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SUPPLEMENTARY INFORMATION

Copper-Catalysed Electrophilic Carboamination of Terminal Alkynes with Benzyne Looked at through the Computational Lens

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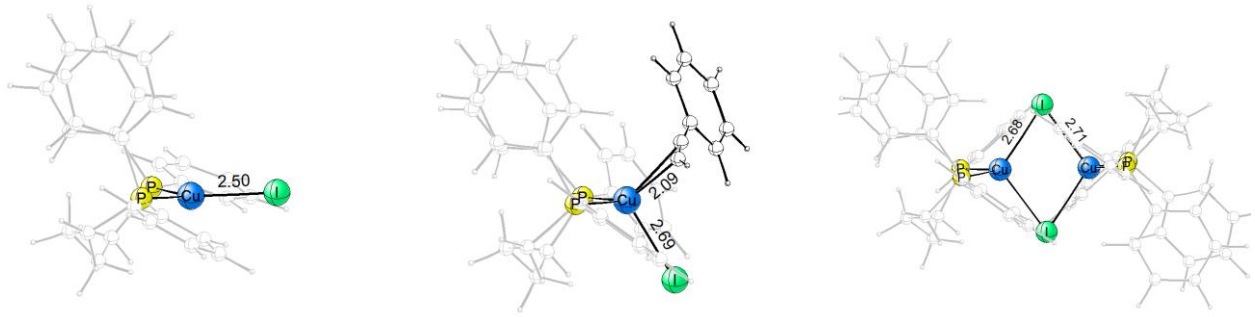
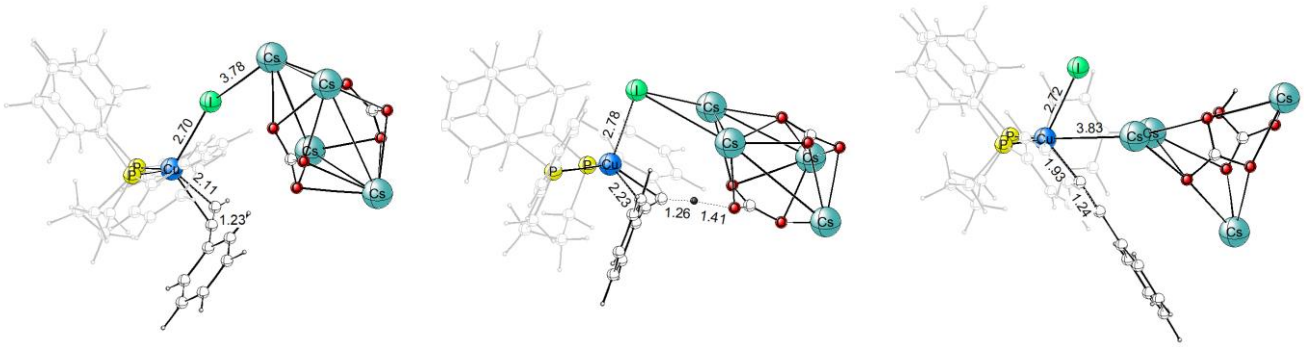


0 **0•S** **0dim**

Fig. S1 Selected structural parameter (angstrom) of the optimised structures of various forms of {P^P}Cu^{I} iodide **0**.

