	0.015278	-3.295978	4.118923
C	-0.053699	-2.609774	2.914622
H	-0.821896	0.483684	4.101194
H	-0.677477	-0.738981	6.240707
H	-0.146671	-3.162405	6.262745
H	0.259850	-4.354235	4.121743
H	0.145727	-3.133086	1.981756
C	-2.117965	1.915761	-1.650434
C	-2.536406	3.241096	-1.726096
C	-1.645108	4.236760	-2.110266
C	-0.325645	3.906756	-2.412894
C	0.101586	2.588521	-2.322058
H	-2.818398	1.143877	-1.344284
H	-3.563356	3.494031	-1.478386
H	-1.974426	5.270377	-2.167468
H	0.376999	4.681098	-2.707248
H	1.139295	2.336040	-2.530398
C	-0.659213	-0.144895	-4.572562
C	-0.472075	-0.633936	-5.861144
C	0.430662	-1.668535	-6.092451
C	1.155780	-2.209028	-5.033992
C	0.979111	-1.717777	-3.745540
H	-1.358707	0.667931	-4.394198
H	-1.030763	-0.203703	-6.687544
H	0.577802	-2.045552	-7.100553
H	1.873798	-3.003693	-5.214251
H	1.569152	-2.111971	-2.920659
C	5.507766	-0.363427	0.375164
C	4.059176	-0.419700	0.883775
O	3.217362	-0.267007	-0.231365
C	3.806525	-1.772671	1.568468
C	3.826912	0.713012	1.897228
H	5.685670	0.595174	-0.123322
H	5.670819	-1.160854	-0.357221
H	6.233539	-0.477885	1.189275
H	4.514477	0.655052	2.750510
H	2.799076	0.659238	2.280590
H	3.961372	1.681691	1.402672
H	2.777015	-1.808024	1.948201
H	4.489202	-1.945709	2.410110
H	3.932976	-2.581643	0.840509

1•T
E_t = -3945.927029 a.u.

Cu	1.002642	0.030460	0.017386
P	-0.776064	-0.125027	1.416097
P	-0.462117	0.158364	-1.664671
C	-1.825934	-1.206543	0.354793
C	-1.714686	-1.054314	-1.042967
C	-2.521602	-1.828434	-1.879612
C	-3.407817	-2.757050	-1.344469
C	-3.498530	-2.922483	0.034344
C	-2.713523	-2.145653	0.879155
H	-2.440697	-1.719682	-2.957574
H	-4.022209	-3.359068	-2.008074
H	-4.180197	-3.657156	0.453263
H	-2.781384	-2.277085	1.955515
C	-1.928427	1.227654	1.878532
C	-0.545879	-1.042502	2.984300
C	-1.430441	1.721692	-1.749215
C	-0.243524	-0.306938	-3.426415
C	-3.126791	1.457860	1.196989
C	-3.905399	2.570780	1.498220
C	-3.506165	3.462019	2.487642
C	-2.319090	3.232935	3.181003
C	-1.532904	2.130255	2.875015
H	-3.452071	0.770789	0.422045
H	-4.829133	2.738796	0.951778
H	-4.116468	4.329426	2.721899
H	-2.002833	3.918304	3.962380
H	-0.610997	1.958553	3.425914
C	-1.501652	-1.078078	4.005881
C	-1.249646	-1.798960	5.167720
C	-0.045529	-2.483789	5.317747
C	0.911650	-2.438061	4.308484
C	0.671445	-1.714739	3.143896
H	-2.435134	-0.531605	3.896057
H	-1.993591	-1.824679	5.959146
H	0.148698	-3.044874	6.227754
H	1.857726	-2.958195	4.430449
H	1.425047	-1.649855	2.354874
C	-2.686829	1.782322	-2.360552
C	-3.416030	2.964651	-2.343052
C	-2.897737	4.094697	-1.712894
C	-1.648463	4.039797	-1.105682
C	-0.915145	2.856330	-1.120045
H	-3.097585	0.900172	-2.845815
H	-4.393109	3.004383	-2.816764
H	-3.473183	5.016121	-1.692313
H	-1.245987	4.915967	-0.605695
H	0.052919	2.802154	-0.627062
C	-0.320189	0.640653	-4.452184
C	-0.019953	0.284468	-5.763744
C	0.360560	-1.017732	-6.069213
C	0.449367	-1.964985	-5.051419
C	0.160486	-1.612308	-3.740089
H	-0.617880	1.660564	-4.226802
H	-0.086649	1.031360	-6.549844
H	0.593053	-1.293622	-7.093629
H	0.754466	-2.982651	-5.277718
H	0.249691	-2.357091	-2.953293
C	1.786399	-3.176730	-0.301182
C	2.926800	-2.144850	-0.236726
O	2.528465	-1.003289	0.470277
C	4.119809	-2.766308	0.508943
C	3.360882	-1.772920	-1.665085
H	1.499028	-3.486301	0.710240
H	2.063498	-4.072473	-0.871672
H	0.903839	-2.721088	-0.768304
H	3.673979	-2.647528	-2.249661
H	4.199671	-1.067940	-1.624391
H	2.531568	-1.284026	-2.190966
H	3.820807	-3.027265	1.530509
H	4.936767	-2.038972	0.570985
H	4.493375	-3.669741	0.011766
O	2.099023	2.027055	0.340550
C	2.383153	2.315674	1.722535
H	1.499894	2.029615	2.300714
H	2.559120	3.398345	1.839115
C	3.630159	1.500455	2.035374

1•T (cont)

H	4.187251	1.905092	2.885891
H	3.347411	0.463493	2.235681
C	4.423450	1.561206	0.713217
H	5.240832	2.288023	0.763659
H	4.833024	0.577981	0.473280
C	3.380604	1.990107	-0.336499
H	3.591218	2.993736	-0.734135
H	3.281395	1.280281	-1.161588

1•S

E_t = -4292.097626 a.u.

Cu	0.835340	-0.351309	-0.332313
P	-1.127452	-0.462356	0.992799
P	-0.946132	-0.228054	-2.127855
C	-2.249966	-1.516146	-0.014609
C	-2.212372	-1.354968	-1.409874
C	-3.097681	-2.083918	-2.208360
C	-3.994251	-2.976744	-1.634680
C	-4.008879	-3.157615	-0.254316
C	-3.143083	-2.428278	0.551138
H	-3.071136	-1.962228	-3.287450
H	-4.673716	-3.540389	-2.267623
H	-4.694817	-3.869346	0.196469
H	-3.148113	-2.577347	1.627580
C	-2.186660	1.015389	1.266752
C	-1.068901	-1.347060	2.587994
C	-1.841221	1.353458	-2.371513
C	-0.748461	-0.914947	-3.814361
C	-1.632363	2.278291	1.054324
C	-2.410387	3.422713	1.195858
C	-3.751160	3.313230	1.546800
C	-4.314696	2.055855	1.753023
C	-3.539010	0.911611	1.609014
H	-0.591020	2.354906	0.759017
H	-1.969873	4.399126	1.015847
H	-4.361791	4.205889	1.651098
H	-5.364086	1.965844	2.019715
H	-3.990059	-0.066878	1.752372
C	-1.632237	-0.866013	3.769447
C	-1.522289	-1.608188	4.942670
C	-0.845686	-2.822850	4.943362
C	-0.269480	-3.296912	3.765646
C	-0.373573	-2.563916	2.591239
H	-2.148556	0.089321	3.779205
H	-1.964635	-1.229845	5.860222
H	-0.763162	-3.399107	5.860802
H	0.267729	-4.241499	3.763247
H	0.082858	-2.910629	1.664324
C	-3.183001	1.530330	-2.024427
C	-3.777118	2.783246	-2.132571
C	-3.045456	3.871021	-2.597050
C	-1.709573	3.703297	-2.953072
C	-1.108230	2.456527	-2.829755
H	-3.761644	0.689160	-1.654373
H	-4.817293	2.908483	-1.845684
H	-3.512452	4.848342	-2.679107
H	-1.131216	4.547326	-3.318176
H	-0.061170	2.333931	-3.100464
C	-0.974003	-0.191444	-4.986954
C	-0.744168	-0.783945	-6.226151
C	-0.293632	-2.097498	-6.305170
C	-0.071704	-2.823230	-5.136362
C	-0.291135	-2.236761	-3.897505
H	-1.343773	0.828581	-4.937320
H	-0.927921	-0.215702	-7.133710
H	-0.118213	-2.556440	-7.273895
H	0.279140	-3.850180	-5.189357
H	-0.116175	-2.793182	-2.979533
C	2.577107	0.646014	-0.348169
C	1.530702	1.532859	-0.351641
C	2.487120	1.604601	0.824940
C	2.054869	1.159127	2.191927
C	3.485755	2.729126	0.798573
H	3.404491	0.389829	-0.999695
H	1.124294	2.289522	-1.014891
C	3.842170	3.338196	-0.413652
C	5.388032	4.804102	0.718940
C	4.112799	3.177771	1.967993
C	5.052304	4.201555	1.927150
H	5.526845	4.528712	2.848204
H	3.862877	2.716835	2.918163
C	4.777978	4.364888	-0.451821
H	3.388163	2.999986	-1.340338
H	6.121654	5.604432	0.688996
H	5.034861	4.821510	-1.403766
C	2.500206	-0.040706	2.740057
C	1.327091	0.422215	4.795144
C	1.241206	1.991065	2.967291
C	0.877419	1.626246	4.257419
H	0.240330	2.281988	4.844896

1•S (cont)

H	0.909353	2.942310	2.558191
C	2.135644	-0.411230	4.031991
H	3.136523	-0.686833	2.145802
H	1.037502	0.130429	5.800320
H	2.482135	-1.356543	4.439807
C	3.068621	-2.905047	0.447632
C	2.064001	-3.041942	-0.706254
O	0.930189	-2.236101	-0.501751
C	2.781108	-2.700202	-2.023149
C	1.563024	-4.495293	-0.765031
H	2.561476	-3.053718	1.407800
H	3.504572	-1.900657	0.437858
H	3.885013	-3.632931	0.364898
H	0.814896	-4.600372	-1.558344
H	1.085575	-4.765974	0.183388
H	2.380792	-5.199567	-0.958627
H	3.059205	-1.641147	-2.031933
H	2.128743	-2.880020	-2.882184
H	3.693072	-3.295983	-2.152508

1•B

E_t = -4316.996615 a.u.

Cu	0.458811	-0.386335	0.123580
P	-1.264489	-0.598156	1.610051
P	-1.075105	-0.305357	-1.479966
C	-2.232949	-1.787080	0.587371
C	-2.177480	-1.635842	-0.815631
C	-2.914182	-2.502861	-1.624382
C	-3.676922	-3.519184	-1.058557
C	-3.711104	-3.681810	0.323118
C	-2.993197	-2.816198	1.141482
H	-2.873575	-2.395209	-2.704812
H	-4.238362	-4.191780	-1.700958
H	-4.295299	-4.483863	0.764997
H	-3.014450	-2.945892	2.220199
C	-2.505163	0.671793	2.070845
C	-0.939845	-1.450571	3.198334
C	-2.190357	1.155949	-1.466007
C	-0.878941	-0.723921	-3.252252
C	-3.807647	0.688428	1.566613
C	-4.669236	1.733416	1.886390
C	-4.245693	2.765049	2.716546
C	-2.948779	2.751941	3.226880
C	-2.081521	1.718530	2.899740
H	-4.147656	-0.109832	0.913599
H	-5.676413	1.739336	1.479346
H	-4.920937	3.578941	2.964670
H	-2.610494	3.554125	3.876858
H	-1.066260	1.718268	3.291399
C	-1.872831	-1.512802	4.239171
C	-1.551418	-2.169406	5.421899
C	-0.299740	-2.761673	5.574642
C	0.635106	-2.687556	4.546111
C	0.324687	-2.028859	3.360244
H	-2.844257	-1.037601	4.126602
H	-2.278505	-2.216372	6.227826
H	-0.051275	-3.272257	6.501002
H	1.617624	-3.134956	4.669256
H	1.059035	-1.939770	2.556298
C	-3.437112	1.142157	-2.098784
C	-4.278627	2.244235	-2.008567
C	-3.885057	3.364828	-1.279594
C	-2.652232	3.378283	-0.637017
C	-1.809214	2.275271	-0.725383
H	-3.750748	0.266074	-2.661431
H	-5.246162	2.227271	-2.502516
H	-4.547411	4.222807	-1.203885
H	-2.351696	4.240539	-0.048986
H	-0.857216	2.266347	-0.200771
C	-1.149081	0.193110	-4.270334
C	-0.871510	-0.127927	-5.595703
C	-0.318430	-1.360903	-5.920040
C	-0.032735	-2.275556	-4.908114
C	-0.301029	-1.957477	-3.584108
H	-1.562846	1.166790	-4.028916
H	-1.084488	0.596582	-6.376702
H	-0.102334	-1.608096	-6.955444
H	0.410403	-3.237353	-5.149681
H	-0.059357	-2.672327	-2.801466
B	2.623370	1.609363	-0.501060
O	1.690740	1.809720	0.503253
O	3.922726	1.282735	-0.259975
C	2.094252	1.674972	1.886104
C	3.590298	1.916367	2.086143
C	4.322973	1.011457	1.093082
C	2.185607	1.899650	-1.976134
C	3.943413	3.389476	1.850500
C	3.964406	1.498792	3.509176
H	1.502796	2.404094	2.455651
H	5.406207	1.177258	1.143423
H	4.090623	-0.038606	1.309695
H	1.837253	0.660723	2.216561
H	3.665155	3.720564	0.844882
H	5.021088	3.549324	1.966925
H	3.423777	4.028899	2.573188
H	3.413496	2.092965	4.247574
H	5.034230	1.654310	3.688362
H	3.736932	0.440842	3.682369
C	1.199087	2.854111	-2.260263
C	1.453925	2.489876	-4.626698
C	2.803727	1.255213	-3.057068

1•B (cont)

C	2.435046	1.536618	-4.367490
H	2.914015	1.013257	-5.190476
H	3.580104	0.521096	-2.862188
C	0.838553	3.153590	-3.569668
H	0.721216	3.385307	-1.442071
H	1.169194	2.713272	-5.651621
H	0.076868	3.904376	-3.764516
C	1.395400	-3.476538	-0.068118
C	2.508545	-2.415741	-0.002340
O	2.054257	-1.253832	0.647159
C	3.684277	-2.985681	0.808492
C	2.985757	-2.081240	-1.422874
H	1.722092	-4.387731	-0.584931
H	0.524465	-3.069079	-0.597510
H	1.068349	-3.750789	0.941429
H	3.798173	-1.348554	-1.369167
H	2.164700	-1.631405	-1.994972
H	3.344238	-2.967591	-1.961913
H	3.363013	-3.187245	1.837012
H	4.505920	-2.262182	0.841318
H	4.065441	-3.917302	0.373693

TS[**1**•B–XSi]
E_t = -4316.991247 a.u.

Cu	0.422819	0.126847	-0.444487
P	-1.367176	0.011729	1.023479
P	-1.127314	0.291429	-2.072820
C	-2.340209	-1.160814	-0.018754
C	-2.264720	-1.006717	-1.420895
C	-2.952411	-1.896332	-2.245962
C	-3.701291	-2.933156	-1.696971
C	-3.767493	-3.091361	-0.316628
C	-3.088332	-2.208344	0.517340
H	-2.882068	-1.793325	-3.325143
H	-4.221671	-3.626015	-2.351909
H	-4.339450	-3.908428	0.113713
H	-3.118228	-2.344764	1.595478
C	-2.584919	1.355096	1.328167
C	-1.212293	-0.854591	2.627826
C	-2.158234	1.810774	-2.068011
C	-1.000987	-0.059830	-3.876771
C	-3.938740	1.104952	1.572408
C	-4.822799	2.161430	1.759664
C	-4.365692	3.475530	1.693706
C	-3.022310	3.730205	1.439704
C	-2.135445	2.674631	1.257557
H	-4.304801	0.081802	1.601147
H	-5.873967	1.958911	1.945189
H	-5.061201	4.300266	1.822513
H	-2.665262	4.752876	1.357440
H	-1.093822	2.870130	1.021278
C	-1.962631	-0.540997	3.763740
C	-1.765240	-1.251430	4.945383
C	-0.821783	-2.272559	5.000673
C	-0.058523	-2.571049	3.873865
C	-0.240660	-1.861865	2.693390
H	-2.696920	0.258328	3.732089
H	-2.352780	-1.003848	5.825006
H	-0.672513	-2.826312	5.923519
H	0.697512	-3.350770	3.919228
H	0.393424	-2.039146	1.824064
C	-3.529275	1.799536	-1.805052
C	-4.242994	2.992998	-1.771982
C	-3.596844	4.202836	-2.004320
C	-2.230540	4.217830	-2.272763
C	-1.513749	3.028195	-2.301424
H	-4.035447	0.859298	-1.604654
H	-5.304768	2.975771	-1.544411
H	-4.154844	5.134020	-1.962978
H	-1.717406	5.159889	-2.445525
H	-0.443155	3.042175	-2.482844
C	-1.991610	0.337071	-4.781785
C	-1.857204	0.054070	-6.136570
C	-0.732286	-0.621571	-6.603664
C	0.263217	-1.006591	-5.711493
C	0.132250	-0.721196	-4.356225
H	-2.865548	0.875324	-4.424731
H	-2.632211	0.366195	-6.830763
H	-0.628467	-0.838676	-7.663012
H	1.149865	-1.522140	-6.069311
H	0.918503	-1.008764	-3.665851
O	2.339271	0.124629	2.276201
O	4.101887	-0.054354	0.617319
O	1.573587	-1.355666	0.101184
C	4.905126	-0.841973	1.494126
C	4.558005	-0.621003	2.970464
C	3.041805	-0.796862	3.102394
C	2.464855	1.711871	-1.190712
C	5.265906	-1.674897	3.820439
C	4.972794	0.788350	3.406546
H	4.781963	-1.905679	1.241986
H	2.761783	-1.824045	2.818337
H	2.716449	-0.625406	4.136890
H	5.952719	-0.572530	1.303305
H	6.353044	-1.614347	3.693229
B	2.813704	0.289376	0.989102
H	5.046529	-1.524850	4.883837
H	4.500457	1.552702	2.782272
H	6.059204	0.909585	3.327691
H	4.681603	0.973592	4.446698
C	2.180102	1.498957	0.173793
C	1.581495	3.956170	-1.087191
C	1.549923	2.550455	0.872338

TS[**1**•B–XSi] (cont)

C	1.263345	3.763548	0.255561
H	0.807193	4.569514	0.825861
H	1.328437	2.409904	1.927893
C	2.165408	2.922732	-1.814109
H	2.983911	0.934265	-1.744862
H	1.369656	4.909548	-1.565227
H	2.405585	3.064678	-2.864725
C	2.884677	-2.121776	-1.775398
C	1.880104	-2.492973	-0.677476
H	4.947842	-2.687972	3.546891
C	0.607141	-3.084112	-1.305406
C	2.487439	-3.572863	0.233842
H	3.801898	-1.733839	-1.322210
H	2.461927	-1.320701	-2.391939
H	3.130298	-2.970287	-2.425407
H	1.766071	-3.865897	1.005698
H	3.384900	-3.194966	0.729897
H	2.762930	-4.469422	-0.334349
H	0.136847	-2.366606	-1.984075
H	-0.122572	-3.330438	-0.525010
H	0.825396	-3.995965	-1.875556

XSi
E_t = -4317.013137 a.u.