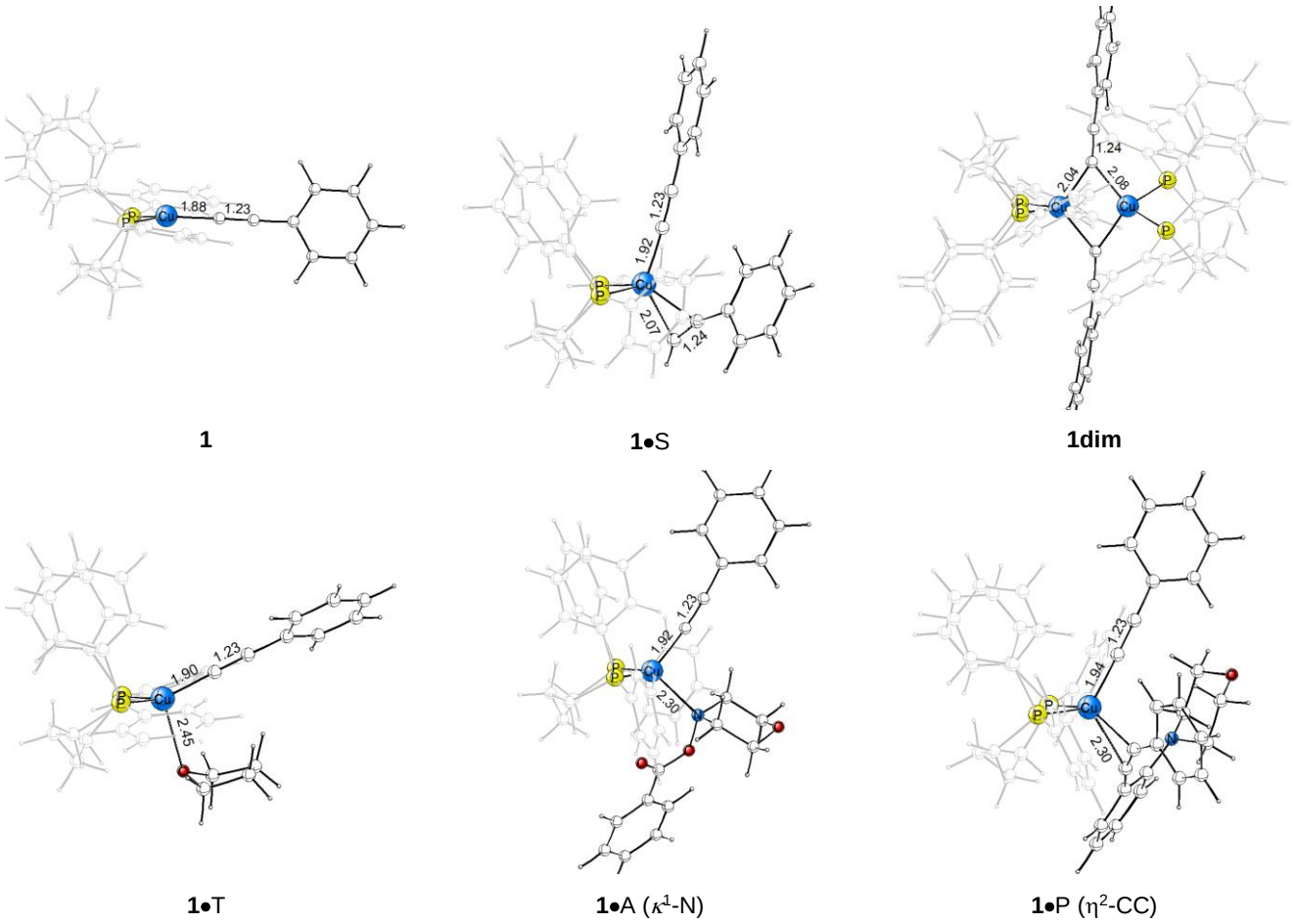
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



0•S•{Cs} TS[**0•S•{Cs}**–**1•{CsI}•{Cs'}**] **1•{CsI}•{Cs'}**

Fig. S2 Selected structural parameter (angstrom) of the optimised structures of key stationary points for $[Cs_2CO_3]_2$-triggered transmetalation of {PP}Cu^{I} iodide **0** by alkyne S.