Cu	0.207591	0.162193	-0.340619
P	-1.567459	-0.003467	1.094363
P	-1.333062	0.307312	-1.993398
C	-2.717286	-0.998405	0.055671
C	-2.636402	-0.834052	-1.344214
C	-3.512477	-1.544873	-2.167012
C	-4.433492	-2.431442	-1.619836
C	-4.489272	-2.617384	-0.241943
C	-3.638242	-1.899173	0.590731
H	-3.458432	-1.422416	-3.245101
H	-5.101143	-2.985571	-2.273488
H	-5.196558	-3.321681	0.186433
H	-3.681516	-2.046486	1.666157
C	-2.554016	1.489872	1.493363
C	-1.450218	-0.860063	2.706204
C	-2.214347	1.918926	-2.038479
C	-1.154861	-0.148698	-3.759109
C	-1.942038	2.468005	2.286069
C	-2.610796	3.648617	2.581153
C	-3.891251	3.872264	2.079393
C	-4.500652	2.905666	1.287076
C	-3.838547	1.717107	0.995269
H	-0.936181	2.303253	2.663653
H	-2.128059	4.399999	3.199758
H	-4.410364	4.799619	2.304434
H	-5.496071	3.075992	0.886915
H	-4.320055	0.972053	0.368757
C	-2.466350	-0.797120	3.667261
C	-2.315213	-1.457499	4.880537
C	-1.147654	-2.171032	5.146453
C	-0.127456	-2.213848	4.202044
C	-0.271381	-1.558252	2.982701
H	-3.365148	-0.217377	3.471117
H	-3.105098	-1.407120	5.624706
H	-1.029203	-2.678985	6.099614
H	0.797183	-2.742446	4.415542
H	0.548538	-1.556657	2.267767
C	-3.435079	2.070507	-2.704222
C	-4.100963	3.288891	-2.668285
C	-3.556022	4.362708	-1.965381
C	-2.345278	4.214511	-1.299520
C	-1.676843	2.994395	-1.332096
H	-3.865689	1.234231	-3.249430
H	-5.049701	3.401227	-3.185530
H	-4.082781	5.312453	-1.933273
H	-1.922510	5.041743	-0.736928
H	-0.740138	2.873925	-0.795240
C	-1.103782	0.835012	-4.752343
C	-0.829016	0.488461	-6.071436
C	-0.599536	-0.839130	-6.416302
C	-0.637409	-1.822690	-5.431004
C	-0.903507	-1.481534	-4.111417
H	-1.281475	1.875097	-4.494851
H	-0.795340	1.262957	-6.832319
H	-0.385941	-1.107135	-7.446813
H	-0.450802	-2.861217	-5.688677
H	-0.917491	-2.258616	-3.351779
O	2.813818	-0.811890	2.011596
O	3.929338	-0.673871	-0.180830
O	1.561834	-1.317943	-0.038377
C	5.171897	-0.992499	0.407487
C	5.260187	-0.646852	1.897785
C	4.028132	-1.266910	2.565469
C	2.128368	1.609986	-0.906343
C	6.524518	-1.272056	2.488187
C	5.285637	0.871388	2.099137
H	5.380696	-2.074699	0.292555
H	4.109579	-2.368763	2.485570
H	4.023581	-1.019830	3.639377
H	5.961098	-0.456949	-0.145013
H	7.419474	-0.896723	1.977735
B	2.710798	-0.509707	0.591502
H	6.620473	-1.023944	3.551906
H	4.425923	1.353160	1.627211
H	6.195855	1.298759	1.661884
H	5.270607	1.120949	3.167088
C	2.132089	1.033706	0.385217
C	1.568996	3.784954	-0.017283
C	1.784151	1.882878	1.456624

XSi (cont)

C	1.514748	3.233511	1.265005
H	1.281626	3.870031	2.115684
H	1.782116	1.457998	2.459237
C	1.863028	2.970693	-1.103547
H	2.448424	1.000369	-1.750483
H	1.380346	4.845554	-0.164474
H	1.900144	3.391201	-2.105712
C	2.163680	-2.601615	-1.996118
C	1.632971	-2.656463	-0.562368
H	6.513893	-2.364261	2.393432
C	0.207855	-3.208519	-0.540746
C	2.524450	-3.533326	0.317156
H	3.178531	-2.196412	-2.000282
H	1.529747	-1.943911	-2.602599
H	2.167397	-3.598671	-2.452979
H	2.179852	-3.504306	1.355989
H	3.561545	-3.194130	0.283290
H	2.491180	-4.570326	-0.035208
H	-0.463260	-2.556659	-1.110320
H	-0.171161	-3.265908	0.485587
H	0.172130	-4.210623	-0.982121

TS[**XSi**–**2**•OB[1]]
E_t = -4316.986489 a.u.

Cu	0.159683	-0.140629	-0.110918
P	-1.604930	-0.281543	1.289161
P	-1.360061	-0.010568	-1.778967
C	-2.890538	-1.124929	0.270458
C	-2.805223	-0.967482	-1.128802
C	-3.786204	-1.543054	-1.940062
C	-4.817730	-2.290135	-1.381178
C	-4.884101	-2.466464	-0.002052
C	-3.928162	-1.878613	0.819464
H	-3.730967	-1.424521	-3.018667
H	-5.566585	-2.741337	-2.026090
H	-5.681660	-3.060276	0.435282
H	-3.982277	-2.013701	1.896201
C	-2.408834	1.314707	1.705840
C	-1.561273	-1.181955	2.882221
C	-2.020653	1.705808	-1.877446
C	-1.229334	-0.520645	-3.534130
C	-1.719201	2.187931	2.555551
C	-2.215069	3.459691	2.808688
C	-3.399755	3.881709	2.208493
C	-4.093168	3.016679	1.369916
C	-3.604873	1.737328	1.121124
H	-0.786860	1.870051	3.014476
H	-1.667416	4.128751	3.466317
H	-3.776893	4.883740	2.392128
H	-5.014398	3.338623	0.893060
H	-4.149546	1.076266	0.453949
C	-2.508675	-0.990187	3.893961
C	-2.409352	-1.703355	5.083566
C	-1.363589	-2.604475	5.273146
C	-0.410030	-2.783796	4.275707
C	-0.500617	-2.071088	3.084213
H	-3.312727	-0.271689	3.754611
H	-3.145481	-1.550626	5.867794
H	-1.285167	-3.155421	6.206297
H	0.420726	-3.466330	4.430469
H	0.266881	-2.174030	2.320813
C	-3.243037	1.981476	-2.499470
C	-3.745621	3.276573	-2.507477
C	-3.032925	4.305917	-1.893519
C	-1.815368	4.036984	-1.279951
C	-1.307667	2.740858	-1.269474
H	-3.805532	1.181524	-2.974433
H	-4.697132	3.483789	-2.989333
H	-3.432429	5.316479	-1.892548
H	-1.254744	4.829670	-0.793325
H	-0.363035	2.533927	-0.774949
C	-0.965376	0.429066	-4.527588
C	-0.703587	0.027395	-5.833517
C	-0.700365	-1.323269	-6.167148
C	-0.952854	-2.275322	-5.182253
C	-1.205057	-1.880213	-3.874717
H	-0.964649	1.486242	-4.277343
H	-0.501856	0.776830	-6.593554
H	-0.497116	-1.634088	-7.187729
H	-0.946527	-3.332741	-5.431349
H	-1.384040	-2.635292	-3.113697
O	2.613027	-0.694367	1.992688
O	3.735443	-0.912145	-0.122954
O	1.484271	-1.772549	0.235127
C	4.926440	-0.959986	0.664007
C	4.970591	0.149704	1.714297
C	3.690408	0.035576	2.582894
C	2.384858	1.568326	-1.261654
C	6.199867	-0.052128	2.606513
C	5.067569	1.512436	1.018945
H	5.002267	-1.942540	1.162241
H	3.924893	-0.489311	3.518758
H	3.337501	1.044330	2.842482
H	5.775102	-0.861556	-0.024639
H	7.124493	0.044619	2.025656
B	2.551485	-0.895638	0.617365
H	6.227266	0.704906	3.399001
H	4.236904	1.670020	0.329100
H	6.003473	1.582691	0.451529
H	5.055936	2.323861	1.755402
C	1.862303	1.119267	-0.030446
C	2.740265	3.802864	-0.420080
C	1.837093	2.078185	1.001565

TS[**XSi**–**2**•OB[1]] (cont)

C	2.253924	3.396890	0.819826
H	2.199416	4.108361	1.641834
H	1.469250	1.779965	1.982345
C	2.817441	2.876940	-1.460976
H	2.452986	0.867648	-2.094465
H	3.064996	4.828951	-0.573885
H	3.205775	3.184394	-2.429853
C	1.932159	-2.458627	-2.073303
C	1.607362	-2.917369	-0.653580
H	6.193178	-1.039740	3.082373
C	0.235289	-3.586399	-0.603519
C	2.673016	-3.870174	-0.115076
H	2.923403	-2.002634	-2.114056
H	1.195035	-1.721479	-2.409000
H	1.900850	-3.310059	-2.762451
H	2.464216	-4.117064	0.931458
H	3.666741	-3.421891	-0.184552
H	2.672193	-4.798428	-0.696934
H	-0.545587	-2.868407	-0.879844
H	0.016860	-3.948927	0.406422
H	0.194799	-4.432761	-1.296575

2•OB[1]

E_t = -4317.007489 a.u.

Cu	0.207069	0.289802	0.312869
P	-1.590031	0.130826	1.757988
P	-1.366148	0.438753	-1.306160
C	-3.005075	-0.485209	0.744757
C	-2.866938	-0.418921	-0.657206
C	-3.844601	-0.985409	-1.475781
C	-4.962320	-1.597661	-0.918172
C	-5.116677	-1.635292	0.464589
C	-4.143705	-1.082554	1.290791
H	-3.719953	-0.958173	-2.555472
H	-5.711677	-2.046416	-1.564138
H	-5.991618	-2.106228	0.903769
H	-4.260226	-1.130640	2.369826
C	-1.948321	1.909411	2.041752
C	-1.890917	-0.619679	3.411187
C	-1.969667	2.172207	-1.440138
C	-1.254705	-0.157085	-3.036305
C	-0.885666	2.732441	2.431520
C	-1.101778	4.087456	2.656325
C	-2.367769	4.634290	2.468428
C	-3.422194	3.821369	2.062706
C	-3.217258	2.461287	1.856580
H	0.113613	2.314683	2.531684
H	-0.271296	4.718501	2.959759
H	-2.531136	5.696757	2.626923
H	-4.407841	4.247654	1.899020
H	-4.041621	1.831339	1.533365
C	-2.017451	0.155661	4.567393
C	-2.148521	-0.453808	5.812136
C	-2.158352	-1.839930	5.920056
C	-2.031843	-2.619469	4.772241
C	-1.889297	-2.016214	3.530020
H	-2.019594	1.239174	4.496206
H	-2.248441	0.162781	6.700966
H	-2.261912	-2.312383	6.892520
H	-2.037517	-3.703416	4.845305
H	-1.784838	-2.635750	2.643802
C	-3.265703	2.481821	-1.864249
C	-3.683185	3.805878	-1.929176
C	-2.814852	4.830908	-1.561578
C	-1.529960	4.527802	-1.125191
C	-1.107869	3.203687	-1.061721
H	-3.954557	1.685979	-2.135171
H	-4.691945	4.037658	-2.259475
H	-3.145959	5.864895	-1.604140
H	-0.855166	5.320462	-0.815523
H	-0.117001	2.962540	-0.684822
C	-1.588610	0.632849	-4.139396
C	-1.473224	0.119689	-5.428487
C	-1.028489	-1.182708	-5.626666
C	-0.680321	-1.967576	-4.529899
C	-0.778898	-1.458068	-3.241636
H	-1.935511	1.651500	-3.995338
H	-1.731245	0.744124	-6.279272
H	-0.939851	-1.581481	-6.633319
H	-0.311074	-2.978288	-4.678803
H	-0.456525	-2.061716	-2.397601
O	2.293666	-0.787519	-2.018237
O	3.407716	-1.616772	-0.040392
O	1.071241	-1.976855	-0.451629
C	4.594808	-0.890312	-0.398541
C	4.758870	-0.786188	-1.916290
C	3.486921	-0.133126	-2.464869
C	2.511536	2.116017	-0.090778
C	5.952210	0.119332	-2.223798
C	4.964663	-2.173614	-2.534741
H	4.538251	0.110749	0.050279
H	3.449361	0.917302	-2.148623
H	3.477707	-0.170493	-3.561911
H	5.442293	-1.427583	0.045187
H	6.882066	-0.322779	-1.848241
B	2.286890	-1.426483	-0.805050
H	6.063924	0.261403	-3.305019
H	4.109071	-2.830095	-2.346900
H	5.856497	-2.654161	-2.116509
H	5.096758	-2.094658	-3.619754
C	1.916723	1.148724	0.744781
C	4.335290	2.513112	1.441073
C	2.603964	0.907641	1.953135

2•OB[1] (cont)

C	3.784695	1.563462	2.299511
H	4.277926	1.335514	3.242550
H	2.208133	0.171247	2.653113
C	3.689232	2.789657	0.239680
H	2.046043	2.353309	-1.048325
H	5.253544	3.031060	1.706534
H	4.103881	3.530661	-0.441904
C	-0.590293	-3.414582	0.379624
C	0.887542	-3.051878	0.507999
H	5.828929	1.103772	-1.757897
C	1.209295	-2.569274	1.920040
C	1.757753	-4.245307	0.114019
H	-0.800924	-3.829646	-0.611721
H	-1.210715	-2.520979	0.510034
H	-0.871786	-4.158699	1.132011
H	2.818901	-4.012461	0.233986
H	1.568510	-4.520448	-0.929305
H	1.517397	-5.107169	0.745785
H	0.611353	-1.682902	2.160388
H	2.265122	-2.305341	2.007733
H	0.974512	-3.352514	2.649324

2

E_t = -3712.058763 a.u.

Cu	1.555471	-0.030467	0.056748
P	-0.219015	-0.176198	1.451287
P	0.025406	0.110573	-1.600374
C	-1.370057	-1.184407	0.426449
C	-1.246806	-1.070828	-0.973877
C	-2.056118	-1.851310	-1.801305
C	-2.982117	-2.730468	-1.250428
C	-3.103944	-2.842084	0.132457
C	-2.298228	-2.075435	0.967094
H	-1.946197	-1.781884	-2.880577
H	-3.603714	-3.337300	-1.902763
H	-3.820764	-3.535859	0.562335
H	-2.378235	-2.177908	2.046159
C	-1.153061	1.344804	1.858007
C	-0.126261	-1.085362	3.039129
C	-0.901657	1.689300	-1.719490
C	0.289719	-0.433071	-3.329640
C	-2.447734	1.591892	1.397512
C	-3.061520	2.812968	1.659825
C	-2.395539	3.790723	2.390526
C	-1.104990	3.547928	2.856323
C	-0.481735	2.337561	2.583124
H	-2.973138	0.834410	0.822893
H	-4.064530	2.999249	1.286710
H	-2.877443	4.742793	2.593602
H	-0.577557	4.308812	3.424529
H	0.534191	2.159408	2.929676
C	-0.984158	-0.841625	4.115214
C	-0.855226	-1.579235	5.287872
C	0.124956	-2.562495	5.391941
C	0.984589	-2.804156	4.323398
C	0.867016	-2.063814	3.152924
H	-1.747193	-0.071442	4.036617
H	-1.521819	-1.384160	6.123213
H	0.225092	-3.134324	6.310153
H	1.759821	-3.560361	4.405780
H	1.557412	-2.226167	2.326770
C	-2.215396	1.758164	-2.192622
C	-2.893457	2.971376	-2.197509
C	-2.269236	4.122052	-1.721668
C	-0.964281	4.059120	-1.244503
C	-0.282294	2.847045	-1.242739
H	-2.712401	0.858126	-2.546476
H	-3.914734	3.017876	-2.565203
H	-2.804668	5.067320	-1.715979
H	-0.478879	4.951500	-0.860803
H	0.731576	2.789905	-0.852156
C	-0.077824	0.321325	-4.445545
C	0.218979	-0.137485	-5.726770
C	0.878446	-1.348645	-5.903599
C	1.255475	-2.100693	-4.792191
C	0.974789	-1.641552	-3.512784
H	-0.590845	1.269844	-4.316374
H	-0.066979	0.457845	-6.589264
H	1.109339	-1.702822	-6.904070
H	1.784412	-3.040312	-4.922748
H	1.297723	-2.215141	-2.645794
C	3.423350	-0.488018	0.244229
C	4.236609	-0.773048	-0.871406
C	6.167483	-1.211751	0.509237
C	4.057502	-0.585711	1.499279
C	5.400073	-0.935705	1.637531
H	5.849665	-0.995093	2.626865
H	3.486557	-0.378683	2.404830
C	5.579255	-1.128307	-0.749963
H	3.810272	-0.711523	-1.872709
H	7.214217	-1.487913	0.610137
H	6.170354	-1.339158	-1.639045

2•T

E_t = -3944.461442 a.u.

Cu	1.023783	-0.160259	0.115768
P	-0.765427	-0.337812	1.488442
P	-0.480770	-0.036747	-1.566330
C	-1.835010	-1.406785	0.436395
C	-1.689446	-1.293524	-0.959256
C	-2.452566	-2.107048	-1.798341
C	-3.351927	-3.022202	-1.262076
C	-3.497260	-3.132596	0.118232
C	-2.739522	-2.329885	0.963779
H	-2.326878	-2.038247	-2.875643
H	-3.935863	-3.655388	-1.924188
H	-4.195840	-3.850885	0.537833
H	-2.840114	-2.426181	2.041690
C	-1.817152	1.118106	1.862168
C	-0.708678	-1.265184	3.070181
C	-1.560325	1.441697	-1.777632
C	-0.117239	-0.594282	-3.273541
C	-3.152591	1.220546	1.464793
C	-3.863503	2.394668	1.692948
C	-3.254950	3.471777	2.328339
C	-1.923842	3.376301	2.728756
C	-1.205380	2.212621	2.485782
H	-3.634362	0.386655	0.962477
H	-4.897399	2.467186	1.367425
H	-3.812831	4.387035	2.505111
H	-1.440053	4.216157	3.219628
H	-0.156448	2.153122	2.769110
C	-1.412416	-0.889320	4.216578
C	-1.300398	-1.644109	5.381492
C	-0.494912	-2.778123	5.407601
C	0.207368	-3.156564	4.264888
C	0.109539	-2.401291	3.103549
H	-2.049886	-0.009643	4.198388
H	-1.849653	-1.345492	6.270070
H	-0.410191	-3.364825	6.317946
H	0.843844	-4.036682	4.280743
H	0.677009	-2.680639	2.217794
C	-2.764127	1.393745	-2.488306
C	-3.585105	2.512924	-2.551726
C	-3.214143	3.689097	-1.902666
C	-2.022199	3.741224	-1.189457
C	-1.198686	2.621006	-1.122808
H	-3.063967	0.475927	-2.987679
H	-4.520111	2.466308	-3.103103
H	-3.861208	4.560794	-1.947306
H	-1.737890	4.648649	-0.664782
H	-0.287232	2.648940	-0.531627
C	-0.266826	0.226436	-4.394217
C	0.140450	-0.219813	-5.649205
C	0.697499	-1.484962	-5.798071
C	0.858011	-2.304567	-4.681806
C	0.464981	-1.860368	-3.427019
H	-0.703245	1.215612	-4.288631
H	0.018658	0.426874	-6.513653
H	1.013090	-1.830815	-6.778125
H	1.302623	-3.290026	-4.787620
H	0.616211	-2.493000	-2.554596
C	2.640370	-1.253186	0.257929
O	1.881814	2.008649	0.292067
C	2.515565	2.490413	-0.909238
H	2.529063	3.592949	-0.890895
H	1.911779	2.151511	-1.756966
C	3.924846	1.906711	-0.875284
H	3.926195	0.911414	-1.326504
H	4.639638	2.537969	-1.411325
C	4.238378	1.795609	0.635235
H	4.593096	0.790596	0.876287
H	4.994340	2.520420	0.951952
C	2.891343	2.078586	1.323346
H	2.626064	1.335948	2.081210
H	2.867586	3.084918	1.769338
C	3.228712	-1.569212	1.500070
C	5.092629	-2.708364	0.471744
C	3.344151	-1.721145	-0.870846
C	4.542249	-2.429142	-0.776590
H	5.049825	-2.763782	-1.679529
H	2.951130	-1.517040	-1.867697
C	4.426916	-2.274933	1.614909
H	2.739502	-1.249406	2.421545

2•T (cont)

H	6.026651	-3.258766	0.552371
H	4.842664	-2.486857	2.598375

2•S

E_t = -4290.643251 a.u.

Cu	0.836471	-0.386840	-0.322093
P	-1.092452	-0.534555	0.962315
P	-0.777796	-0.242841	-2.126778
C	-2.206426	-1.541981	-0.110382
C	-2.091858	-1.373314	-1.504438
C	-2.896867	-2.130573	-2.356526
C	-3.804062	-3.048614	-1.838621
C	-3.910742	-3.221342	-0.461833
C	-3.116149	-2.470496	0.398050
H	-2.795205	-2.016455	-3.432291
H	-4.417440	-3.639825	-2.512529
H	-4.606522	-3.949675	-0.054952
H	-3.183724	-2.622047	1.472266
C	-2.135227	0.957895	1.248602
C	-1.124832	-1.420146	2.565582
C	-1.642970	1.350651	-2.389343
C	-0.451993	-0.837491	-3.831508
C	-3.522192	0.869802	1.408783
C	-4.281695	2.019419	1.590472
C	-3.665629	3.268558	1.609302
C	-2.287374	3.362444	1.451884
C	-1.525582	2.212251	1.271318
H	-4.012780	-0.099638	1.380876
H	-5.358551	1.940264	1.711645
H	-4.261814	4.167180	1.741788
H	-1.801651	4.334011	1.457405
H	-0.452442	2.279501	1.130373
C	-1.761187	-0.916008	3.701440
C	-1.730394	-1.632360	4.894577
C	-1.068651	-2.853570	4.962484
C	-0.420109	-3.352029	3.835120
C	-0.434469	-2.635893	2.645238
H	-2.275146	0.039372	3.659404
H	-2.226284	-1.230691	5.773910
H	-1.049946	-3.412297	5.894146
H	0.113264	-4.297188	3.883732
H	0.100913	-3.013171	1.777075
C	-2.965613	1.575298	-2.002247
C	-3.525964	2.843780	-2.119866
C	-2.778797	3.896466	-2.635985
C	-1.462425	3.677317	-3.037883
C	-0.894609	2.416875	-2.907105
H	-3.557840	0.759676	-1.598575
H	-4.552171	3.006303	-1.802950
H	-3.218368	4.885550	-2.726790
H	-0.873943	4.493539	-3.447319
H	0.135632	2.252467	-3.217338
C	-1.147466	-0.361815	-4.948124
C	-0.857295	-0.859000	-6.214383
C	0.123655	-1.833887	-6.375474
C	0.820910	-2.306384	-5.267208
C	0.543753	-1.806679	-3.999460
H	-1.913118	0.399798	-4.825975
H	-1.400655	-0.484278	-7.077333
H	0.347959	-2.220543	-7.365664
H	1.592405	-3.061437	-5.387290
H	1.095915	-2.168457	-3.135234
C	1.558856	-2.226690	-0.532054
C	0.731705	-3.352688	-0.709554
C	2.609787	-4.855952	-0.929617
C	2.940732	-2.488898	-0.570006
C	3.461252	-3.768968	-0.762809
H	4.539358	-3.914577	-0.783939
H	3.650195	-1.672739	-0.449652
C	1.235870	-4.638743	-0.902320
H	-0.350643	-3.238745	-0.710627
H	3.010006	-5.855066	-1.080714
H	0.548645	-5.471926	-1.034863
C	1.447461	1.585829	-0.261699
C	2.493856	0.727634	-0.452635
C	2.513700	1.546705	0.822465
C	3.503857	2.676670	0.846580
C	2.200549	0.919185	2.150939
H	0.959920	2.392010	-0.799805
H	3.247397	0.525619	-1.205722
C	2.627888	-0.370071	2.462479
C	1.623989	-0.208579	4.650737
C	1.486685	1.641780	3.111940
C	1.195581	1.082215	4.350255

2•S (cont)

H	0.630446	1.652884	5.082336
H	1.169784	2.657876	2.886874
C	2.340207	-0.931463	3.703888
H	3.174550	-0.941785	1.719193
H	1.387386	-0.652649	5.613251
H	2.670571	-1.942278	3.925725
C	4.259458	2.961805	1.990762
C	5.396719	4.761031	0.850125
C	3.725381	3.454303	-0.298992
C	4.656952	4.485438	-0.295866
H	4.807997	5.075261	-1.195919
H	3.165989	3.244934	-1.206123
C	5.194539	3.990721	1.990871
H	4.113414	2.368090	2.887582
H	6.126725	5.565247	0.852294
H	5.770785	4.189686	2.890332

2•B

E_t = -4315.530989 a.u.