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

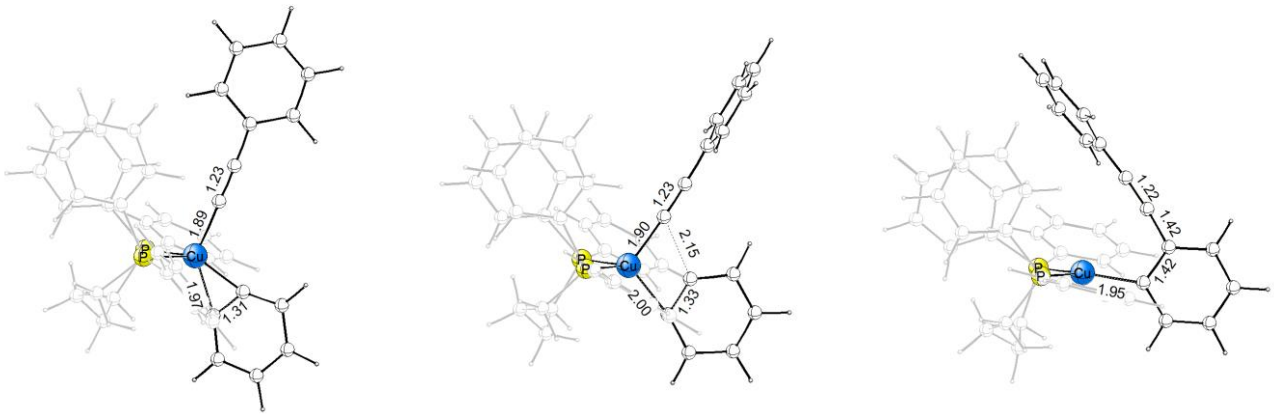


1 **1●S** **1dim**

1●T **1●A** (κ^1-N) **1●P** (η^2-CC)

Fig. S3 Selected structural parameter (angstrom) of the optimised structures of various forms of the catalytically competent {P^P}Cu^{I} alkynyl **1**.

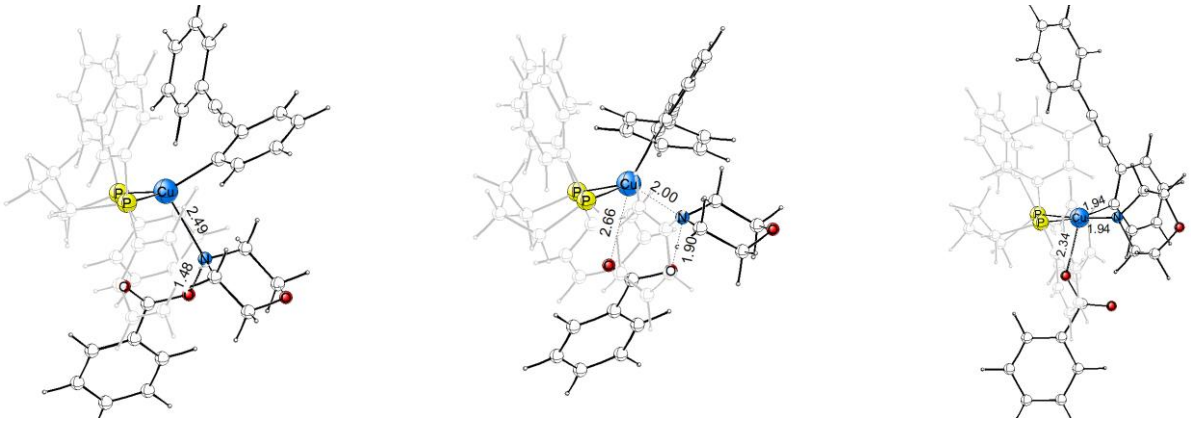
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



1●B TS[**1●B**–**2**] **2**

Fig. S4 Selected structural parameter (angstrom) of the optimised structures of key stationary points for benzyne C≡C bond insertion into the Cu–$C_{alkynyl}$ linkage at benzyne adduct **1**•B of the {P^P}Cu^{I} alkynyl.

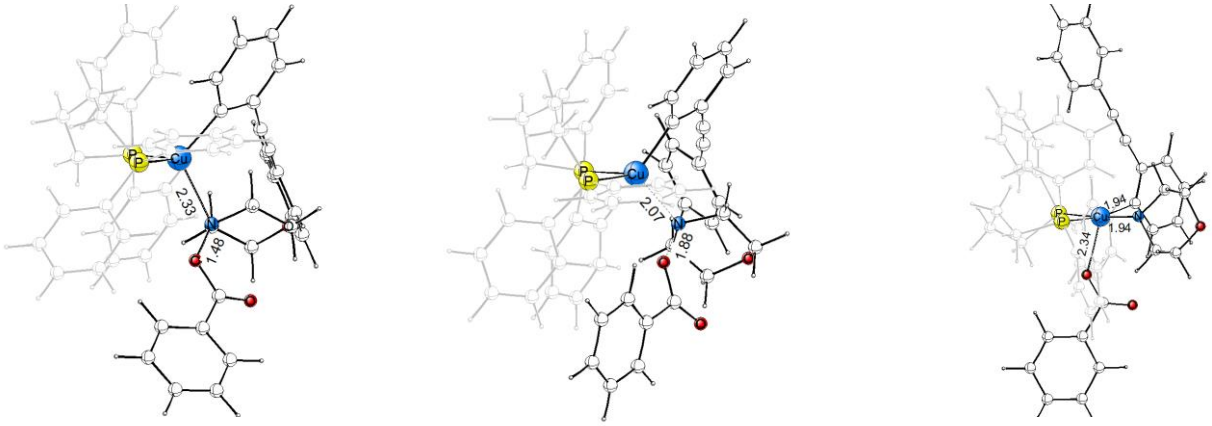
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



2$_1$•A TS[**2**$_1$•A–**3**] **3**

Fig. S5 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 multicentre TS structure at amine adduct **2**•A of the arylcopper.

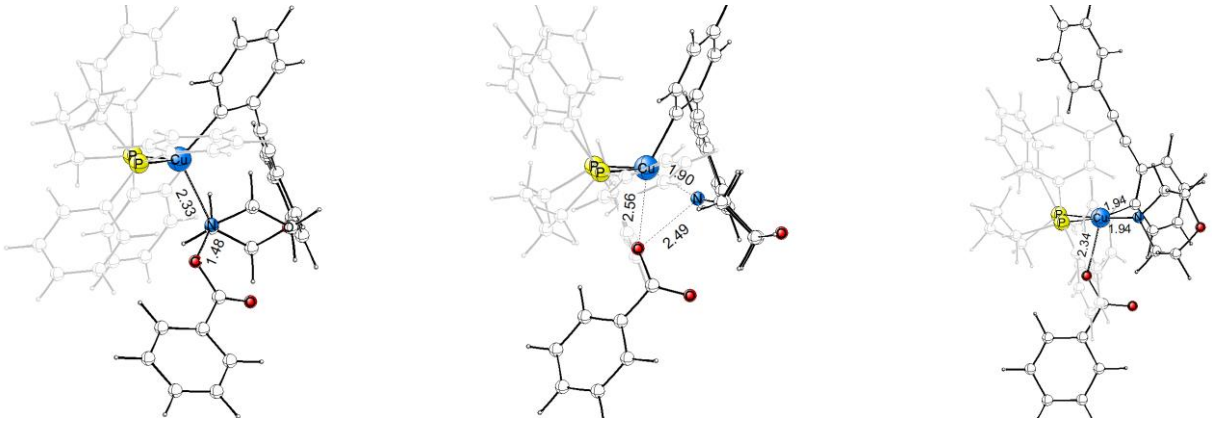
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



2$_2$•A TS[**2**$_2$•A–**3**] **3**

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 classic TS structure at amine adduct **2**•A of the arylcopper.