Cu	0.665309	-0.647204	0.093336
P	-1.119892	-0.841611	1.475229
P	-0.850639	-0.538163	-1.575977
C	-1.946964	-2.120288	0.433262
C	-1.872345	-1.942967	-0.965401
C	-2.469296	-2.878420	-1.810934
C	-3.129851	-3.983464	-1.281881
C	-3.189481	-4.166680	0.096244
C	-2.599923	-3.238660	0.950116
H	-2.399770	-2.750531	-2.888015
H	-3.585915	-4.709128	-1.949267
H	-3.689818	-5.037928	0.509486
H	-2.631777	-3.390364	2.026199
C	-2.487591	0.360619	1.751941
C	-0.903627	-1.652809	3.103275
C	-2.012323	0.874253	-1.717787
C	-0.470853	-0.981094	-3.313139
C	-3.818160	-0.041248	1.908505
C	-4.819669	0.906170	2.087397
C	-4.502449	2.262254	2.107764
C	-3.181727	2.667210	1.947796
C	-2.177660	1.721555	1.767312
H	-4.073518	-1.097412	1.882589
H	-5.850913	0.585218	2.207027
H	-5.287094	3.001950	2.241713
H	-2.926230	3.723058	1.953558
H	-1.149703	2.042620	1.627904
C	-1.620242	-1.290115	4.246502
C	-1.344155	-1.902262	5.466520
C	-0.357941	-2.879453	5.553962
C	0.364090	-3.238295	4.417029
C	0.103982	-2.622400	3.199590
H	-2.388044	-0.524241	4.186447
H	-1.903745	-1.612031	6.351508
H	-0.144924	-3.354918	6.507284
H	1.145681	-3.990028	4.479752
H	0.696385	-2.873245	2.321383
C	-3.396148	0.744550	-1.582309
C	-4.210980	1.872451	-1.599681
C	-3.655271	3.136760	-1.762971
C	-2.276068	3.274504	-1.900482
C	-1.459510	2.151909	-1.865700
H	-3.835373	-0.239656	-1.443737
H	-5.284377	1.760981	-1.475882
H	-4.293839	4.015510	-1.770641
H	-1.833977	4.260294	-2.014848
H	-0.379602	2.266971	-1.935394
C	-1.207963	-0.522712	-4.408304
C	-0.835655	-0.886308	-5.699476
C	0.266827	-1.711001	-5.904399
C	1.005987	-2.167234	-4.814899
C	0.647890	-1.796771	-3.524163
H	-2.070127	0.120047	-4.250193
H	-1.411110	-0.525562	-6.547510
H	0.554091	-1.993346	-6.913379
H	1.871751	-2.804712	-4.970170
H	1.237317	-2.128953	-2.670143
C	2.169378	-1.890962	0.180934
C	2.025842	-3.262426	-0.115956
C	4.357232	-3.726100	0.313246
C	3.469677	-1.491774	0.548423
C	4.543139	-2.379941	0.615971
H	5.528098	-2.021562	0.910174
H	3.660265	-0.445306	0.793319
C	3.087485	-4.164705	-0.053874
H	1.045386	-3.647520	-0.403190
H	5.189093	-4.423881	0.364784
H	2.924562	-5.213974	-0.293270
B	1.922030	2.534582	0.247370
O	1.962923	1.295813	-0.346755
O	2.316425	3.671504	-0.402142
C	2.536299	1.130106	-1.661606
C	3.546531	2.229982	-1.976622
C	2.847414	3.570169	-1.733950
C	1.404380	2.618778	1.714595
C	4.786538	2.094266	-1.083807
C	3.942110	2.126678	-3.450636
H	2.997418	0.135642	-1.673734
H	3.549128	4.403529	-1.860514

2•B (cont)

H	2.025006	3.701481	-2.453714
H	1.718157	1.134675	-2.396836
H	5.263762	1.121677	-1.243933
H	4.540422	2.171813	-0.019931
H	5.514337	2.879408	-1.316408
H	4.416888	1.160749	-3.653769
H	4.657648	2.913115	-3.715475
H	3.069729	2.220081	-4.107416
C	0.883939	3.813312	2.233167
C	0.371448	2.726114	4.322995
C	1.416626	1.485094	2.543083
C	0.907824	1.537149	3.836542
H	0.919574	0.646256	4.458608
H	1.825050	0.546834	2.170879
C	0.364169	3.866157	3.522078
H	0.878436	4.704273	1.609758
H	-0.038948	2.765685	5.328457
H	-0.048487	4.795563	3.905204

2•P

E_t = -4809.409145 a.u.

Cu	-0.061663	-0.617412	-0.769844
P	-1.830110	-0.815937	0.621418
P	-1.617746	-0.518970	-2.543763
C	-2.910875	-1.870181	-0.440334
C	-2.791092	-1.761932	-1.839525
C	-3.553996	-2.597962	-2.658358
C	-4.429398	-3.525364	-2.104609
C	-4.550762	-3.627479	-0.722128
C	-3.795148	-2.803779	0.104275
H	-3.449378	-2.526599	-3.737707
H	-5.011043	-4.173167	-2.754286
H	-5.227514	-4.356220	-0.285005
H	-3.878378	-2.898580	1.183325
C	-2.935424	0.549619	1.162357
C	-1.617336	-1.789682	2.168992
C	-2.735164	0.865161	-3.046840
C	-1.179131	-1.251597	-4.176098
C	-4.083755	0.896912	0.447566
C	-4.801134	2.043420	0.777601
C	-4.389525	2.850283	1.832911
C	-3.252317	2.503044	2.560918
C	-2.525552	1.368650	2.224685
H	-4.420225	0.271830	-0.372974
H	-5.687317	2.302089	0.204709
H	-4.951766	3.743273	2.090325
H	-2.921148	3.120106	3.391799
H	-1.634537	1.119603	2.796801
C	-2.499585	-1.731588	3.252756
C	-2.240673	-2.464362	4.406568
C	-1.106172	-3.268256	4.488123
C	-0.227348	-3.335584	3.410524
C	-0.475537	-2.592562	2.261055
H	-3.381648	-1.099278	3.201072
H	-2.928159	-2.406354	5.245883
H	-0.906163	-3.837440	5.391620
H	0.662424	-3.956641	3.467943
H	0.223414	-2.617322	1.427672
C	-4.130063	0.776354	-3.060911
C	-4.905873	1.879279	-3.404386
C	-4.302026	3.084468	-3.749116
C	-2.913229	3.180453	-3.754148
C	-2.137152	2.083086	-3.399513
H	-4.616087	-0.161334	-2.807139
H	-5.989104	1.792301	-3.408936
H	-4.910307	3.943915	-4.015992
H	-2.427063	4.112824	-4.027144
H	-1.053454	2.181513	-3.401551
C	-1.383888	-0.573142	-5.382045
C	-0.974076	-1.139090	-6.585858
C	-0.361079	-2.387638	-6.602411
C	-0.161120	-3.070280	-5.405837
C	-0.559681	-2.508570	-4.199329
H	-1.873854	0.395420	-5.389277
H	-1.143183	-0.600756	-7.514331
H	-0.042042	-2.827254	-7.543288
H	0.321125	-4.043534	-5.400695
H	-0.381691	-3.047581	-3.274248
C	1.019194	-2.175266	-1.290722
C	2.101230	-2.031717	-2.180561
C	2.400676	-4.416594	-2.414148
C	0.660073	-3.509049	-1.006291
C	1.331768	-4.608238	-1.542498
H	1.008281	-5.617152	-1.292210
H	-0.201637	-3.714825	-0.369858
C	2.779701	-3.115983	-2.733133
H	2.433912	-1.035871	-2.470083
H	2.924234	-5.267342	-2.843418
H	3.607153	-2.944869	-3.419492
C	1.371282	0.863908	2.047380
C	1.627305	1.734777	0.850812
C	2.780481	0.956078	1.447403
C	3.789479	1.782505	2.199573
C	3.408279	-0.278816	0.861308
C	4.455972	-0.146121	-0.056527
C	4.785036	-2.532720	-0.074532
C	3.084330	-1.552979	1.322350
C	3.762725	-2.673207	0.854163
H	3.478390	-3.660978	1.204510
H	2.299308	-1.670523	2.063025

2•P (cont)

C	5.133437	-1.262864	-0.526423
H	4.760826	0.847110	-0.379220
H	5.302666	-3.409013	-0.452468
H	5.937886	-1.142575	-1.246660
C	4.262503	1.317833	3.429352
C	5.706585	3.238110	3.631653
C	4.294821	2.979760	1.694556
C	5.249312	3.703998	2.404185
H	5.635584	4.633408	1.995096
H	3.942483	3.348886	0.734499
C	5.209836	2.040474	4.141512
H	3.871239	0.384835	3.826986
H	6.447496	3.803815	4.189035
H	5.560128	1.671025	5.101011
H	0.878095	-0.067150	1.768153
C	1.002984	1.360217	3.395838
H	1.704825	2.799544	1.076829
C	-0.284623	2.342701	-0.428061
C	0.040434	3.780888	-0.810253
O	0.762244	3.841220	-2.042066
C	1.989804	3.123709	-1.919291
C	1.730413	1.657509	-1.610925
N	0.908591	1.439801	-0.388770
H	-0.769986	2.311468	0.553152
H	-0.993528	1.938097	-1.153880
H	-0.894070	4.330800	-0.965811
H	0.613595	4.303070	-0.024008
H	2.508098	3.220316	-2.879344
H	2.619060	3.593795	-1.142108
H	1.181809	1.214459	-2.453356
H	2.667390	1.104342	-1.495631
C	0.465674	0.450554	4.315222
C	0.239830	2.188522	5.970939
C	1.159460	2.691483	3.794861
C	0.781540	3.099902	5.069097
H	0.914736	4.138350	5.359254
H	1.592142	3.418244	3.113645
C	0.084667	0.859683	5.587819
H	0.333096	-0.588288	4.021755
H	-0.056018	2.511678	6.964746
H	-0.337508	0.135089	6.278754

2dim

E_t = -7424.190259 a.u.

Cu	-1.170349	-0.013621	0.491275
C	0.055366	-1.816935	0.826011
C	-0.071688	1.541920	1.382163
Cu	1.173639	-0.079582	0.457837
P	-3.240183	-0.012543	1.403031
P	-2.227651	0.203486	-1.539733
C	-4.159622	1.115421	0.265582
C	-5.252628	1.883789	0.673307
C	-5.905146	2.717468	-0.227494
C	-5.471919	2.788334	-1.548221
C	-4.384256	2.029604	-1.965619
C	-3.717064	1.192974	-1.068757
C	-4.230425	-1.560950	1.322379
C	-3.614884	0.678214	3.054292
C	-2.945202	-1.302073	-2.309857
C	-1.570865	1.107689	-3.002991
P	3.208473	0.026675	1.449073
P	2.336063	-0.176299	-1.522116
C	4.291034	-0.944228	0.328444
C	5.464600	-1.569513	0.757715
C	6.272013	-2.245195	-0.148437
C	5.918876	-2.288129	-1.495249
C	4.752174	-1.671078	-1.930240
C	3.920024	-1.006662	-1.025499
C	4.028480	1.674390	1.462811
C	3.558755	-0.676204	3.103365
C	2.961486	1.424157	-2.193367
C	1.859061	-1.149112	-3.007666
C	-3.405708	2.540724	4.580526
C	-3.201217	1.988924	3.323097
H	-4.510700	-1.101436	3.878653
H	-4.852547	-0.117545	6.118373
H	-4.156054	2.220651	6.574151
H	-3.078928	3.558261	4.775390
H	-2.707663	2.573909	2.549955
C	-5.629600	-1.563596	1.319091
C	-4.261465	-1.706567	-2.078338
C	-4.721815	-2.920625	-2.579868
C	-3.878962	-3.736596	-3.326220
C	-2.569449	-3.329813	-3.575919
C	-2.102312	-2.125759	-3.067227
H	-4.931415	-1.078858	-1.498957
H	-5.745033	-3.226019	-2.380166
H	-4.240135	-4.684188	-3.715795
H	-1.901948	-3.953133	-4.164809
H	-1.079393	-1.819501	-3.272606
C	-6.324940	-2.760369	1.197019
C	-2.068363	0.940453	-4.300063
C	-1.541971	1.682785	-5.351588
C	-0.518245	2.600314	-5.121481
C	-0.008453	2.760910	-3.836941
C	-0.526852	2.008751	-2.787295
H	-2.861987	0.222014	-4.487217
H	-1.935006	1.546264	-6.355542
H	-0.110194	3.178886	-5.945708
H	0.813622	3.447057	-3.650968
H	-0.098773	2.091391	-1.793196
H	-6.747722	3.317517	0.104670
H	-2.455012	-2.769724	1.187355
H	-3.687803	-4.895727	0.991227
H	-6.176322	-4.897557	0.978829
H	-7.411542	-2.755299	1.189729
H	-6.177131	-0.628111	1.400275
C	-3.540215	-2.768010	1.205798
H	4.474033	-1.727892	-2.978694
H	6.550737	-2.809687	-2.208736
H	7.179632	-2.733869	0.194490
H	5.741294	-1.523708	1.807750
C	-4.240034	-3.965631	1.089639
C	-5.629856	-3.963723	1.080468
C	-4.393417	0.477592	5.333923
C	3.763548	1.521410	-3.334373
C	4.244425	2.758436	-3.747670
C	3.943934	3.907197	-3.017238
C	3.156350	3.815213	-1.874653
C	2.663217	2.579373	-1.468158
H	4.009210	0.630381	-3.905869
H	4.863565	2.826098	-4.637946
H	4.329184	4.871013	-3.338623

2dim (cont)

H	2.926718	4.701331	-1.289838
H	2.050292	2.504477	-0.572318
C	-4.003156	1.788415	5.589242
C	1.381142	-0.545059	-4.175039
C	0.921541	-1.321406	-5.235127
C	0.926283	-2.709387	-5.145210
C	1.387645	-3.319852	-3.980428
C	1.844536	-2.549111	-2.919002
H	1.362837	0.536056	-4.261324
H	0.552763	-0.830795	-6.131464
H	0.568142	-3.312743	-5.974651
H	1.389277	-4.402950	-3.893978
H	2.188182	-3.037348	-2.010932
H	-4.040022	2.102366	-2.993134
C	5.273007	1.907526	0.870937
C	5.799427	3.194905	0.829340
C	5.095395	4.259683	1.382239
C	3.855539	4.033168	1.974334
C	3.318520	2.751900	2.005789
H	5.828297	1.087840	0.425406
H	6.762490	3.364727	0.356140
H	5.508346	5.264117	1.344938
H	3.288935	4.856426	2.400933
H	2.336006	2.592455	2.439908
C	-4.201170	-0.078423	4.072419
C	3.216705	-2.018250	3.316811
C	3.394899	-2.594504	4.567247
C	3.897443	-1.836644	5.623560
C	4.226142	-0.500661	5.419173
C	4.061080	0.080302	4.164554
H	2.799731	-2.606423	2.502708
H	3.130561	-3.637265	4.719373
H	4.028853	-2.286921	6.603375
H	4.618831	0.095248	6.238359
H	4.328260	1.121739	4.009918
H	-5.974976	3.443440	-2.253897
C	-0.154833	-2.764752	-0.199055
C	-0.360492	-4.121895	0.042578
C	-0.358289	-4.603059	1.349206
C	-0.160048	-3.706961	2.398586
C	0.034415	-2.352463	2.135656
H	-0.171957	-2.426885	-1.230628
H	-0.532223	-4.800703	-0.791207
H	-0.514973	-5.660134	1.550045
H	-0.164885	-4.064412	3.426581
H	0.179103	-1.692038	2.988556
H	-5.578448	1.844341	1.709374
C	-0.198877	2.879725	0.948128
C	-0.168225	3.971501	1.818270
C	-0.006335	3.774286	3.186277
C	0.110077	2.470884	3.667472
C	0.073599	1.395809	2.784489
H	-0.348090	3.095942	-0.107856
H	-0.275027	4.980090	1.423339
H	0.020665	4.620458	3.868465
H	0.222064	2.290606	4.734527
H	0.161545	0.396706	3.206257

TS[**2**•S–**3**]

E_t = -4290.624227 a.u.

Cu	0.545177	-0.139752	-0.443384
P	-1.280198	-0.323533	0.952471
P	-1.019064	0.018509	-2.109608
C	-2.546199	-1.155003	-0.104799
C	-2.441819	-0.970082	-1.495110
C	-3.392396	-1.542539	-2.343384
C	-4.431093	-2.305638	-1.822074
C	-4.529124	-2.498058	-0.446624
C	-3.595679	-1.921520	0.407184
H	-3.309132	-1.399952	-3.417297
H	-5.160409	-2.754463	-2.490249
H	-5.334450	-3.100411	-0.035565
H	-3.672297	-2.080607	1.479268
C	-2.081279	1.316605	1.217229
C	-1.483951	-1.206945	2.547518
C	-1.696399	1.713342	-2.296516
C	-0.802729	-0.587743	-3.825791
C	-1.332401	2.468139	0.969815
C	-1.918039	3.724227	1.095042
C	-3.254797	3.838896	1.459127
C	-4.010495	2.692545	1.697513
C	-3.428805	1.436274	1.573559
H	-0.299638	2.362508	0.640176
H	-1.329637	4.612980	0.885363
H	-3.714186	4.820008	1.544302
H	-5.058365	2.777561	1.971411
H	-4.028693	0.546134	1.745306
C	-1.930521	-0.586974	3.716061
C	-2.023867	-1.308854	4.902361
C	-1.659013	-2.650042	4.939000
C	-1.204872	-3.272923	3.778496
C	-1.118304	-2.558501	2.590534
H	-2.202448	0.463709	3.702685
H	-2.377506	-0.815083	5.803381
H	-1.725981	-3.209352	5.867882
H	-0.914664	-4.319601	3.798232
H	-0.771132	-3.053585	1.686859
C	-3.048869	2.012809	-2.122067
C	-3.484730	3.333117	-2.176467
C	-2.581222	4.360621	-2.424671
C	-1.231707	4.067566	-2.606769
C	-0.788113	2.753567	-2.524557
H	-3.760322	1.217950	-1.918226
H	-4.534847	3.557618	-2.012772
H	-2.924701	5.390600	-2.461704
H	-0.518986	4.866748	-2.789553
H	0.272281	2.530370	-2.617046
C	-0.793054	0.263105	-4.933729
C	-0.533775	-0.245029	-6.203887
C	-0.287899	-1.602570	-6.381028
C	-0.301614	-2.456011	-5.279588
C	-0.549363	-1.953988	-4.008722
H	-0.997300	1.322356	-4.807988
H	-0.530615	0.425601	-7.058472
H	-0.086798	-1.995798	-7.373353
H	-0.112027	-3.517932	-5.408239
H	-0.542476	-2.623891	-3.153028
C	1.682176	-1.817695	-0.679145
C	2.007859	-2.245302	-1.974669
C	2.183111	-4.537948	-1.243181
C	1.659786	-2.782137	0.336141
C	1.897208	-4.127067	0.055826
H	1.859452	-4.857788	0.860993
H	1.448032	-2.483588	1.357751
C	2.242921	-3.585718	-2.259236
H	2.070917	-1.516776	-2.782293
H	2.370763	-5.585681	-1.460582
H	2.474609	-3.887343	-3.278486
C	1.923498	1.336142	-0.196352
C	2.567564	0.067556	-0.421321
C	2.880181	0.814666	0.854638
C	4.253275	1.430476	0.914713
C	2.345780	0.354496	2.178911
H	2.138612	2.217893	-0.795621
H	3.324175	-0.196118	-1.150403
C	1.468717	1.163447	2.901502
C	1.435341	-0.433185	4.707951
C	2.780148	-0.843240	2.747902
C	2.316616	-1.243136	3.998274

TS[**2**•S–**3**] (cont)

H	2.645822	-2.188710	4.420967
H	3.485861	-1.461395	2.198672
C	1.019288	0.776651	4.159086
H	1.146299	2.103561	2.463362
H	1.064832	-0.748653	5.678940
H	0.333184	1.416320	4.707970
C	4.890015	1.884446	-0.250099
C	6.799437	2.640137	1.019999
C	4.921634	1.607129	2.133090
C	6.175936	2.206760	2.184528
H	6.667043	2.334581	3.145510
H	4.451707	1.275553	3.053177
C	6.146972	2.474186	-0.198835
H	4.393168	1.783596	-1.210624
H	7.779899	3.105750	1.060518
H	6.618703	2.811049	-1.118082

3

E_t = -4290.711073 a.u.

Cu	0.291311	0.398909	-0.161205
P	-1.475821	0.241341	1.241499
P	-1.272696	0.532064	-1.816873
C	-2.810197	-0.543945	0.233397
C	-2.718855	-0.396627	-1.165074
C	-3.686483	-0.978233	-1.986692
C	-4.741128	-1.692885	-1.431148
C	-4.837370	-1.832144	-0.048554
C	-3.877642	-1.260646	0.779284
H	-3.603506	-0.877219	-3.065691
H	-5.486422	-2.146617	-2.078167
H	-5.658360	-2.394862	0.386761
H	-3.944742	-1.389603	1.856190
C	-2.141119	1.915989	1.591317
C	-1.587060	-0.647597	2.838590
C	-1.854047	2.263576	-1.949884
C	-1.130070	-0.035701	-3.551208
C	-1.292616	3.011922	1.418900
C	-1.767829	4.304052	1.618207
C	-3.091546	4.508127	1.992058
C	-3.942287	3.418827	2.167324
C	-3.471425	2.127391	1.964461
H	-0.261079	2.847389	1.112226
H	-1.104084	5.150668	1.470471
H	-3.464296	5.517433	2.142542
H	-4.977519	3.577007	2.456255
H	-4.141988	1.280698	2.088072
C	-1.391588	-2.034110	2.838522
C	-1.386933	-2.743468	4.030984
C	-1.555592	-2.076594	5.242388
C	-1.726649	-0.696269	5.251540
C	-1.743108	0.018505	4.056662
H	-1.236675	-2.560650	1.899442
H	-1.231659	-3.818194	4.015539
H	-1.543681	-2.631151	6.176233
H	-1.850744	-0.168830	6.193137
H	-1.880103	1.095905	4.073186
C	-3.161042	2.658048	-1.658207
C	-3.509189	4.004736	-1.697450
C	-2.562087	4.964553	-2.038006
C	-1.257137	4.576332	-2.332986
C	-0.900058	3.235237	-2.277726
H	-3.904889	1.914190	-1.387042
H	-4.525450	4.303089	-1.456345
H	-2.837269	6.015007	-2.067470
H	-0.511404	5.321831	-2.593938
H	0.125579	2.935341	-2.482777
C	-1.655398	0.676061	-4.633343
C	-1.507135	0.183461	-5.926389
C	-0.840285	-1.018607	-6.146098
C	-0.314117	-1.727780	-5.069241
C	-0.448741	-1.236894	-3.776535
H	-2.177315	1.614266	-4.465342
H	-1.915349	0.741461	-6.764394
H	-0.724786	-1.398580	-7.157278
H	0.217706	-2.661097	-5.230278
H	-0.017936	-1.784754	-2.942494
C	2.220687	-1.967583	-1.261096
C	2.611982	-2.749752	-2.355180
C	0.814784	-4.314304	-1.967908
C	1.116785	-2.407346	-0.513693
C	0.422896	-3.559498	-0.864279
H	-0.431780	-3.873734	-0.270115
H	0.814760	-1.849700	0.372093
C	1.919886	-3.904491	-2.708106
H	3.467715	-2.434052	-2.947716
H	0.268763	-5.212026	-2.242711
H	2.245025	-4.484545	-3.568076
C	2.238719	0.495992	-0.369193
C	2.943729	-0.704300	-0.984115
C	3.315654	-0.214243	0.431322
C	4.664984	0.440164	0.555121
C	2.932346	-1.052118	1.611902
H	2.615598	1.438337	-0.777891
H	3.730749	-0.521031	-1.716440
C	3.396711	-2.362451	1.742528
C	2.301801	-2.570421	3.880704
C	2.152096	-0.511870	2.634800
C	1.841643	-1.261641	3.764401

3 (cont)

H	1.227075	-0.829715	4.549913
H	1.788400	0.507048	2.527932
C	3.080934	-3.119849	2.865872
H	4.004589	-2.786835	0.946979
H	2.050072	-3.160041	4.758272
H	3.441799	-4.141610	2.948000
C	5.429716	0.312546	1.722556
C	7.185776	1.697584	0.809082
C	5.199259	1.223450	-0.480448
C	6.438498	1.837396	-0.357631
H	6.823101	2.432586	-1.181851
H	4.640024	1.363097	-1.401067
C	6.669522	0.932835	1.847623
H	5.049101	-0.280494	2.547537
H	8.154424	2.179518	0.904919
H	7.234093	0.812739	2.768606

3_1•A
E_t = -4997.906887 a.u.

Cu	0.153543	-0.288311	-0.167026
P	-1.668894	-0.429514	1.212936
P	-1.385958	-0.174855	-1.863914
C	-2.615074	-1.622500	0.161575
C	-2.465381	-1.527634	-1.237035
C	-3.097397	-2.455869	-2.064648
C	-3.885330	-3.463349	-1.518787
C	-4.048307	-3.547009	-0.139629
C	-3.415221	-2.633004	0.696523
H	-2.951083	-2.403549	-3.140348
H	-4.365109	-4.187451	-2.170941
H	-4.660319	-4.335069	0.290124
H	-3.530105	-2.713400	1.773941
C	-2.851384	0.977144	1.359005
C	-1.775542	-1.202733	2.879091
C	-2.588096	1.172392	-2.238111
C	-0.828332	-0.768010	-3.499359
C	-2.426126	2.135547	2.018413
C	-3.267065	3.238924	2.112264
C	-4.539220	3.200817	1.547551
C	-4.970276	2.050009	0.896649
C	-4.133104	0.943130	0.802498
H	-1.431693	2.172111	2.455707
H	-2.920428	4.135399	2.618887
H	-5.190771	4.067758	1.614001
H	-5.959503	2.012559	0.449175
H	-4.477523	0.053780	0.283230
C	-0.802870	-2.142815	3.230870
C	-0.886778	-2.812641	4.446680
C	-1.922705	-2.531782	5.331515
C	-2.880114	-1.577062	4.997399
C	-2.811971	-0.917328	3.775045
H	0.027007	-2.349245	2.561444
H	-0.123908	-3.541822	4.702124
H	-1.980668	-3.049446	6.285060
H	-3.687050	-1.347938	5.687916
H	-3.568187	-0.182026	3.514845
C	-2.367989	2.425180	-1.661542
C	-3.270459	3.464414	-1.863409
C	-4.403947	3.257770	-2.641523
C	-4.635342	2.009074	-3.215300
C	-3.733890	0.970389	-3.013609
H	-1.503572	2.574587	-1.019796
H	-3.099179	4.425551	-1.386747
H	-5.115209	4.064869	-2.793571
H	-5.524457	1.843050	-3.817254
H	-3.924582	-0.003783	-3.456504
C	-0.966912	-0.019298	-4.671780
C	-0.390066	-0.463511	-5.858923
C	0.327072	-1.654853	-5.888063
C	0.474493	-2.401206	-4.719893
C	-0.087628	-1.959085	-3.530141
H	-1.528431	0.910898	-4.659957
H	-0.505998	0.125015	-6.764810
H	0.774824	-1.999488	-6.815705
H	1.039026	-3.329307	-4.731545
H	0.058521	-2.529528	-2.615236
C	1.499709	-3.901320	-0.213759
C	2.114636	-5.160946	-0.242751
C	0.173554	-6.181510	0.761899
C	0.203482	-3.816548	0.288079
C	-0.454604	-4.940638	0.776726
H	-1.464627	-4.841628	1.166058
H	-0.284210	-2.847301	0.282939
C	1.462905	-6.287332	0.242416
H	3.123043	-5.247439	-0.643985
H	-0.337111	-7.061204	1.143499
H	1.960831	-7.253087	0.215418
C	1.784091	-1.288125	-0.710158
C	2.243799	-2.723750	-0.736990
C	2.959741	-1.713699	0.177271
C	4.346453	-1.297405	-0.217172
C	2.732125	-1.779554	1.657677
H	2.165854	-0.797981	-1.614612
H	2.876278	-3.015249	-1.578813
C	2.269457	-0.654149	2.343375
C	2.510427	-1.792175	4.454834
C	3.072977	-2.916265	2.393679
C	2.954740	-2.926574	3.781591

3_1•A (cont)

H	3.219089	-3.822256	4.337830
H	3.437647	-3.796458	1.871765
C	2.166393	-0.654201	3.729941
H	1.980052	0.229322	1.781824
H	2.420235	-1.798734	5.537808
H	1.803096	0.233385	4.240962
C	5.295232	-0.923206	0.745999
C	6.909978	-0.354518	-0.960450
C	4.726526	-1.191496	-1.566521
C	5.983521	-0.728649	-1.931091
H	6.238539	-0.653532	-2.984778
H	4.024767	-1.456717	-2.352631
C	6.555346	-0.458768	0.379262
H	5.040226	-0.989868	1.798580
H	7.891787	0.010895	-1.246964
H	7.263699	-0.175517	1.153590
C	-0.795295	6.142977	2.965593
C	-1.367736	6.947811	1.983026
C	-1.272308	6.585272	0.641783
C	-0.604116	5.422889	0.278379
H	0.302398	4.324301	3.360584
C	-0.139215	4.972616	2.609932
H	-0.863819	6.428075	4.011236
H	-1.885877	7.860629	2.262669
H	-1.716521	7.214425	-0.124003
H	-0.524727	5.139683	-0.765843
C	0.635521	3.322460	0.947678
C	-0.041429	4.607823	1.264803
O	0.931196	3.249512	-0.369886
O	0.896592	2.466733	1.764759
N	1.468603	1.939792	-0.799556
C	1.352232	2.009049	-2.273647
C	2.906484	1.900993	-0.428905
H	1.635943	1.012648	-2.632186
C	2.243684	3.065965	-2.912848
H	0.300770	2.174965	-2.533471
C	3.747905	2.958621	-1.124440
H	3.247759	0.904480	-0.725153
H	2.991691	1.972107	0.658717
H	2.196752	2.974108	-4.003213
H	1.904978	4.078479	-2.633951
H	4.805385	2.777190	-0.906731
H	3.483343	3.971199	-0.773919
O	3.604790	2.883448	-2.543120

TS[**3_1•A**–**4**]
E_t = -4997.872622 a.u.

Cu	0.398811	0.128959	-0.128778
P	-1.532173	-0.002439	1.212338
P	-1.278703	0.285778	-1.833019
C	-2.559580	-1.133914	0.182558
C	-2.467711	-0.967103	-1.215386
C	-3.214298	-1.789643	-2.061334
C	-4.034507	-2.780431	-1.536017
C	-4.116526	-2.951350	-0.158334
C	-3.391915	-2.127316	0.694911
H	-3.126001	-1.673051	-3.137796
H	-4.595358	-3.428797	-2.202977
H	-4.733963	-3.741454	0.258694
H	-3.446950	-2.289010	1.765369
C	-2.615816	1.488279	1.308987
C	-1.662243	-0.565100	2.960383
C	-2.245011	1.820007	-2.116306
C	-0.822696	-0.293450	-3.501943
C	-3.856576	1.582169	0.673649
C	-4.595027	2.758630	0.753681
C	-4.104596	3.848136	1.465947
C	-2.876896	3.752956	2.116793
C	-2.138611	2.578459	2.041847
H	-4.242275	0.745702	0.098701
H	-5.548545	2.826735	0.237507
H	-4.674377	4.772437	1.508169
H	-2.480655	4.597963	2.673006
H	-1.178770	2.505796	2.544872
C	-2.889071	-0.663730	3.627579
C	-2.932978	-1.106034	4.944984
C	-1.754869	-1.431843	5.615490
C	-0.529959	-1.283121	4.973860
C	-0.485425	-0.840181	3.655620
H	-3.808723	-0.380103	3.122312
H	-3.889172	-1.190950	5.453695
H	-1.794036	-1.786236	6.641918
H	0.396803	-1.517638	5.490033
H	0.471265	-0.708963	3.161555
C	-3.425354	1.852582	-2.862744
C	-4.142803	3.037452	-2.979528
C	-3.687714	4.195503	-2.351703
C	-2.511553	4.170035	-1.610142
C	-1.792484	2.986073	-1.492624
H	-3.788200	0.946727	-3.342010
H	-5.065591	3.056077	-3.552431
H	-4.260684	5.115265	-2.429511
H	-2.166643	5.060278	-1.092021
H	-0.893598	2.957205	-0.879852
C	-0.374619	-1.613390	-3.659199
C	0.175250	-2.030092	-4.864671
C	0.299983	-1.137347	-5.927264
C	-0.140194	0.174204	-5.777883
C	-0.697037	0.596609	-4.574734
H	-0.453398	-2.309370	-2.828437
H	0.514656	-3.056854	-4.972669
H	0.738835	-1.462874	-6.865702
H	-0.050054	0.876289	-6.601907
H	-1.034066	1.624317	-4.467221
C	0.054955	-3.699173	0.158893
C	-0.668974	-4.773234	-0.376218
C	-1.881030	-5.061705	1.690493
C	-0.236444	-3.310785	1.470149
C	-1.180019	-3.988318	2.231078
H	-1.374551	-3.658828	3.249206
H	0.292435	-2.473707	1.900915
C	-1.630183	-5.441563	0.375075
H	-0.474795	-5.087143	-1.399951
H	-2.623626	-5.588330	2.283680
H	-2.183166	-6.264768	-0.069551
C	1.329774	-1.541867	-0.729507
C	1.068229	-3.029117	-0.691528
C	2.406232	-2.444866	-0.161823
C	3.630782	-2.634539	-1.017555
C	2.667428	-2.516696	1.313065
H	1.615254	-1.260715	-1.750651
H	1.188551	-3.558816	-1.639229
C	2.921223	-3.755663	1.909361
C	3.226475	-2.700985	4.057351
C	2.693652	-1.375805	2.112503
C	2.980797	-1.463117	3.473190

TS[**3**$_1$•A–**4**] (cont)

H	2.996504	-0.557657	4.075528
H	2.440870	-0.414209	1.677526
C	3.189847	-3.850175	3.269089
H	2.886111	-4.651286	1.293746
H	3.440367	-2.773020	5.120313
H	3.364377	-4.823437	3.718919
C	3.544082	-2.725147	-2.416685
C	5.949100	-2.764403	-2.632730
C	4.914087	-2.614851	-0.454072
C	6.054791	-2.676155	-1.250163
H	7.034032	-2.648422	-0.779679
H	5.022408	-2.535504	0.622743
C	4.681725	-2.790993	-3.209334
H	2.574888	-2.718650	-2.908120
H	6.838476	-2.805737	-3.254423
H	4.575398	-2.851720	-4.289202
C	-0.367626	5.697132	3.289435
C	-0.520413	6.772996	2.416410
C	-0.144581	6.644461	1.081417
C	0.393145	5.448520	0.620961
H	0.267287	3.638260	3.485198
C	0.155083	4.496093	2.828303
H	-0.660514	5.794393	4.330934
H	-0.930043	7.711751	2.777806
H	-0.263999	7.481617	0.399477
H	0.700521	5.336930	-0.414137
C	1.079119	3.047477	1.022125
C	0.538545	4.367897	1.492175
O	1.732732	3.138190	-0.100948
O	0.883651	2.019367	1.677040
N	1.811315	1.364157	-0.814885
C	1.699307	1.692564	-2.245566
C	3.214643	1.030246	-0.499870
H	1.740715	0.731669	-2.783829
C	2.794715	2.599667	-2.797716
H	0.715593	2.138547	-2.428099
C	4.255718	1.959024	-1.113884
H	3.380409	0.016003	-0.891071
H	3.324513	1.005790	0.586757
H	2.697302	2.650616	-3.887690
H	2.688170	3.613389	-2.382105
H	5.250284	1.530293	-0.953955
H	4.209506	2.950485	-0.638230
O	4.085380	2.080796	-2.521579

4

E_t = -4997.914449 a.u.

Cu	0.118095	-0.622380	0.327284
P	-1.977577	-0.793549	1.737413
P	-1.622107	-0.534485	-1.299871
C	-2.991513	-1.913841	0.673994
C	-2.807453	-1.819273	-0.715280
C	-3.564934	-2.620942	-1.573902
C	-4.497701	-3.511939	-1.058130
C	-4.697875	-3.593485	0.317992
C	-3.953960	-2.794020	1.176976
H	-3.416190	-2.551665	-2.647720
H	-5.075036	-4.138808	-1.731784
H	-5.436438	-4.279263	0.723155
H	-4.118058	-2.852410	2.249048
C	-3.176778	0.571838	2.077044
C	-1.813460	-1.733415	3.294576
C	-2.696191	0.953025	-1.408637
C	-1.296409	-0.984500	-3.038544
C	-2.786692	1.682028	2.838696
C	-3.661717	2.744971	3.034117
C	-4.928879	2.731552	2.462314
C	-5.318612	1.640577	1.693390
C	-4.453618	0.569954	1.501479
H	-1.792447	1.724085	3.268086
H	-3.337209	3.594145	3.629128
H	-5.605724	3.568759	2.608256
H	-6.301023	1.620000	1.230155
H	-4.779222	-0.263067	0.887970
C	-1.616343	-3.117816	3.238745
C	-1.439492	-3.853675	4.405638
C	-1.427308	-3.213562	5.639614
C	-1.590854	-1.832157	5.698711
C	-1.779083	-1.093928	4.536653
H	-1.619299	-3.624766	2.279704
H	-1.297659	-4.929359	4.346729
H	-1.284433	-3.786915	6.551022
H	-1.571846	-1.321718	6.657141
H	-1.895337	-0.018970	4.601610
C	-3.917821	0.905166	-2.088402
C	-4.734929	2.027236	-2.130350
C	-4.342488	3.200288	-1.488182
C	-3.131485	3.248686	-0.807978
C	-2.304915	2.129175	-0.765179
H	-4.232630	-0.010378	-2.582917
H	-5.682928	1.985022	-2.659267
H	-4.988810	4.073328	-1.512990
H	-2.828404	4.154035	-0.290061
H	-1.369646	2.158923	-0.211053
C	-1.410957	-0.054148	-4.074824
C	-1.067653	-0.411156	-5.373982
C	-0.606394	-1.692609	-5.651767
C	-0.481600	-2.621029	-4.622633
C	-0.814179	-2.267536	-3.322395
H	-1.770592	0.949478	-3.868489
H	-1.154725	0.321778	-6.170820
H	-0.325526	-1.964005	-6.664722
H	-0.103394	-3.617201	-4.830247
H	-0.704353	-2.996465	-2.521998
C	3.881601	0.008567	0.100116
C	5.187815	-0.420877	0.368442
C	5.523852	1.410535	1.898201
C	3.418948	1.161218	0.738890
C	4.230417	1.850823	1.631748
H	3.840684	2.740068	2.120648
H	2.417232	1.515919	0.538438
C	6.001468	0.270700	1.258732
H	5.566590	-1.315964	-0.120418
H	6.154458	1.951288	2.598178
H	7.009132	-0.085472	1.454691
C	1.599746	-0.953323	-0.980088
C	3.082448	-0.794073	-0.865009
C	2.286175	-0.127705	-2.045758
C	2.489222	-0.774226	-3.391159
C	2.227209	1.366938	-2.095056
H	1.312860	-1.929155	-1.374071
H	3.653464	-1.667428	-1.181462
C	3.400491	2.114359	-2.235336
C	2.115249	4.147141	-2.416699
C	1.004732	2.029690	-2.123597
C	0.942563	3.410055	-2.287813

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H	-0.024988	3.905708	-2.306431
H	0.092465	1.455283	-2.017790
C	3.345995	3.494166	-2.386851
H	4.359438	1.603705	-2.216118
H	2.072231	5.225984	-2.539039
H	4.266837	4.062458	-2.481407
C	2.439617	-0.017228	-4.569040
C	3.005121	-1.944652	-5.910574
C	2.774182	-2.143939	-3.516591
C	3.033853	-2.717826	-4.753850
H	3.266586	-3.777915	-4.811519
H	2.803807	-2.783883	-2.639005
C	2.697285	-0.593670	-5.808468
H	2.206447	1.040703	-4.513704
H	3.218906	-2.391332	-6.877417
H	2.659093	0.025582	-6.700780
C	1.495900	5.285101	1.693150
C	1.599189	5.694234	3.020530
C	1.306417	4.798555	4.047018
C	0.913982	3.499386	3.747218
H	1.028909	3.654256	0.361165
C	1.099137	3.987181	1.391989
H	1.732416	5.977040	0.889156
H	1.912541	6.707841	3.255790
H	1.392221	5.113991	5.083332
H	0.697725	2.779530	4.530806
C	0.406701	1.665359	2.107864
C	0.805975	3.085557	2.417495
O	0.189241	0.880495	3.052210
O	0.316594	1.376828	0.861834
N	0.824133	-2.129959	1.322758
C	1.161876	-3.363695	0.649672
C	1.909273	-1.773354	2.226831
H	0.347364	-3.668888	-0.025268
C	1.379523	-4.479428	1.692646
H	2.100859	-3.300129	0.062745
C	2.096202	-2.897324	3.254232
H	1.661670	-0.843954	2.750894
H	2.869688	-1.646967	1.698257
H	0.437477	-4.670476	2.230803
H	1.699552	-5.399282	1.189809
H	1.184725	-3.004260	3.861882
H	2.946455	-2.669291	3.905086
O	2.404839	-4.130183	2.602548

3_2•A
E_t = -4997.905362 a.u.