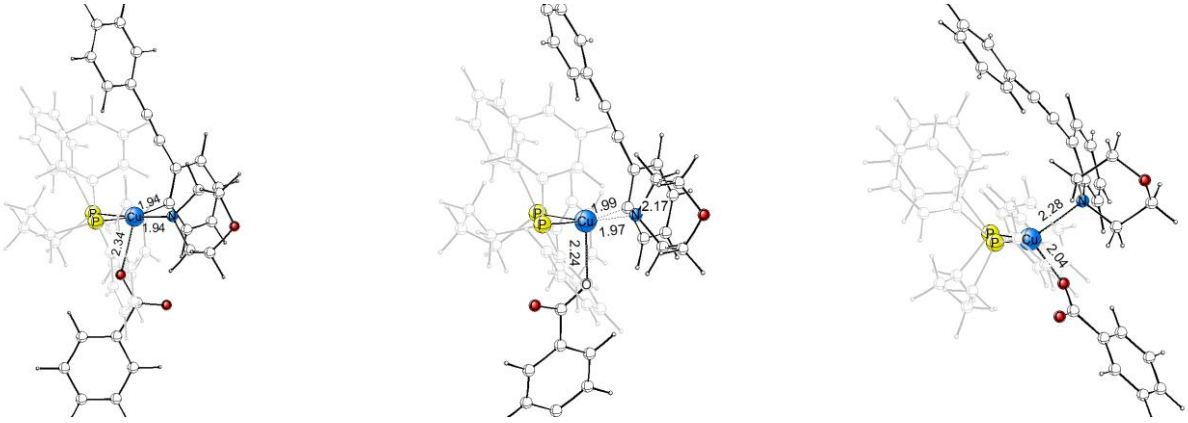
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



2$_2$•A TS$_{OA}$[**2**$_2$•A–**3**] **3**

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

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



3 TS[**3**–**4**•P] **4**•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 **3**.

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

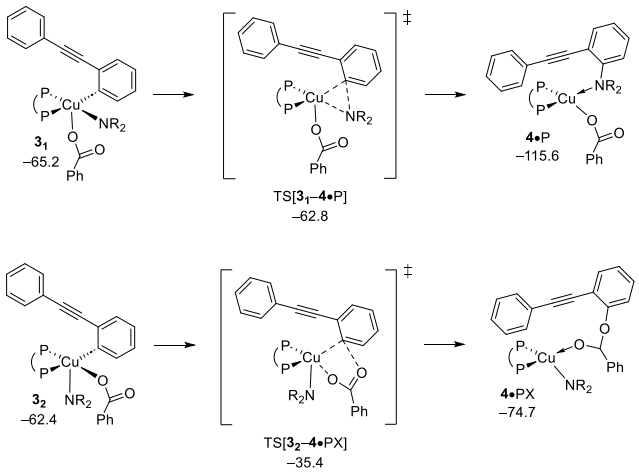
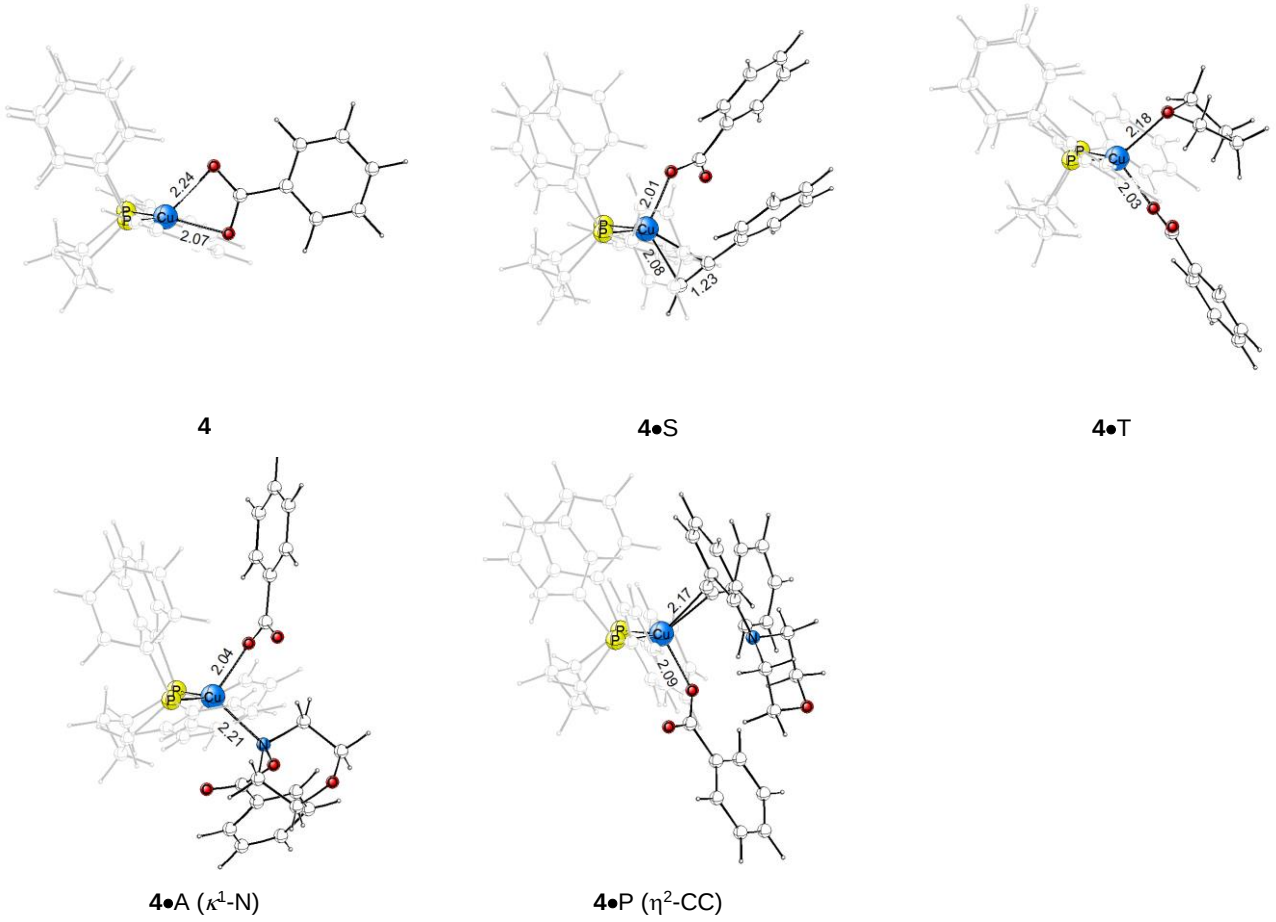