Cu	0.053416	0.382293	-0.413790
P	-1.707292	0.222112	1.007240
P	-1.463890	0.512100	-2.137223
C	-2.934904	-0.662680	-0.058992
C	-2.841595	-0.512226	-1.453818
C	-3.801870	-1.105339	-2.275759
C	-4.818980	-1.879153	-1.730726
C	-4.892431	-2.054010	-0.351987
C	-3.962407	-1.440558	0.479220
H	-3.745426	-0.967959	-3.352304
H	-5.551796	-2.346798	-2.381926
H	-5.680954	-2.663967	0.079675
H	-4.033202	-1.570016	1.555390
C	-2.623439	1.761715	1.446816
C	-1.796933	-0.712953	2.597687
C	-2.416461	1.877976	-2.944620
C	-0.817782	-0.419374	-3.576303
C	-2.033039	2.643147	2.363145
C	-2.644407	3.849566	2.678238
C	-3.852062	4.201375	2.077435
C	-4.446539	3.331331	1.170522
C	-3.840096	2.116691	0.858098
H	-1.093188	2.378461	2.839242
H	-2.173854	4.517699	3.394179
H	-4.327555	5.147227	2.320592
H	-5.390164	3.593121	0.699960
H	-4.316262	1.448908	0.146207
C	-0.873189	-1.739103	2.820880
C	-0.927543	-2.491280	3.990494
C	-1.889471	-2.214955	4.957204
C	-2.796594	-1.177969	4.753683
C	-2.753758	-0.431804	3.580826
H	-0.092731	-1.943748	2.093614
H	-0.200859	-3.283702	4.141681
H	-1.927356	-2.799983	5.872130
H	-3.543198	-0.949146	5.509111
H	-3.466341	0.374248	3.429782
C	-2.870139	1.824496	-4.266445
C	-3.601150	2.880668	-4.800477
C	-3.893847	3.998064	-4.023056
C	-3.444820	4.059411	-2.707269
C	-2.702353	3.010823	-2.176578
H	-2.642497	0.959846	-4.883563
H	-3.945714	2.828730	-5.829540
H	-4.464587	4.820624	-4.444412
H	-3.663261	4.928364	-2.092602
H	-2.348056	3.066617	-1.150751
C	0.039913	0.270827	-4.444894
C	0.688747	-0.396887	-5.474149
C	0.497392	-1.767005	-5.647759
C	-0.342206	-2.458319	-4.783273
C	-0.992411	-1.792819	-3.747248
H	0.198157	1.340098	-4.316189
H	1.348245	0.152230	-6.140262
H	1.008478	-2.291352	-6.450083
H	-0.482324	-3.529619	-4.893882
H	-1.609032	-2.359375	-3.056924
C	0.660621	-3.247638	-1.398628
C	0.774699	-4.459946	-2.091605
C	-1.187584	-5.332150	-0.988410
C	-0.396548	-3.107285	-0.500718
C	-1.311657	-4.132088	-0.293383
H	-2.129254	-3.986980	0.408655
H	-0.499360	-2.157164	0.011247
C	-0.136884	-5.490039	-1.890693
H	1.588933	-4.586765	-2.802773
H	-1.901496	-6.135791	-0.831655
H	-0.029730	-6.420697	-2.442136
C	1.523025	-0.743457	-1.164697
C	1.635975	-2.162454	-1.668710
C	2.627685	-1.639596	-0.608877
C	4.035178	-1.393186	-1.077095
C	2.538267	-2.161170	0.792692
H	1.964268	-0.092592	-1.926855
H	2.111259	-2.302816	-2.641619
C	2.553344	-1.275266	1.872541
C	2.655765	-3.112969	3.431631
C	2.570902	-3.532572	1.057405
C	2.614886	-4.006700	2.365375

3_2•A (cont)

H	2.633689	-5.077520	2.549733
H	2.566396	-4.231383	0.226122
C	2.628111	-1.743546	3.180751
H	2.519833	-0.207380	1.674479
H	2.713876	-3.480087	4.453095
H	2.662061	-1.038208	4.006475
C	4.304120	-0.929183	-2.376928
C	6.678148	-0.848374	-1.933856
C	5.133603	-1.580609	-0.225586
C	6.432665	-1.310073	-0.646855
H	7.258276	-1.464746	0.042894
H	4.971051	-1.942659	0.784105
C	5.600633	-0.664407	-2.797337
H	3.489580	-0.771990	-3.079389
H	7.691458	-0.637483	-2.262886
H	5.770306	-0.311412	-3.811393
C	1.898830	2.753565	6.234536
C	1.211767	1.570269	6.501900
C	0.738193	0.785343	5.454539
C	0.945933	1.181657	4.139268
H	2.636607	4.075588	4.693274
C	2.106491	3.156816	4.923341
H	2.272253	3.362723	7.052292
H	1.048359	1.259473	7.529995
H	0.206307	-0.141130	5.651788
H	0.588296	0.558607	3.327740
C	1.852827	2.871456	2.484669
C	1.626310	2.373093	3.869300
O	1.242574	2.032400	1.589073
O	2.466630	3.874867	2.207461
N	1.256854	2.324447	0.150352
C	0.607651	3.627860	-0.108038
C	2.646169	2.307769	-0.361089
H	-0.427230	3.568307	0.248531
C	0.645249	3.865908	-1.614427
H	1.130118	4.447805	0.398747
C	2.593658	2.629817	-1.852571
H	3.055353	1.301690	-0.215860
H	3.267607	3.052566	0.149068
H	0.072502	3.082955	-2.137569
H	0.197348	4.838751	-1.840134
H	2.044307	1.845226	-2.395801
H	3.614803	2.679391	-2.241882
O	1.983751	3.894493	-2.089867

TS[**3_2•A**–**4**]
E_t = -4997.866608 a.u.

Cu	0.378297	-0.065401	-0.250937
P	-1.294252	-0.237750	1.413929
P	-1.476603	0.005739	-1.758600
C	-2.693884	-1.059209	0.533665
C	-2.753100	-0.991503	-0.869460
C	-3.775646	-1.660333	-1.547313
C	-4.746290	-2.366355	-0.845983
C	-4.698566	-2.418182	0.544647
C	-3.672304	-1.777426	1.227786
H	-3.809758	-1.629633	-2.632850
H	-5.535661	-2.880970	-1.386727
H	-5.450963	-2.972997	1.098063
H	-3.616275	-1.845645	2.310750
C	-2.042469	1.317704	2.050022
C	-1.192062	-1.221266	2.973121
C	-2.426048	1.517084	-2.212142
C	-1.347776	-0.821217	-3.402048
C	-3.418188	1.554146	2.091965
C	-3.913639	2.708984	2.692791
C	-3.043925	3.633954	3.260153
C	-1.670640	3.409977	3.212588
C	-1.174881	2.263855	2.605304
H	-4.107304	0.831306	1.665305
H	-4.985958	2.882164	2.719758
H	-3.431895	4.537229	3.721590
H	-0.983456	4.137086	3.634950
H	-0.102328	2.098324	2.562031
C	-0.726899	-2.537863	2.885776
C	-0.602967	-3.318427	4.026417
C	-0.923594	-2.791340	5.274728
C	-1.378042	-1.480890	5.371121
C	-1.517362	-0.697338	4.227398
H	-0.448104	-2.952414	1.924206
H	-0.233145	-4.335006	3.932097
H	-0.813821	-3.398351	6.169159
H	-1.632931	-1.060786	6.340181
H	-1.882867	0.320253	4.320962
C	-3.755081	1.730735	-1.839850
C	-4.428556	2.874382	-2.263025
C	-3.785145	3.816453	-3.055942
C	-2.455132	3.617503	-3.418163
C	-1.780103	2.480460	-2.996504
H	-4.274823	0.998890	-1.229264
H	-5.462561	3.026823	-1.966298
H	-4.308376	4.712989	-3.374642
H	-1.936915	4.358001	-4.020295
H	-0.742132	2.338150	-3.284727
C	-0.329471	-1.762839	-3.586113
C	-0.196092	-2.426310	-4.801662
C	-1.065436	-2.145586	-5.851134
C	-2.070253	-1.196648	-5.681436
C	-2.212248	-0.536253	-4.465810
H	0.361812	-1.972101	-2.774526
H	0.595741	-3.158860	-4.929357
H	-0.956037	-2.658582	-6.802426
H	-2.746534	-0.966495	-6.499923
H	-2.991507	0.211340	-4.345847
C	0.679666	-3.915140	-0.049074
C	-0.644084	-3.707051	-0.440438
C	-1.374709	-5.632677	0.808438
C	0.962520	-5.024940	0.753659
C	-0.055829	-5.866403	1.190684
H	0.183219	-6.715238	1.826114
H	1.988440	-5.232454	1.036616
C	-1.663397	-4.556263	-0.024369
H	-0.872929	-2.858493	-1.073726
H	-2.168538	-6.291093	1.149644
H	-2.683756	-4.366197	-0.344359
C	1.691437	-1.538484	-0.677956
C	1.752502	-3.040921	-0.611826
C	2.758194	-2.213592	0.200444
C	4.174253	-2.142021	-0.307658
C	2.652425	-2.183319	1.700546
H	2.167643	-1.205714	-1.605475
H	2.219438	-3.542636	-1.464601
C	3.167984	-3.240149	2.461508
C	2.657702	-2.079756	4.514886
C	2.160485	-1.074255	2.383920
C	2.163798	-1.014056	3.774462

TS[**3**$_2$•A–**4**] (cont)

H	1.758651	-0.140205	4.278184
H	1.748985	-0.254599	1.804252
C	3.161367	-3.196496	3.850057
H	3.613113	-4.090460	1.951707
H	2.647682	-2.044730	5.600542
H	3.560194	-4.032843	4.417844
C	5.226857	-1.759816	0.537816
C	6.816156	-1.833487	-1.279391
C	4.488923	-2.358406	-1.659472
C	5.785690	-2.212111	-2.135458
H	5.990906	-2.393261	-3.187154
H	3.711275	-2.637265	-2.364945
C	6.524302	-1.605736	0.059637
H	5.027323	-1.573286	1.588099
H	7.828480	-1.713330	-1.653319
H	7.310759	-1.300878	0.744775
C	-2.185417	7.174448	-0.657012
C	-3.391132	6.625980	-0.221298
C	-3.457459	5.277679	0.114171
C	-2.328463	4.473634	0.012155
H	-0.101097	6.782178	-1.080966
C	-1.052574	6.376976	-0.751556
H	-2.129472	8.227412	-0.918680
H	-4.276519	7.251462	-0.143909
H	-4.394245	4.842566	0.451008
H	-2.381263	3.419111	0.256280
C	0.136890	4.200033	-0.544449
C	-1.121372	5.021193	-0.417949
O	-0.067342	2.921207	-0.327174
O	1.208775	4.731174	-0.828141
N	1.363144	1.683030	-0.447844
C	1.924599	1.942085	-1.779863
C	2.270937	2.198222	0.579538
H	1.294138	1.453256	-2.531779
C	3.361501	1.373425	-1.878714
H	1.982508	3.019874	-1.961632
C	3.657280	1.547852	0.401011
H	1.870639	1.961475	1.570027
H	2.398342	3.280511	0.472275
H	3.362275	0.277597	-1.828023
H	3.780991	1.687313	-2.840150
H	3.597177	0.455799	0.503482
H	4.330773	1.946482	1.166610
O	4.186667	1.905925	-0.861791

TS[**4**–**5**•P]
E_t = -4997.906999 a.u.

Cu	0.089351	-0.609018	0.164966
P	-2.025930	-0.781658	1.850731
P	-1.708037	-0.519497	-1.215563
C	-3.180065	-1.761091	0.797798
C	-2.993530	-1.692291	-0.595502
C	-3.830470	-2.420055	-1.446431
C	-4.847340	-3.209501	-0.922978
C	-5.052441	-3.261787	0.453802
C	-4.225566	-2.539440	1.305208
H	-3.683744	-2.369743	-2.521633
H	-5.488204	-3.776031	-1.592761
H	-5.859467	-3.862070	0.864202
H	-4.389704	-2.575042	2.378766
C	-3.068688	0.665973	2.327717
C	-1.866931	-1.797160	3.371025
C	-2.661456	1.055609	-1.182689
C	-1.568750	-0.929520	-2.994141
C	-4.385157	0.810400	1.874537
C	-5.111595	1.959405	2.167513
C	-4.541047	2.981916	2.918019
C	-3.230612	2.850783	3.365705
C	-2.494066	1.710463	3.065415
H	-4.847347	0.031899	1.276696
H	-6.129398	2.054167	1.799153
H	-5.110779	3.879113	3.143527
H	-2.763426	3.646778	3.939155
H	-1.461757	1.641546	3.390929
C	-1.886144	-3.195634	3.295910
C	-1.611573	-3.972837	4.416664
C	-1.299858	-3.367605	5.628811
C	-1.266479	-1.978138	5.709333
C	-1.540180	-1.197733	4.592684
H	-2.124847	-3.686316	2.356997
H	-1.633467	-5.056134	4.335752
H	-1.077721	-3.973430	6.502303
H	-1.014880	-1.493002	6.648057
H	-1.480021	-0.119168	4.672484
C	-3.942249	1.131566	-1.742568
C	-4.666522	2.314079	-1.670382
C	-4.126024	3.425399	-1.025435
C	-2.860514	3.349934	-0.456645
C	-2.125517	2.169439	-0.533119
H	-4.376753	0.262304	-2.230002
H	-5.659800	2.365875	-2.107454
H	-4.700581	4.344992	-0.956314
H	-2.442277	4.203203	0.069686
H	-1.147248	2.105204	-0.062052
C	-1.845591	-0.008947	-4.007453
C	-1.675207	-0.365804	-5.341840
C	-1.227017	-1.637979	-5.676330
C	-0.931452	-2.554605	-4.670597
C	-1.089613	-2.199100	-3.338636
H	-2.196630	0.987205	-3.756222
H	-1.890678	0.359137	-6.121649
H	-1.087209	-1.911571	-6.717889
H	-0.555925	-3.540937	-4.925090
H	-0.847801	-2.916124	-2.556295
C	4.141839	-0.194936	-0.220254
C	3.699003	0.913496	0.506807
C	5.893585	1.199884	1.475386
C	5.480298	-0.582959	-0.093654
C	6.349295	0.105972	0.746631
H	7.383378	-0.216280	0.832117
H	5.844216	-1.440804	-0.655211
C	4.565278	1.598973	1.349305
H	2.668054	1.236039	0.424879
H	6.567709	1.737416	2.136054
H	4.190786	2.451595	1.909945
C	1.810824	-1.234402	-1.026190
C	3.278824	-0.988603	-1.144930
C	2.317972	-0.280432	-2.140227
C	2.274606	-0.884132	-3.521392
C	2.247231	1.214050	-2.147330
H	1.486340	-2.157221	-1.494440
H	3.852009	-1.805494	-1.584660
C	1.023592	1.874053	-2.095434
C	2.108292	3.996513	-2.442365
C	3.405743	1.964466	-2.367937
C	3.338367	3.345665	-2.505159

TS[**4**–**5**•P] (cont)

H	4.249388	3.915671	-2.662833
H	4.365069	1.457843	-2.423916
C	0.948048	3.255131	-2.241752
H	0.120301	1.294491	-1.947993
H	2.055257	5.076147	-2.552702
H	-0.020151	3.747135	-2.193716
C	1.959580	-0.097838	-4.638467
C	2.351511	-1.951527	-6.137244
C	2.600778	-2.231782	-3.753294
C	2.641301	-2.755004	-5.039298
H	2.912497	-3.797670	-5.181762
H	2.843498	-2.894068	-2.927560
C	2.002734	-0.623242	-5.924740
H	1.692491	0.943956	-4.500607
H	2.394859	-2.357410	-7.143862
H	1.762388	0.019034	-6.767728
C	1.517231	4.617822	4.121133
C	1.781298	5.534879	3.105479
C	1.697952	5.136289	1.773297
C	1.345858	3.828738	1.456740
H	0.975625	2.573332	4.580388
C	1.171720	3.308641	3.805558
H	1.587230	4.925100	5.161095
H	2.055604	6.556945	3.352689
H	1.911184	5.845501	0.977757
H	1.283749	3.505329	0.422133
C	0.701917	1.481779	2.142685
C	1.078718	2.905919	2.471343
O	0.524886	0.670963	3.070891
O	0.587443	1.227920	0.888928
N	1.253277	-1.987438	0.826822
C	1.317725	-3.385046	0.439039
C	2.292776	-1.711228	1.803760
H	0.514439	-3.627280	-0.269078
C	1.133290	-4.264860	1.687831
H	2.293213	-3.644542	-0.017932
C	2.031581	-2.592234	3.031845
H	2.256453	-0.666429	2.113071
H	3.296973	-1.949348	1.416011
H	0.120990	-4.114807	2.089043
H	1.263137	-5.317584	1.409804
H	1.049840	-2.347261	3.465384
H	2.813950	-2.419364	3.777767
O	2.101090	-3.972884	2.676174

5•P

E_t = -4998.002901 a.u.

Cu	0.162191	0.701719	-0.377511
P	-1.654652	0.495330	1.136158
P	-1.451302	0.806453	-1.979231
C	-3.012870	-0.205393	0.094235
C	-2.900741	-0.109078	-1.304852
C	-3.892819	-0.664593	-2.119025
C	-4.990507	-1.304760	-1.557865
C	-5.115002	-1.379931	-0.173236
C	-4.135772	-0.830882	0.645023
H	-3.795750	-0.608075	-3.199499
H	-5.750061	-1.739562	-2.201505
H	-5.976287	-1.869040	0.272744
H	-4.237459	-0.896570	1.723571
C	-2.214353	2.222534	1.428944
C	-1.990247	-0.332290	2.751180
C	-2.120241	2.507011	-2.204080
C	-1.336745	0.159131	-3.692809
C	-3.420367	2.718710	0.928383
C	-3.754001	4.056995	1.109060
C	-2.891600	4.909544	1.790405
C	-1.694865	4.417369	2.304174
C	-1.356045	3.082001	2.123515
H	-4.095542	2.068031	0.380985
H	-4.687310	4.434817	0.701400
H	-3.149460	5.957177	1.918446
H	-1.008681	5.074111	2.831871
H	-0.419634	2.704055	2.524253
C	-1.924609	-1.730804	2.808195
C	-2.178344	-2.400666	3.995876
C	-2.475771	-1.685084	5.152996
C	-2.523463	-0.297183	5.109163
C	-2.287738	0.379337	3.914106
H	-1.682637	-2.303986	1.917543
H	-2.118981	-3.484649	4.020641
H	-2.661095	-2.209477	6.086119
H	-2.755375	0.269948	6.006394
H	-2.351073	1.462615	3.890752
C	-3.363871	2.735142	-2.802212
C	-3.850035	4.030403	-2.926807
C	-3.100589	5.106203	-2.453556
C	-1.865644	4.881894	-1.857203
C	-1.372463	3.586058	-1.728991
H	-3.957254	1.900666	-3.166281
H	-4.817749	4.201267	-3.390194
H	-3.486589	6.117768	-2.545418
H	-1.285545	5.714397	-1.469161
H	-0.424441	3.408896	-1.226806
C	-1.205892	-1.222957	-3.883861
C	-0.981002	-1.740361	-5.152334
C	-0.864494	-0.885747	-6.246975
C	-0.980474	0.487588	-6.062376
C	-1.216316	1.010613	-4.793851
H	-1.274580	-1.898073	-3.033994
H	-0.887360	-2.814635	-5.285018
H	-0.679384	-1.289997	-7.237830
H	-0.886258	1.160728	-6.909618
H	-1.301067	2.085097	-4.659690
C	3.931898	-3.333628	-0.275391
C	3.409055	-4.066660	-1.350544
C	5.604205	-4.896632	-1.934919
C	5.315907	-3.417384	-0.055379
C	6.141771	-4.178876	-0.872458
H	7.209138	-4.213279	-0.673113
H	5.750504	-2.867343	0.775885
C	4.233561	-4.835058	-2.163825
H	2.349413	-4.038081	-1.568322
H	6.243689	-5.496603	-2.575444
H	3.794552	-5.390330	-2.988240
C	2.287633	-1.247883	0.482243
C	3.170845	-2.490445	0.693189
C	1.661024	-2.502294	1.025407
C	1.393131	-2.477816	2.524871
C	0.682314	-3.364070	0.281154
H	2.469304	-0.513075	1.261059
H	3.762262	-2.360770	1.598696
C	0.825945	-4.755519	0.234275
C	-1.312787	-4.981672	-0.863563
C	-0.474101	-2.803603	-0.265587
C	-1.467578	-3.599359	-0.827623

5•P (cont)

H	-2.369869	-3.135187	-1.219647
H	-0.595186	-1.721775	-0.239212
C	-0.158101	-5.554650	-0.337297
H	1.731549	-5.212959	0.621115
H	-2.086419	-5.608885	-1.297113
H	-0.021402	-6.631906	-0.370044
C	1.204764	-1.279307	3.217199
C	1.062537	-2.467546	5.314927
C	1.393466	-3.672851	3.251944
C	1.228922	-3.669151	4.631602
H	1.240747	-4.610028	5.175293
H	1.534125	-4.619658	2.740767
C	1.049001	-1.277216	4.600486
H	1.175397	-0.329486	2.691148
H	0.937629	-2.462972	6.394143
H	0.899462	-0.330876	5.112253
C	2.094983	6.428693	0.907478
C	2.579044	6.722834	2.180163
C	2.760282	5.698187	3.106286
C	2.457556	4.385780	2.761843
H	1.406536	4.872902	-0.421505
C	1.786626	5.117120	0.565457
H	1.959203	7.225467	0.181039
H	2.817818	7.748422	2.448451
H	3.141334	5.924489	4.098425
H	2.592970	3.570231	3.465639
C	1.593108	2.663479	1.153763
C	1.963954	4.085919	1.490578
O	1.804778	1.767883	1.994505
O	1.051803	2.487211	0.005219
N	2.039011	-0.474996	-0.743529
C	3.214920	0.458620	-0.836695
C	2.020074	-1.245532	-2.017527
H	3.228302	1.084416	0.059109
C	3.159227	1.320987	-2.080173
H	4.135855	-0.148678	-0.860391
C	1.995594	-0.313143	-3.219379
H	1.148329	-1.907016	-2.036824
H	2.929239	-1.852442	-2.093961
H	2.272886	1.973823	-2.049598
H	4.056426	1.946781	-2.127468
H	1.093185	0.313172	-3.207280
H	1.991999	-0.908610	-4.138468
O	3.146867	0.519023	-3.259435

3$_3$•A

E_t = -4997.905362 a.u.

Cu	-0.184852	-0.000884	0.155125
P	-1.986353	-0.131531	1.552915
P	-1.758777	0.130346	-1.510525
C	-3.112787	-1.185736	0.528718
C	-2.990135	-1.073698	-0.870484
C	-3.773911	-1.874178	-1.702588
C	-4.689679	-2.767202	-1.159874
C	-4.836110	-2.857326	0.221496
C	-4.053480	-2.071206	1.060009
H	-3.657262	-1.801319	-2.780335
H	-5.289678	-3.391786	-1.815470
H	-5.556424	-3.548347	0.650391
H	-4.160723	-2.163662	2.136745
C	-2.978265	1.404290	1.765748
C	-2.084399	-0.914633	3.212959
C	-2.717498	1.676602	-1.744012
C	-1.463436	-0.446927	-3.227533
C	-4.317673	1.357510	2.165532
C	-5.058348	2.528200	2.263037
C	-4.469338	3.754279	1.958825
C	-3.138921	3.805058	1.560434
C	-2.392733	2.633609	1.461510
H	-4.783215	0.402766	2.396228
H	-6.099550	2.484682	2.570160
H	-5.052947	4.668254	2.026187
H	-2.678681	4.755694	1.307587
H	-1.363179	2.671428	1.117194
C	-2.285464	-0.145024	4.363361
C	-2.289002	-0.744357	5.619401
C	-2.100511	-2.117213	5.742986
C	-1.879157	-2.885479	4.603584
C	-1.852633	-2.288277	3.350601
H	-2.453605	0.924756	4.277353
H	-2.451760	-0.134122	6.503429
H	-2.114652	-2.584928	6.723281
H	-1.701296	-3.953348	4.688781
H	-1.645295	-2.899855	2.476577
C	-4.105642	1.742596	-1.602653
C	-4.766450	2.957125	-1.758328
C	-4.051678	4.109472	-2.068800
C	-2.667387	4.047830	-2.206134
C	-1.997937	2.842983	-2.030591
H	-4.671087	0.847273	-1.359675
H	-5.844814	3.000756	-1.634307
H	-4.571074	5.055847	-2.191593
H	-2.099275	4.947025	-2.429095
H	-0.911986	2.821159	-2.077210
C	-0.517945	-1.463083	-3.403362
C	-0.254197	-1.960336	-4.673993
C	-0.915376	-1.434595	-5.781845
C	-1.848737	-0.415419	-5.612600
C	-2.127421	0.076536	-4.340598
H	0.007895	-1.866598	-2.541722
H	0.474392	-2.757340	-4.793689
H	-0.701396	-1.815960	-6.776352
H	-2.364056	-0.000551	-6.474393
H	-2.857686	0.871238	-4.212711
C	1.199960	-3.091683	-0.751972
C	0.005516	-3.186699	-0.028230
C	-0.626715	-5.186606	-1.222918
C	1.470596	-4.091292	-1.695812
C	0.569420	-5.124559	-1.932137
H	0.799080	-5.879646	-2.679433
H	2.397005	-4.042406	-2.264999
C	-0.899591	-4.213154	-0.264875
H	-0.210704	-2.424791	0.716154
H	-1.338462	-5.984502	-1.413850
H	-1.833848	-4.246890	0.291542
C	1.686483	-0.581523	-0.127381
C	2.134070	-1.948895	-0.621402
C	2.643579	-1.402541	0.725264
C	4.091693	-0.994419	0.753817
C	2.174052	-2.036570	1.996811
H	2.257160	0.199768	-0.640376
H	2.916168	-1.985636	-1.381577
C	1.607005	-1.252558	3.001395
C	1.547925	-3.145862	4.491349
C	2.404102	-3.390219	2.250018
C	2.088240	-3.944255	3.486894

3$_3$•A (cont)

H	2.271536	-4.999900	3.668955
H	2.842002	-4.005970	1.468203
C	1.304654	-1.797670	4.243837
H	1.419604	-0.203346	2.794037
H	1.305029	-3.574523	5.460098
H	0.859813	-1.174726	5.015857
C	4.724187	-0.445499	-0.374094
C	6.810215	-0.205405	0.819665
C	4.862688	-1.124377	1.917144
C	6.198549	-0.735379	1.949307
H	6.764281	-0.853480	2.870135
H	4.410644	-1.535801	2.813378
C	6.058812	-0.063134	-0.344159
H	4.168036	-0.308299	-1.297304
H	7.855647	0.089382	0.841895
H	6.515927	0.348342	-1.240755
C	2.789677	2.308706	3.467032
C	4.178273	2.359822	3.377373
C	4.792994	2.530382	2.140550
C	4.025869	2.648331	0.990301
C	2.630959	2.591032	1.076720
C	2.016894	2.418701	2.320568
H	2.310224	2.166181	4.431013
H	4.783929	2.253985	4.272880
H	5.875502	2.543658	2.066865
H	4.506356	2.756863	0.025359
H	0.933409	2.362705	2.368118
C	1.753914	2.665010	-0.112082
O	2.461221	2.948110	-1.236129
O	0.552888	2.473563	-0.097279
N	1.640991	3.054166	-2.444864
C	1.624112	1.722270	-3.069716
C	2.388164	3.987498	-3.292196
H	1.056582	1.035779	-2.430008
C	0.942144	1.855872	-4.426361
H	2.647631	1.330200	-3.200310
C	1.675495	4.057888	-4.638954
H	2.392098	4.973332	-2.812884
H	3.430357	3.655734	-3.441751
H	-0.104346	2.174358	-4.294122
H	0.946686	0.889818	-4.939283
H	0.652972	4.450549	-4.500271
H	2.222388	4.725192	-5.312245
O	1.631850	2.782627	-5.262485

TS[**3**$_3$•A–**7**]
E_t = -4997.848927 a.u.

Cu	-0.063333	0.253409	0.163067
P	-1.926392	0.079910	1.543783
P	-1.653383	0.361105	-1.541754
C	-3.141461	-0.820624	0.492059
C	-2.968627	-0.762950	-0.904165
C	-3.804217	-1.513386	-1.732602
C	-4.814786	-2.298559	-1.190235
C	-5.011544	-2.327446	0.187505
C	-4.177933	-1.592721	1.023612
H	-3.650349	-1.494265	-2.807799
H	-5.449770	-2.887883	-1.845680
H	-5.806688	-2.931431	0.614980
H	-4.318943	-1.636169	2.099519
C	-2.697680	1.701050	1.907435
C	-2.048898	-0.816306	3.146908
C	-2.586863	1.946660	-1.554777
C	-1.502908	-0.126645	-3.296225
C	-1.869507	2.716198	2.398175
C	-2.395731	3.972832	2.673644
C	-3.741339	4.234071	2.431211
C	-4.560968	3.233561	1.917416
C	-4.045862	1.967340	1.663779
H	-0.806082	2.530470	2.522821
H	-1.745558	4.756334	3.052585
H	-4.146971	5.223514	2.623001
H	-5.604536	3.441517	1.699498
H	-4.686315	1.193350	1.250523
C	-1.896528	-2.207884	3.163226
C	-1.985670	-2.911877	4.355677
C	-2.188039	-2.237065	5.556193
C	-2.300959	-0.850894	5.552827
C	-2.240608	-0.142118	4.355681
H	-1.699905	-2.752561	2.244803
H	-1.867096	-3.991386	4.345937
H	-2.248191	-2.788970	6.489936
H	-2.452963	-0.313783	6.484773
H	-2.357041	0.937371	4.364674
C	-2.009572	3.069678	-0.959687
C	-2.718773	4.265341	-0.894286
C	-4.004863	4.346604	-1.415093
C	-4.589645	3.225259	-1.999910
C	-3.887516	2.027646	-2.063028
H	-1.016084	2.989661	-0.524450
H	-2.269422	5.127144	-0.409000
H	-4.560958	5.277912	-1.350321
H	-5.599217	3.280224	-2.397043
H	-4.355953	1.149750	-2.500639
C	-1.814024	0.729018	-4.357588
C	-1.539316	0.347319	-5.668955
C	-0.962061	-0.890792	-5.935872
C	-0.660357	-1.750759	-4.881733
C	-0.921737	-1.370981	-3.571237
H	-2.265914	1.696496	-4.160771
H	-1.774837	1.025335	-6.484420
H	-0.743903	-1.181584	-6.959399
H	-0.207696	-2.719758	-5.073438
H	-0.662005	-2.040393	-2.755942
C	0.762698	-3.065533	-0.986313
C	0.856733	-4.086188	-1.941572
C	-1.360513	-4.871932	-1.396130
C	-0.406633	-2.993146	-0.223002
C	-1.457094	-3.878056	-0.426065
H	-2.370259	-3.774387	0.155437
H	-0.488755	-2.198206	0.511374
C	-0.193239	-4.976152	-2.148480
H	1.757190	-4.163236	-2.547299
H	-2.188763	-5.553749	-1.565804
H	-0.103804	-5.748662	-2.907413
C	1.624877	-0.662197	-0.374184
C	1.847308	-2.062282	-0.882472
C	2.464850	-1.606156	0.464898
C	3.955070	-1.411192	0.458609
C	1.931426	-2.144663	1.754995
H	2.257245	0.074614	-0.874691
H	2.598742	-2.204290	-1.661726
C	1.949146	-3.510496	2.040308
C	1.259116	-3.069802	4.310753
C	1.539359	-1.253347	2.755454
C	1.216773	-1.707820	4.028475

TS[**3**$_3$•A–**7**] (cont)

H	0.911280	-1.001051	4.795944
H	1.521190	-0.192570	2.524630
C	1.607684	-3.971600	3.308921
H	2.246240	-4.209616	1.262825
H	0.997200	-3.427297	5.302712
H	1.623349	-5.037745	3.518345
C	4.726301	-1.664342	1.601442
C	6.760296	-1.050857	0.450611
C	4.631671	-0.950144	-0.683636
C	6.009482	-0.778136	-0.689729
H	6.499274	-0.420680	-1.591910
H	4.077095	-0.709246	-1.586514
C	6.105907	-1.487738	1.596268
H	4.239672	-1.997905	2.511617
H	7.837867	-0.912370	0.447882
H	6.670883	-1.688781	2.502823
C	5.347057	1.881532	1.666841
C	5.042556	1.743980	3.017752
C	3.723122	1.857981	3.446976
C	2.712324	2.095356	2.524546
C	3.009782	2.216143	1.164561
C	4.337380	2.119738	0.743073
H	6.371807	1.770540	1.327701
H	5.831889	1.534546	3.734493
H	3.479699	1.743817	4.499785
H	1.677553	2.173507	2.842929
H	4.561744	2.205943	-0.314274
C	1.889604	2.392210	0.175118
O	2.220402	2.755124	-0.995281
O	0.716477	2.151986	0.583581
N	0.715988	2.026445	-2.450706
C	1.504848	1.180867	-3.305672
C	0.461564	3.293769	-3.083553
H	0.848972	0.870722	-4.143671
C	2.728613	1.867569	-3.925957
H	1.783402	0.267346	-2.769085
C	1.688245	3.948589	-3.731993
H	-0.282247	3.101931	-3.883452
H	-0.001442	3.976640	-2.362542
H	3.195588	1.209135	-4.665316
H	3.449072	2.096657	-3.126494
H	1.383402	4.812391	-4.331339
H	2.366859	4.275640	-2.931588
O	2.346373	3.049959	-4.613016

TS[**7**–**5**]
E_t = -4997.868295 a.u.

Cu	0.007568	0.073362	0.299441
P	-1.822717	-0.070082	1.746215
P	-1.596973	0.227244	-1.372672
C	-3.186793	-0.735950	0.700540
C	-3.065816	-0.647991	-0.701010
C	-4.055388	-1.203967	-1.514622
C	-5.157333	-1.837891	-0.954153
C	-5.292549	-1.902761	0.429946
C	-4.315716	-1.350583	1.250346
H	-3.952179	-1.155178	-2.594735
H	-5.912110	-2.278053	-1.599517
H	-6.158126	-2.386626	0.873349
H	-4.420691	-1.410874	2.329537
C	-2.309072	1.665824	2.073840
C	-2.059571	-0.951073	3.338896
C	-2.168210	1.971477	-1.452035
C	-1.495329	-0.283238	-3.125381
C	-1.354351	2.503776	2.660964
C	-1.618241	3.860000	2.812747
C	-2.826738	4.390536	2.371070
C	-3.780748	3.557668	1.794815
C	-3.527859	2.198273	1.647396
H	-0.392191	2.104384	2.972825
H	-0.859412	4.504985	3.246295
H	-3.017931	5.456284	2.460273
H	-4.718637	3.969477	1.433813
H	-4.267034	1.560290	1.172012
C	-2.038544	-2.350590	3.340652
C	-2.180068	-3.054493	4.528227
C	-2.304000	-2.372940	5.736144
C	-2.292276	-0.982063	5.744877
C	-2.179768	-0.271101	4.552858
H	-1.897557	-2.899785	2.413949
H	-2.164727	-4.140599	4.510913
H	-2.400224	-2.924654	6.666993
H	-2.380243	-0.442198	6.683322
H	-2.189788	0.814511	4.570104
C	-3.440041	2.307121	-1.925516
C	-3.843480	3.636328	-1.943214
C	-2.984712	4.635642	-1.487043
C	-1.720163	4.304189	-1.015821
C	-1.310847	2.974524	-0.996700
H	-4.116687	1.529077	-2.269346
H	-4.834928	3.893164	-2.304961
H	-3.309718	5.672297	-1.488329
H	-1.046103	5.069338	-0.640173
H	-0.334748	2.714558	-0.595542
C	-1.305009	0.670172	-4.131538
C	-1.060441	0.270065	-5.441157
C	-1.006421	-1.082495	-5.763730
C	-1.208884	-2.036238	-4.768652
C	-1.446651	-1.643910	-3.457204
H	-1.342600	1.727866	-3.887609
H	-0.909959	1.021450	-6.211242
H	-0.810616	-1.392251	-6.786214
H	-1.173957	-3.095485	-5.007799
H	-1.593490	-2.399793	-2.692391
C	0.311785	-3.330888	-1.120577
C	0.194466	-4.360858	-2.061763
C	-2.017942	-4.903282	-1.267742
C	-0.751029	-3.126385	-0.237004
C	-1.906961	-3.894522	-0.315700
H	-2.738735	-3.688102	0.353316
H	-0.675490	-2.335589	0.503741
C	-0.955122	-5.140166	-2.135809
H	1.008015	-4.530499	-2.763262
H	-2.926044	-5.495391	-1.333656
H	-1.026748	-5.926611	-2.882017
C	1.613326	-1.064398	-0.717334
C	1.530205	-2.480328	-1.160695
C	2.364593	-2.061597	0.073572
C	3.868112	-2.111248	0.021564
C	1.842348	-2.384553	1.448416
H	2.138260	-2.669936	-2.044510
H	1.819308	-0.086521	-1.141719
C	1.673391	-3.714408	1.837792
C	1.117477	-3.000774	4.075565
C	1.627019	-1.365704	2.379089
C	1.270319	-1.674986	3.689376

TS[**7**–**5**] (cont)

H	1.110253	-0.867709	4.398857
H	1.773827	-0.320262	2.114531
C	1.310093	-4.020102	3.144198
H	1.835819	-4.506278	1.111226
H	0.830631	-3.240557	5.095272
H	1.181582	-5.058056	3.438454
C	4.555658	-2.988034	-0.813567
C	6.668943	-2.139828	-0.010108
C	4.598098	-1.255036	0.853234
C	5.987421	-1.269191	0.837281
H	6.538647	-0.592703	1.484497
H	4.072503	-0.565625	1.509043
C	5.947801	-2.998412	-0.833452
H	4.001443	-3.660785	-1.460311
H	7.754886	-2.151454	-0.024845
H	6.469293	-3.684662	-1.494731
N	3.094017	-0.635306	-2.532616
C	4.183450	0.273369	-2.236829
C	2.199141	-0.020509	-3.496606
H	4.794720	0.362868	-3.156591
C	3.725908	1.677890	-1.847764
H	4.822709	-0.154676	-1.457899
C	1.784021	1.420602	-3.159838
H	2.726588	0.001371	-4.469302
H	1.306565	-0.649031	-3.622936
H	4.576454	2.355813	-1.724975
H	3.172474	1.628666	-0.895849
H	1.271194	1.882839	-4.009204
H	1.084177	1.411488	-2.302957
O	2.903935	2.245608	-2.869770
C	2.161316	5.662266	-0.303211
C	2.330829	6.514051	0.785452
C	2.310550	5.996893	2.079435
C	2.119825	4.635473	2.281855
H	1.818547	3.640896	-0.950974
C	1.949947	4.302368	-0.100340
H	2.192561	6.056541	-1.315414
H	2.485690	7.577679	0.626259
H	2.448110	6.657613	2.931012
H	2.110622	4.206185	3.279359
C	1.638957	2.321883	1.457800
C	1.924393	3.779716	1.195526
O	1.806566	1.861711	2.595236
O	1.190078	1.670154	0.436861

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E_t = -3900.661730 a.u.

Cu	1.080167	-0.539838	-0.017462
P	-0.655073	-0.722719	1.378688
P	-0.373868	-0.417900	-1.703959
C	-1.964050	-1.479939	0.328850
C	-1.824789	-1.368001	-1.069832
C	-2.772688	-1.964456	-1.903331
C	-3.846812	-2.663798	-1.363287
C	-3.984925	-2.772318	0.017467
C	-3.047232	-2.183690	0.858903
H	-2.657544	-1.896853	-2.981989
H	-4.572917	-3.130223	-2.023071
H	-4.819841	-3.322992	0.441288
H	-3.147806	-2.280581	1.936708
C	-1.250172	0.979020	1.711122
C	-0.840524	-1.588411	2.983880
C	-1.035578	1.290148	-1.839016
C	-0.213003	-1.003378	-3.432276
C	-2.545328	1.406658	1.412304
C	-2.910526	2.730520	1.635709
C	-1.991479	3.629415	2.167116
C	-0.698102	3.206806	2.463396
C	-0.320906	1.891275	2.224478
H	-3.264303	0.709991	0.989821
H	-3.915290	3.060107	1.387157
H	-2.278965	4.663033	2.338508
H	0.028343	3.909086	2.862049
H	0.704459	1.576288	2.402415
C	-1.576126	-1.064924	4.050142
C	-1.675575	-1.775125	5.242916
C	-1.046850	-3.009054	5.378359
C	-0.307045	-3.531331	4.320021
C	-0.195199	-2.820965	3.131357
H	-2.067469	-0.101144	3.947452
H	-2.246538	-1.361203	6.069231
H	-1.124333	-3.559704	6.311449
H	0.196758	-4.487628	4.426449
H	0.404398	-3.215233	2.313629
C	-2.312498	1.554601	-2.343301
C	-2.791828	2.858166	-2.378619
C	-2.002981	3.903904	-1.903978
C	-0.734353	3.643956	-1.397919
C	-0.247212	2.340605	-1.362487
H	-2.937086	0.739267	-2.699338
H	-3.785677	3.058097	-2.769270
H	-2.383177	4.921588	-1.922783
H	-0.121575	4.454572	-1.014799
H	0.735609	2.133632	-0.943286
C	-0.321056	-0.151977	-4.534018
C	-0.114146	-0.644067	-5.820166
C	0.198524	-1.984229	-6.017884
C	0.316483	-2.835844	-4.920901
C	0.123586	-2.347895	-3.635969
H	-0.565804	0.896017	-4.388510
H	-0.199184	0.026647	-6.670415
H	0.358888	-2.364845	-7.022377
H	0.571655	-3.881437	-5.067161
H	0.235434	-3.012577	-2.781859
C	6.504727	2.142278	1.160936
C	7.471936	1.140387	1.127898
C	7.101381	-0.174849	0.856855
C	5.768754	-0.488804	0.619956
C	4.796351	0.513448	0.652685
C	5.171444	1.831133	0.924193
H	6.793111	3.168429	1.371523
H	8.514486	1.384613	1.312867
H	7.855354	-0.956666	0.830399
H	5.459365	-1.506794	0.406582
C	3.363252	0.181768	0.400035
H	4.401740	2.596062	0.943830
O	2.487360	1.097212	0.436235
O	3.043870	-1.027336	0.154405

5•T

E_t = -4133.060922 a.u.

Cu	0.622157	0.096882	0.014972
P	-1.122549	-0.086592	1.421337
P	-0.850978	0.215549	-1.666179
C	-2.223603	-1.124791	0.365155
C	-2.118350	-0.966597	-1.033317
C	-2.916665	-1.746126	-1.871563
C	-3.807109	-2.672161	-1.337450
C	-3.904808	-2.832677	0.041218
C	-3.114125	-2.062904	0.888193
H	-2.826748	-1.639978	-2.949102
H	-4.415880	-3.278657	-2.001965
H	-4.588595	-3.566084	0.459119
H	-3.171113	-2.206436	1.964392
C	-2.165085	1.382090	1.778943
C	-1.026362	-1.028059	2.986927
C	-1.747453	1.817779	-1.740202
C	-0.651707	-0.232686	-3.432111
C	-3.524053	1.286550	2.093864
C	-4.275467	2.436453	2.306135
C	-3.678955	3.690331	2.196489
C	-2.330691	3.792331	1.871128
C	-1.576058	2.643038	1.659914
H	-3.999421	0.311027	2.158924
H	-5.331260	2.354510	2.549066
H	-4.270290	4.588252	2.352991
H	-1.867559	4.768557	1.762108
H	-0.531654	2.720363	1.366159
C	-1.648950	-0.646022	4.177229
C	-1.478059	-1.409781	5.329364
C	-0.689846	-2.555231	5.300957
C	-0.055308	-2.931191	4.118157
C	-0.209636	-2.167772	2.968760
H	-2.263900	0.248793	4.208048
H	-1.964898	-1.106127	6.251905
H	-0.559921	-3.149268	6.201089
H	0.574839	-3.815733	4.094336
H	0.318895	-2.437094	2.056114
C	-3.114466	1.944226	-1.486274
C	-3.716643	3.198849	-1.499841
C	-2.963273	4.334628	-1.775400
C	-1.599208	4.214839	-2.032080
C	-0.992347	2.965800	-2.004777
H	-3.708556	1.062113	-1.263742
H	-4.778460	3.286614	-1.287927
H	-3.435447	5.313013	-1.784098
H	-1.004337	5.098926	-2.243604
H	0.077512	2.877049	-2.180497
C	0.422560	-1.062210	-3.768157
C	0.605721	-1.450192	-5.092115
C	-0.265517	-1.005318	-6.081850
C	-1.324562	-0.162829	-5.750661
C	-1.518677	0.225734	-4.429917
H	1.130779	-1.368141	-2.999753
H	1.444225	-2.090853	-5.349543
H	-0.113778	-1.304400	-7.115366
H	-1.998973	0.195455	-6.523469
H	-2.340314	0.889875	-4.173189
O	1.827517	1.924341	0.199554
C	2.479241	2.137388	1.469056
H	1.846077	1.688273	2.240441
H	2.566232	3.221615	1.649992
C	3.844256	1.479117	1.321524
H	4.584166	1.908136	2.003631
H	3.756965	0.408688	1.522821
C	4.193526	1.723055	-0.163370
H	4.905630	2.546476	-0.274460
H	4.626212	0.829793	-0.619728
C	2.848240	2.079982	-0.824507
H	2.830606	3.123575	-1.170875
H	2.584614	1.402568	-1.641138
C	5.153498	-3.618919	1.784305
C	6.140434	-4.008707	0.882232
C	6.074503	-3.583984	-0.442868
C	5.027104	-2.773083	-0.863475
C	4.033414	-2.380318	0.035564
C	4.104657	-2.808767	1.363509
H	5.203611	-3.947683	2.818948
H	6.960071	-4.641744	1.211456
H	6.843483	-3.886612	-1.148530

5•T (cont)

H	4.954914	-2.427876	-1.890240
C	2.914394	-1.484855	-0.436610
H	3.328075	-2.494598	2.054209
O	2.907214	-1.091208	-1.614457
O	2.046274	-1.178373	0.464173

5•S

E_t = -4479.235328 a.u.

Cu	0.518118	-0.027884	-0.367977
P	-1.393119	-0.163420	0.926211
P	-1.110992	0.120215	-2.195530
C	-2.555987	-1.114177	-0.142887
C	-2.440896	-0.971132	-1.540144
C	-3.291947	-1.699200	-2.374520
C	-4.247393	-2.553976	-1.837292
C	-4.361874	-2.693799	-0.457583
C	-3.517966	-1.979030	0.384087
H	-3.194468	-1.605833	-3.452246
H	-4.896755	-3.119547	-2.499455
H	-5.099844	-3.369681	-0.035088
H	-3.588248	-2.111256	1.460519
C	-2.330710	1.355524	1.351758
C	-1.363801	-1.138867	2.472302
C	-1.903119	1.775582	-2.257161
C	-0.982769	-0.335612	-3.966359
C	-3.704074	1.334430	1.612414
C	-4.377138	2.513956	1.906947
C	-3.686384	3.723290	1.942406
C	-2.319626	3.749381	1.687640
C	-1.643875	2.569755	1.391924
H	-4.250946	0.396011	1.573530
H	-5.445101	2.490381	2.105063
H	-4.216276	4.645119	2.165594
H	-1.777707	4.690418	1.707630
H	-0.579851	2.584213	1.177866
C	-1.766000	-0.618012	3.703066
C	-1.686179	-1.402774	4.850139
C	-1.202416	-2.704343	4.776634
C	-0.791118	-3.222434	3.550093
C	-0.863790	-2.445221	2.401896
H	-2.140104	0.399392	3.768599
H	-2.003495	-0.991657	5.804437
H	-1.143218	-3.314804	5.673420
H	-0.407506	-4.237127	3.486060
H	-0.525855	-2.838621	1.446800
C	-3.199541	2.028558	-1.805814
C	-3.700121	3.327351	-1.798123
C	-2.917799	4.383588	-2.250528
C	-1.628329	4.137484	-2.718472
C	-1.121547	2.844412	-2.715341
H	-3.819581	1.210482	-1.451083
H	-4.706376	3.510750	-1.432455
H	-3.310098	5.396437	-2.242159
H	-1.014180	4.956453	-3.082175
H	-0.114040	2.656553	-3.082287
C	-1.829017	0.198608	-4.944693
C	-1.694386	-0.197015	-6.270640
C	-0.717659	-1.124282	-6.627221
C	0.130305	-1.648631	-5.656733
C	0.008339	-1.253652	-4.327582
H	-2.588956	0.925208	-4.668723
H	-2.352764	0.220448	-7.027392
H	-0.613129	-1.429717	-7.664691
H	0.903390	-2.359980	-5.932673
H	0.695994	-1.635482	-3.574113
C	1.390327	1.821622	-0.347020
C	2.312306	0.899087	-0.702240
C	2.540228	1.589689	0.624479
C	3.627694	2.624550	0.652166
C	2.286999	0.852900	1.908331
H	0.869967	2.680614	-0.756446
H	2.902219	0.535054	-1.533309
C	2.724734	-0.459800	2.074390
C	1.821527	-0.504120	4.310561
C	1.622648	1.484277	2.963222
C	1.386889	0.809987	4.155167
H	0.857314	1.306986	4.963482
H	1.295326	2.515123	2.844816
C	2.490965	-1.135795	3.268593
H	3.233976	-0.957853	1.253911
H	1.625487	-1.036877	5.236452
H	2.831105	-2.161622	3.380708
C	3.859666	3.441146	-0.463646
C	5.679008	4.549098	0.668672
C	4.450330	2.788051	1.772930
C	5.464102	3.739579	1.779487
H	6.092169	3.846235	2.659634

5•S (cont)

H	4.294727	2.160674	2.644897
C	4.871540	4.393328	-0.454001
H	3.246678	3.323522	-1.352637
H	6.471775	5.291445	0.675401
H	5.032807	5.014602	-1.330696
C	3.679971	-5.766612	-1.011895
C	3.498503	-6.198981	0.299926
C	2.777351	-5.412146	1.194287
C	2.230171	-4.204240	0.775676
C	2.408771	-3.766781	-0.538886
C	3.145089	-4.553010	-1.426842
H	4.245949	-6.376726	-1.710522
H	3.922968	-7.144778	0.625562
H	2.643637	-5.741601	2.221450
H	1.672298	-3.577217	1.463982
C	1.852276	-2.444887	-1.003927
H	3.289034	-4.188506	-2.439194
O	2.245834	-1.957110	-2.071716
O	0.987560	-1.915741	-0.203104

5•A

E_t = -4607.871087 a.u.

Cu	0.675428	-0.189835	0.536442
P	-1.013525	-0.399555	1.980829
P	-0.747436	-0.069009	-1.213011
C	-2.538686	-0.126005	0.957737
C	-2.424110	-0.068218	-0.441168
C	-3.583396	-0.051626	-1.224982
C	-4.838563	-0.026420	-0.634474
C	-4.950369	-0.022662	0.754568
C	-3.809183	-0.084131	1.541667
H	-3.493179	-0.064065	-2.308405
H	-5.730068	-0.011237	-1.255048
H	-5.929493	0.009056	1.224121
H	-3.905990	-0.094779	2.623186
C	-1.274080	0.672448	3.443305
C	-1.268648	-2.099012	2.648566
C	-0.723705	1.327616	-2.395439
C	-0.838808	-1.570098	-2.269840
C	-0.747565	0.296303	4.686340
C	-0.784576	1.174895	5.762908
C	-1.341446	2.442566	5.615184
C	-1.864407	2.823812	4.382585
C	-1.829363	1.950042	3.301691
H	-0.311663	-0.691398	4.813680
H	-0.377588	0.866009	6.721726
H	-1.369237	3.128430	6.456878
H	-2.300267	3.811153	4.258220
H	-2.219125	2.265325	2.339221
C	-0.414756	-3.103580	2.181931
C	-0.570789	-4.414913	2.625337
C	-1.565488	-4.730048	3.543768
C	-2.406691	-3.728944	4.025597
C	-2.261265	-2.421035	3.580565
H	0.375494	-2.855801	1.474389
H	0.095911	-5.188487	2.254583
H	-1.682858	-5.752190	3.892713
H	-3.178066	-3.968707	4.752085
H	-2.910499	-1.646329	3.977792
C	-1.732651	2.285293	-2.516644
C	-1.586554	3.347591	-3.404240
C	-0.435886	3.468095	-4.174488
C	0.584152	2.529798	-4.038214
C	0.453953	1.472894	-3.146228
H	-2.628590	2.216842	-1.907991
H	-2.375405	4.090372	-3.484942
H	-0.323971	4.302158	-4.861297
H	1.497443	2.629121	-4.618526
H	1.264184	0.757931	-3.012985
C	-0.728577	-1.555048	-3.661196
C	-0.729517	-2.749952	-4.374589
C	-0.842518	-3.967089	-3.711585
C	-0.966078	-3.986617	-2.325706
C	-0.960707	-2.797790	-1.608879
H	-0.634424	-0.612876	-4.191979
H	-0.634718	-2.726002	-5.456701
H	-0.824499	-4.898097	-4.270545
H	-1.043227	-4.931801	-1.796354
H	-1.036875	-2.825252	-0.524712
C	-0.445984	6.292963	-1.544849
C	0.652345	6.645703	-2.324378
C	1.783272	5.833643	-2.343056
C	1.824916	4.675340	-1.578635
C	0.723233	4.320692	-0.794996
C	-0.414355	5.131286	-0.786619
H	-1.329889	6.923875	-1.531120
H	0.627140	7.554654	-2.918961
H	2.637363	6.104550	-2.956664
H	2.702388	4.038782	-1.596758
C	0.703403	3.108364	0.064104
H	-1.262273	4.832306	-0.178707
O	1.939884	2.555190	0.134691
O	-0.271952	2.697183	0.655107
N	2.078299	1.367416	1.008669
C	3.471242	0.941517	0.704045
C	2.023113	1.870154	2.408533
H	3.475866	0.522103	-0.308105
C	3.912563	-0.106305	1.719015
H	4.135379	1.816380	0.767362
C	2.513187	0.772702	3.344862
H	0.991492	2.141407	2.647754

5•A (cont)

H	2.675138	2.751478	2.502509
H	3.298600	-1.012322	1.622511
H	4.958035	-0.362796	1.523313
H	1.846751	-0.104780	3.274399
H	2.490609	1.147676	4.372973
O	3.850191	0.404279	3.051255
C	2.587765	-5.633797	-1.431288
C	2.855860	-5.770228	-2.791714
C	2.943183	-4.637233	-3.596633
C	2.763445	-3.374244	-3.045128
C	2.482852	-3.231890	-1.685794
C	2.397859	-4.371130	-0.882677
H	2.526227	-6.515955	-0.799286
H	2.999456	-6.757672	-3.222319
H	3.150750	-4.740587	-4.658392
H	2.820717	-2.477611	-3.654103
C	2.229333	-1.858459	-1.121550
H	2.178275	-4.248046	0.173412
O	2.426183	-0.860778	-1.839474
O	1.790657	-1.824949	0.089241

5•P

E_t = -4998.017061 a.u.

Cu	-0.666594	-0.431403	0.088557
P	-2.481478	-0.605973	1.518982
P	-2.156984	-0.296537	-1.593116
C	-3.675669	-1.479434	0.431833
C	-3.514152	-1.373589	-0.959371
C	-4.375929	-2.077077	-1.802868
C	-5.390677	-2.865991	-1.273790
C	-5.555643	-2.961198	0.105142
C	-4.698413	-2.272550	0.954191
H	-4.240161	-2.019589	-2.879279
H	-6.049253	-3.414738	-1.941146
H	-6.344384	-3.581927	0.520341
H	-4.810690	-2.362286	2.031386
C	-3.380184	0.900203	2.057309
C	-2.430165	-1.678382	3.008598
C	-3.008402	1.326225	-1.757195
C	-1.971673	-0.890318	-3.318303
C	-2.820897	1.707941	3.058391
C	-3.417475	2.913746	3.404928
C	-4.567704	3.342911	2.746369
C	-5.124103	2.549878	1.748814
C	-4.540539	1.333168	1.409835
H	-1.908929	1.406881	3.568245
H	-2.974020	3.521017	4.189259
H	-5.027623	4.290549	3.011684
H	-6.019564	2.875474	1.227124
H	-4.987658	0.721600	0.632584
C	-3.027177	-1.358860	4.230666
C	-2.913252	-2.230123	5.310849
C	-2.212300	-3.424462	5.178709
C	-1.625660	-3.751236	3.958139
C	-1.725817	-2.882770	2.878882
H	-3.588400	-0.435807	4.340503
H	-3.381503	-1.974325	6.257266
H	-2.125084	-4.101051	6.024157
H	-1.081534	-4.684347	3.843602
H	-1.278862	-3.145192	1.923079
C	-4.354367	1.453401	-2.114933
C	-4.951041	2.708145	-2.159755
C	-4.211295	3.846616	-1.846763
C	-2.870043	3.727328	-1.498876
C	-2.273267	2.471813	-1.451479
H	-4.940864	0.567411	-2.345145
H	-5.998750	2.797770	-2.433508
H	-4.682770	4.825116	-1.872655
H	-2.286834	4.611369	-1.256324
H	-1.225940	2.372300	-1.180279
C	-2.359401	-0.138914	-4.429087
C	-2.119191	-0.617793	-5.714246
C	-1.494030	-1.847133	-5.897810
C	-1.113580	-2.602177	-4.789419
C	-1.343460	-2.128633	-3.503334
H	-2.833703	0.828634	-4.293023
H	-2.420071	-0.025307	-6.574026
H	-1.303065	-2.216818	-6.901328
H	-0.626982	-3.563831	-4.926255
H	-1.043634	-2.713111	-2.634496
C	3.036216	0.268883	0.029770
C	2.314305	1.315074	0.821480
C	2.761442	1.648944	-0.583932
C	3.923641	2.597102	-0.691855
C	1.825857	1.767635	-1.754826
C	1.504027	0.684760	-2.574179
C	0.294304	2.135127	-4.077998
C	1.365715	3.039889	-2.119836
C	0.599858	3.222069	-3.263779
H	0.251109	4.216810	-3.527515
H	1.646977	3.899764	-1.516593
C	0.753341	0.870256	-3.731967
H	1.859389	-0.310368	-2.325950
H	-0.294002	2.272638	-4.980584
H	0.527161	0.017752	-4.365002
C	4.936475	2.325199	-1.614743
C	6.098326	4.338970	-0.975730
C	4.010972	3.755458	0.079545
C	5.090616	4.623677	-0.060991
H	5.143639	5.522755	0.546701
H	3.225105	3.982834	0.796360
C	6.016435	3.186319	-1.753952

5•P (cont)

H	4.874663	1.420385	-2.214026
H	6.944771	5.011167	-1.082414
H	6.802107	2.954953	-2.467385
H	2.366216	-0.508981	-0.327243
C	4.402585	-0.221025	0.342845
H	2.918942	1.816701	1.579105
C	0.934533	0.320109	2.494181
C	1.331753	1.170037	3.692390
O	0.486995	2.320237	3.800800
C	0.598888	3.127831	2.629759
C	0.194282	2.354617	1.379855
N	0.928337	1.073295	1.202435
H	1.594737	-0.545919	2.376479
H	-0.075597	-0.065859	2.669588
H	1.191720	0.593891	4.613043
H	2.387446	1.488149	3.651264
H	-0.076166	3.979172	2.771958
H	1.628587	3.519807	2.549056
H	-0.875993	2.125150	1.437303
H	0.359469	2.968029	0.486130
C	4.833282	-1.405558	-0.265594
C	6.973154	-1.247017	0.831927
C	5.287648	0.442566	1.198337
C	6.558959	-0.065752	1.439815
H	7.230958	0.467765	2.106195
H	4.994663	1.374645	1.672532
C	6.102806	-1.916408	-0.022989
H	4.154153	-1.938814	-0.926373
H	7.966611	-1.642133	1.023229
H	6.409601	-2.842007	-0.502292
C	2.032632	-6.416505	-0.178938
C	3.247458	-6.147959	0.448992
C	3.515544	-4.864814	0.919304
C	2.575310	-3.853692	0.756623
C	1.359001	-4.114916	0.121778
C	1.091231	-5.406543	-0.337878
H	1.820184	-7.417904	-0.543508
H	3.982117	-6.938864	0.574396
H	4.459333	-4.648409	1.412889
H	2.775258	-2.850216	1.117549
C	0.329376	-3.031058	-0.061112
H	0.134722	-5.594351	-0.815964
O	-0.807294	-3.329109	-0.470461
O	0.714957	-1.842852	0.250382

5•B

E_t = -4504.132911 a.u.

Cu	0.272912	-0.237180	-0.027065
P	-1.455318	-0.523155	1.382347
P	-1.194726	-0.140743	-1.697708
C	-2.558328	-1.529667	0.302046
C	-2.445416	-1.343097	-1.088867
C	-3.249453	-2.086806	-1.952711
C	-4.159086	-3.008432	-1.447043
C	-4.269842	-3.194207	-0.071932
C	-3.473541	-2.458098	0.798361
H	-3.149988	-1.951165	-3.026503
H	-4.775240	-3.588804	-2.127786
H	-4.972123	-3.921673	0.325278
H	-3.545326	-2.623112	1.870136
C	-2.472168	0.977102	1.694157
C	-1.424341	-1.436163	2.965161
C	-2.144874	1.406636	-1.949973
C	-0.777519	-0.734418	-3.376767
C	-3.802095	0.910327	2.120992
C	-4.549572	2.072780	2.266985
C	-3.979144	3.311609	1.980871
C	-2.659748	3.385655	1.548936
C	-1.910050	2.222543	1.404294
H	-4.256511	-0.055273	2.328961
H	-5.583240	2.012405	2.595982
H	-4.569403	4.217815	2.084667
H	-2.217553	4.346457	1.302181
H	-0.890725	2.273123	1.027609
C	-1.800351	-0.867042	4.184803
C	-1.637156	-1.582420	5.368574
C	-1.100014	-2.864951	5.344284
C	-0.713853	-3.430688	4.129874
C	-0.861355	-2.721260	2.945522
H	-2.222902	0.133462	4.212333
H	-1.934866	-1.133664	6.312253
H	-0.975142	-3.421118	6.268992
H	-0.282453	-4.427390	4.105216
H	-0.532977	-3.151010	1.999717
C	-3.508609	1.507340	-1.663480
C	-4.156295	2.734731	-1.766321
C	-3.454598	3.867849	-2.163726
C	-2.095695	3.771790	-2.455635
C	-1.440433	2.552481	-2.339986
H	-4.063761	0.629806	-1.345270
H	-5.214183	2.803069	-1.528882
H	-3.963550	4.824522	-2.242531
H	-1.535870	4.650116	-2.765280
H	-0.376487	2.491756	-2.550918
C	-1.140089	-0.065364	-4.546922
C	-0.703358	-0.538512	-5.781553
C	0.088011	-1.680433	-5.854520
C	0.443062	-2.354749	-4.687095
C	0.022553	-1.882555	-3.450397
H	-1.756078	0.827860	-4.494967
H	-0.985938	-0.012109	-6.689077
H	0.429001	-2.045633	-6.819222
H	1.060506	-3.247051	-4.737944
H	0.307580	-2.399738	-2.534843
B	2.155619	2.519594	0.151086
O	1.597683	1.424077	0.774963
O	2.748380	3.529186	0.853465
C	1.795077	1.192997	2.190771
C	3.003047	1.957246	2.725945
C	2.850657	3.413993	2.282349
C	2.101216	2.590156	-1.404863
C	2.990964	1.890395	4.254058
C	4.302849	1.353031	2.178627
H	0.877154	1.500253	2.712934
H	1.953523	3.857396	2.740054
H	3.721481	4.006651	2.587036
H	1.922095	0.110667	2.309371
H	3.041415	0.850280	4.593958
H	2.081048	2.339023	4.668705
H	3.854964	2.420153	4.670098
H	4.330336	1.351198	1.084434
H	4.405573	0.315108	2.511972
H	5.169729	1.919370	2.536171
C	2.022848	3.822459	-2.069410
C	1.935761	2.706179	-4.204855
C	2.122377	1.416823	-2.176754

5•B (cont)

C	2.043910	1.474360	-3.565236
H	2.053304	0.555893	-4.146059
H	2.213819	0.448960	-1.687231
C	1.931454	3.881823	-3.456101
H	2.024557	4.741634	-1.488226
H	1.860199	2.750458	-5.288093
H	1.858392	4.843836	-3.956329
C	5.228128	-3.852376	0.299247
C	5.027501	-5.230434	0.268914
C	3.737215	-5.740103	0.142780
C	2.652757	-4.876048	0.047903
C	2.847598	-3.493587	0.080458
C	4.143668	-2.987588	0.206050
H	6.234178	-3.452524	0.393932
H	5.875594	-5.906007	0.341555
H	3.578458	-6.814826	0.116995
H	1.638439	-5.249319	-0.054708
C	1.661044	-2.573437	-0.021315
H	4.281838	-1.911157	0.224981
O	0.519726	-3.054490	-0.160613
O	1.922144	-1.314856	0.045374

TS[**5**•B**–XO2**]

E_t = -4504.127836 a.u.

Cu	0.559125	0.554899	-0.596214
P	-1.224622	0.342388	0.827465
P	-0.993600	0.674013	-2.272502
C	-2.272017	-0.754271	-0.233493
C	-2.148804	-0.611788	-1.633246
C	-2.867698	-1.455945	-2.481691
C	-3.706682	-2.434323	-1.957266
C	-3.837598	-2.570847	-0.577218
C	-3.125434	-1.735187	0.278350
H	-2.758120	-1.350887	-3.558708
H	-4.256627	-3.091103	-2.626517
H	-4.491347	-3.334979	-0.164101
H	-3.212573	-1.862726	1.354564
C	-2.286186	1.818333	1.089322
C	-1.129227	-0.524038	2.432187
C	-2.061385	2.152705	-2.468649
C	-0.572963	0.124461	-3.966151
C	-3.605738	1.723048	1.541412
C	-4.396080	2.863207	1.635850
C	-3.877210	4.105893	1.274520
C	-2.565337	4.208085	0.823118
C	-1.772816	3.067946	0.729649
H	-4.015625	0.751852	1.809226
H	-5.422532	2.781812	1.983963
H	-4.502265	4.993386	1.335379
H	-2.164564	5.171826	0.519861
H	-0.758691	3.135299	0.342731
C	-1.330357	0.136267	3.648057
C	-1.098241	-0.527995	4.850807
C	-0.657236	-1.848766	4.852899
C	-0.442650	-2.506635	3.642706
C	-0.668494	-1.848352	2.440523
H	-1.665267	1.170488	3.655532
H	-1.261575	-0.007552	5.791170
H	-0.474525	-2.361822	5.793581
H	-0.084209	-3.533378	3.628746
H	-0.478398	-2.363430	1.502939
C	-3.401339	2.161093	-2.068897
C	-4.141551	3.338492	-2.116645
C	-3.558674	4.516982	-2.571285
C	-2.225628	4.515539	-2.978611
C	-1.477994	3.344694	-2.919304
H	-3.862201	1.249758	-1.698506
H	-5.176117	3.333236	-1.783817
H	-4.138457	5.435964	-2.602606
H	-1.763516	5.432804	-3.335622
H	-0.431894	3.351321	-3.214210
C	-1.160352	0.649742	-5.119464
C	-0.761839	0.191776	-6.373421
C	0.216999	-0.792330	-6.481537
C	0.805540	-1.317722	-5.331745
C	0.422707	-0.856522	-4.077771
H	-1.927366	1.415511	-5.034994
H	-1.223185	0.602378	-7.267823
H	0.524449	-1.148133	-7.461503
H	1.573405	-2.083117	-5.412785
H	0.889154	-1.251230	-3.176605
O	2.043361	0.312067	1.868084
O	4.366374	0.263406	1.160662
O	0.841523	-1.475906	-0.722267
C	4.741246	-0.361285	2.386214
C	3.804027	0.012738	3.546697
C	2.378678	-0.328052	3.096796
C	3.050895	0.826602	-1.759501
C	4.154707	-0.824764	4.778619
C	3.915158	1.509252	3.861883
H	4.739033	-1.456073	2.253327
H	2.278170	-1.419923	2.980020
H	1.644449	-0.004757	3.847435
H	5.770061	-0.048341	2.613649
H	5.179285	-0.623510	5.114347
B	3.003666	0.236118	0.834661
H	3.480844	-0.593985	5.613139
H	3.679015	2.111603	2.979674
H	4.931103	1.765922	4.185013
H	3.221427	1.790783	4.663741
C	2.612174	1.129662	-0.447795
C	2.211408	2.927456	-2.611514
C	1.910229	2.353314	-0.278002

TS[**5**•B**–XO2**] (cont)

C	1.729488	3.246640	-1.351706
H	1.216333	4.192643	-1.186398
H	1.617367	2.651608	0.727567
C	2.859813	1.704072	-2.818045
H	3.561527	-0.120033	-1.922603
H	2.081419	3.619805	-3.441051
H	3.211376	1.441151	-3.812792
H	4.072781	-1.898322	4.568632
C	2.194639	-5.660413	1.124404
C	1.016873	-6.255978	0.676260
C	0.095405	-5.508224	-0.055823
C	0.350016	-4.169729	-0.337155
C	1.531161	-3.566233	0.113815
C	2.450473	-4.321358	0.845305
H	2.913465	-6.242559	1.695622
H	0.817133	-7.301891	0.897524
H	-0.824481	-5.971676	-0.405367
H	-0.365077	-3.570688	-0.895913
C	1.764495	-2.095264	-0.119885
H	3.358221	-3.835767	1.190292
O	2.836165	-1.582226	0.320781

TS[**XO2**–**2**•OB^3]
E_t = -4504.089832 a.u.

Cu	0.290019	0.045108	-0.043833
P	-1.510379	-0.091774	1.298707
P	-1.265279	0.159911	-1.755820
C	-2.770996	-0.976471	0.277684
C	-2.682493	-0.818006	-1.121972
C	-3.600457	-1.470172	-1.947781
C	-4.593775	-2.273989	-1.398415
C	-4.679375	-2.431862	-0.017325
C	-3.773993	-1.782809	0.816777
H	-3.523598	-1.356731	-3.026197
H	-5.297803	-2.783856	-2.050029
H	-5.448005	-3.068208	0.412205
H	-3.830487	-1.921849	1.893559
C	-2.320291	1.525380	1.615644
C	-1.536509	-0.969559	2.901280
C	-1.867070	1.879420	-1.894754
C	-1.024144	-0.388587	-3.482754
C	-3.667997	1.634297	1.971860
C	-4.240502	2.886732	2.162084
C	-3.475703	4.038785	1.989522
C	-2.137458	3.936196	1.626102
C	-1.561760	2.683937	1.438712
H	-4.273521	0.739084	2.089911
H	-5.288708	2.965236	2.436613
H	-3.928597	5.016745	2.127338
H	-1.541532	4.830173	1.467716
H	-0.526660	2.597592	1.117885
C	-1.881832	-0.353691	4.106787
C	-1.735933	-1.040932	5.309377
C	-1.246286	-2.342917	5.318271
C	-0.896680	-2.959392	4.117479
C	-1.029811	-2.276230	2.916478
H	-2.256122	0.665998	4.108570
H	-2.004971	-0.553386	6.242258
H	-1.129009	-2.874925	6.258027
H	-0.499505	-3.970376	4.119538
H	-0.712133	-2.741217	1.986003
C	-3.196423	2.248101	-1.677755
C	-3.560629	3.590815	-1.704660
C	-2.604905	4.570113	-1.957478
C	-1.278206	4.205772	-2.177672
C	-0.903806	2.868523	-2.135261
H	-3.943683	1.486963	-1.469569
H	-4.593381	3.871222	-1.517790
H	-2.891452	5.618144	-1.972730
H	-0.523689	4.964898	-2.364011
H	0.140532	2.592653	-2.268518
C	-1.403949	0.365232	-4.596096
C	-1.093384	-0.082271	-5.877516
C	-0.404510	-1.278245	-6.057758
C	-0.022616	-2.032500	-4.949822
C	-0.323582	-1.586707	-3.669927
H	-1.932566	1.304683	-4.460331
H	-1.387548	0.510851	-6.738909
H	-0.155338	-1.616674	-7.059502
H	0.531837	-2.958543	-5.077666
H	0.000976	-2.153799	-2.802049
O	1.950467	-1.080385	2.050516
O	3.925472	0.038848	1.317499
O	0.807615	-2.115456	-0.423338
C	4.276945	-0.001813	2.707379
C	3.136469	0.454156	3.631819
C	1.793009	-0.080915	3.067570
C	2.512753	0.904994	-1.831644
C	3.390060	-0.113535	5.032756
C	3.089697	1.985177	3.686516
H	4.575762	-1.028821	2.970687
H	1.191422	-0.537824	3.860788
H	1.208632	0.745832	2.632517
H	5.148919	0.649366	2.836313
H	4.379170	0.179823	5.405061
B	2.818066	-0.730695	1.035053
H	2.641739	0.260916	5.740527
H	3.071924	2.401061	2.674107
H	3.969170	2.381897	4.206729
H	2.196643	2.333661	4.219555
C	1.976041	1.144884	-0.549883
C	3.231381	3.193630	-2.093084
C	2.135967	2.460260	-0.071364

TS[**XO2**–**2**•OB^3] (cont)

C	2.741141	3.469142	-0.819404
H	2.824478	4.474629	-0.411266
H	1.765058	2.719585	0.919415
C	3.122176	1.897816	-2.594841
H	2.427785	-0.089458	-2.274111
H	3.697341	3.976238	-2.686425
H	3.502365	1.665028	-3.587294
H	3.336544	-1.208142	5.027137
C	4.160947	-4.250122	-3.060476
C	3.241404	-5.171355	-3.555623
C	1.932718	-5.178118	-3.076143
C	1.541530	-4.257942	-2.113584
C	2.462326	-3.329576	-1.617015
C	3.778717	-3.334960	-2.087417
H	5.180113	-4.244551	-3.435393
H	3.545134	-5.887494	-4.314017
H	1.217663	-5.903120	-3.454126
H	0.526050	-4.249057	-1.729052
C	2.002678	-2.326747	-0.625275
H	4.484967	-2.609972	-1.697237
O	2.990734	-1.670939	-0.034601

XO2
E_t = -4504.137910 a.u.

Cu	0.346435	0.486917	0.492575
P	-1.442272	0.308448	1.930741
P	-1.204174	0.568842	-1.185287
C	-2.514235	-0.769730	0.889541
C	-2.415679	-0.652457	-0.512100
C	-3.203328	-1.472241	-1.323317
C	-4.074566	-2.397556	-0.760240
C	-4.168080	-2.514732	0.623807
C	-3.391882	-1.703701	1.443490
H	-3.114824	-1.401069	-2.404004
H	-4.675463	-3.033566	-1.404137
H	-4.842983	-3.241809	1.066463
H	-3.458413	-1.800626	2.523866
C	-2.498461	1.773542	2.246210
C	-1.375541	-0.566479	3.537595
C	-2.221664	2.083135	-1.384167
C	-0.873002	-0.035019	-2.873850
C	-1.948818	2.828235	2.984548
C	-2.679148	3.990128	3.198971
C	-3.958114	4.121868	2.662218
C	-4.505867	3.080612	1.921382
C	-3.784321	1.908424	1.717385
H	-0.941596	2.736006	3.382450
H	-2.244883	4.799737	3.778965
H	-4.523678	5.035965	2.819414
H	-5.499311	3.178852	1.493243
H	-4.219938	1.103232	1.133322
C	-2.188536	-0.243793	4.626792
C	-2.069249	-0.953608	5.818306
C	-1.147534	-1.990395	5.927341
C	-0.335633	-2.314797	4.842673
C	-0.439124	-1.600879	3.655442
H	-2.913326	0.561432	4.543812
H	-2.702570	-0.696655	6.662795
H	-1.057688	-2.542283	6.858685
H	0.389981	-3.119094	4.923893
H	0.204313	-1.840453	2.811620
C	-3.465096	2.073869	-2.023753
C	-4.224309	3.235633	-2.090077
C	-3.751417	4.413330	-1.514029
C	-2.516881	4.428145	-0.874884
C	-1.754493	3.266190	-0.809098
H	-3.842472	1.154416	-2.464258
H	-5.190256	3.222234	-2.587155
H	-4.350897	5.318265	-1.560161
H	-2.150831	5.340717	-0.413798
H	-0.800790	3.262834	-0.287258
C	-0.983910	0.783116	-4.000029
C	-0.604551	0.303336	-5.251030
C	-0.114569	-0.990970	-5.387023
C	0.008243	-1.805795	-4.263048
C	-0.355327	-1.329822	-3.011326
H	-1.364667	1.795743	-3.901727
H	-0.693702	0.946864	-6.121648
H	0.180898	-1.362280	-6.364032
H	0.406708	-2.811758	-4.359370
H	-0.227042	-1.955901	-2.131238
O	4.456817	0.399223	-0.504227
O	2.265338	0.347877	-1.579235
O	0.767114	-1.551510	0.376837
C	2.849591	-0.099706	-2.791770
C	4.294297	0.393020	-2.949510
C	5.061558	-0.064917	-1.698499
C	1.830816	2.242840	0.613156
C	4.911118	-0.242400	-4.194076
C	4.323238	1.919879	-3.057871
H	2.840752	-1.205351	-2.837934
H	5.118078	-1.170065	-1.700874
H	6.090832	0.321769	-1.724311
H	2.225818	0.268462	-3.619631
H	4.357505	0.048646	-5.095214
B	3.053274	0.130237	-0.385898
H	5.951107	0.080461	-4.323019
H	3.904022	2.377522	-2.157837
H	3.741060	2.257978	-3.923808
H	5.352323	2.279749	-3.175847
C	2.433639	0.983235	0.847983
C	1.748561	2.714834	2.984407
C	2.635247	0.613852	2.196875

XO2 (cont)

C	2.308133	1.460230	3.245387
H	2.494699	1.153045	4.270966
H	3.091988	-0.350971	2.408793
C	1.498231	3.099252	1.676464
H	1.737568	2.590155	-0.414563
H	1.515554	3.387836	3.806061
H	1.065707	4.075637	1.469772
H	4.901580	-1.337182	-4.129827
C	3.386423	-5.540984	0.488687
C	2.254874	-6.298715	0.780959
C	1.011610	-5.679988	0.890993
C	0.899126	-4.307383	0.710737
C	2.033185	-3.544453	0.418301
C	3.278676	-4.167915	0.306673
H	4.356119	-6.023019	0.403885
H	2.341992	-7.372334	0.923146
H	0.128389	-6.270337	1.117625
H	-0.062333	-3.808764	0.791437
C	1.898875	-2.068124	0.235834
H	4.150720	-3.562593	0.082417
O	2.985309	-1.441628	-0.038945

2•OB^3

E_t = -4504.110224 a.u.

Cu	0.491538	0.695070	-0.243135
P	-1.308784	0.514431	1.126324
P	-1.049554	0.776228	-1.915013
C	-2.625952	-0.288638	0.108503
C	-2.513657	-0.147899	-1.288633
C	-3.460858	-0.746058	-2.121669
C	-4.511392	-1.478282	-1.578596
C	-4.626069	-1.613541	-0.197662
C	-3.689523	-1.018713	0.641145
H	-3.366999	-0.646096	-3.199921
H	-5.239582	-1.946725	-2.234943
H	-5.443012	-2.189645	0.227861
H	-3.770035	-1.143568	1.717751
C	-2.029189	2.165935	1.490519
C	-1.388425	-0.375163	2.722930
C	-1.614894	2.516789	-2.022498
C	-0.936358	0.248420	-3.668712
C	-3.351212	2.331262	1.912988
C	-3.860328	3.605214	2.133840
C	-3.055850	4.724501	1.929760
C	-1.740867	4.566858	1.506325
C	-1.228674	3.292044	1.287015
H	-3.986022	1.461830	2.063396
H	-4.889346	3.726412	2.460651
H	-3.458739	5.719847	2.095516
H	-1.113427	5.435849	1.331645
H	-0.208753	3.163448	0.930139
C	-1.441089	0.306200	3.942854
C	-1.347882	-0.394641	5.141850
C	-1.200328	-1.778137	5.135566
C	-1.143371	-2.461007	3.921801
C	-1.228734	-1.766817	2.722758
H	-1.553317	1.386697	3.955816
H	-1.391911	0.144971	6.083743
H	-1.126488	-2.323640	6.072038
H	-1.016950	-3.539873	3.908921
H	-1.147913	-2.298377	1.778747
C	-2.939010	2.911366	-1.823766
C	-3.276971	4.261005	-1.852945
C	-2.300529	5.222660	-2.091085
C	-0.977813	4.833927	-2.291003
C	-0.631839	3.489190	-2.244719
H	-3.704735	2.165043	-1.629896
H	-4.307184	4.560392	-1.682444
H	-2.567561	6.275596	-2.111773
H	-0.209027	5.580976	-2.467047
H	0.406961	3.186945	-2.361721
C	-1.508124	0.965155	-4.723312
C	-1.393847	0.495326	-6.028547
C	-0.716390	-0.692105	-6.290667
C	-0.139401	-1.406338	-5.243504
C	-0.238000	-0.932661	-3.940920
H	-2.040838	1.891027	-4.523437
H	-1.838659	1.059561	-6.843510
H	-0.630207	-1.055356	-7.310842
H	0.399725	-2.329134	-5.439056
H	0.228072	-1.479553	-3.126737
O	3.950894	-1.693974	1.006688
O	1.701311	-1.512733	1.860882
O	0.187255	-1.830640	-0.551402
C	2.123332	-0.609378	2.900376
C	3.586254	-0.829960	3.290978
C	4.428228	-0.777454	2.011671
C	3.327606	0.750568	-1.050025
C	4.024253	0.311260	4.210418
C	3.753217	-2.181632	3.995585
H	1.972940	0.412774	2.527711
H	4.412648	0.231634	1.581985
H	5.467180	-1.056847	2.223321
H	1.458366	-0.783483	3.754795
H	3.419957	0.325504	5.124751
B	2.614523	-1.902792	0.940756
H	5.073076	0.190885	4.504772
H	3.450736	-3.014085	3.352246
H	3.140851	-2.219036	4.903705
H	4.799268	-2.340271	4.280856
C	2.350927	1.265294	-0.172357
C	5.052285	2.211193	-0.196850
C	2.808714	2.284246	0.692485

2•OB^3 (cont)

C	4.120880	2.758564	0.682180
H	4.419709	3.552530	1.364489
H	2.117242	2.732724	1.407827
C	4.648288	1.197437	-1.062162
H	3.052247	-0.035806	-1.753654
H	6.078780	2.569041	-0.207155
H	5.365169	0.756004	-1.751577
H	3.918392	1.279996	3.709251
C	1.477104	-5.883396	-2.731982
C	0.225196	-5.991175	-3.332174
C	-0.764139	-5.047934	-3.060911
C	-0.501998	-3.996420	-2.194758
C	0.755815	-3.884553	-1.591855
C	1.745505	-4.834742	-1.860951
H	2.247445	-6.618469	-2.945490
H	0.019534	-6.812536	-4.012942
H	-1.741013	-5.132890	-3.527612
H	-1.258327	-3.248701	-1.973661
C	1.001059	-2.726682	-0.695990
H	2.718725	-4.738991	-1.392378
O	2.209882	-2.753284	-0.114526