Fig. S9 Alternative pathways for regioisomeric N–C or O–C bond forming reductive elimination commencing at formal {P^P}Cu^{III} intermediate **3**. Free energies are given in kcal mol^{-1} relative to {½×**1dim** + B + A}.

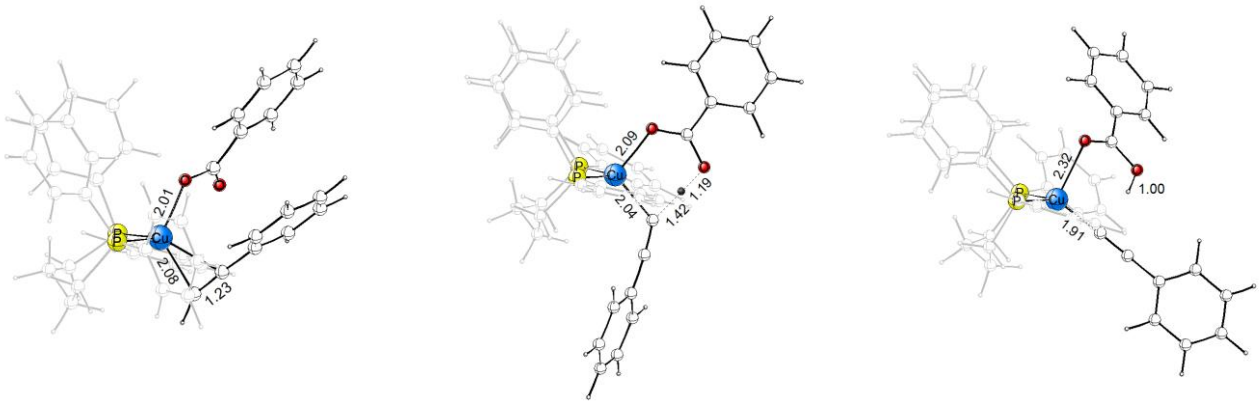


4 **4**•S **4**•T

4•A (κ^1-N) **4**•P (η^2-CC)

Fig. S10 Selected structural parameter (angstrom) of the optimised structures of various forms of {P^P}Cu^{I} benzoate **4**.

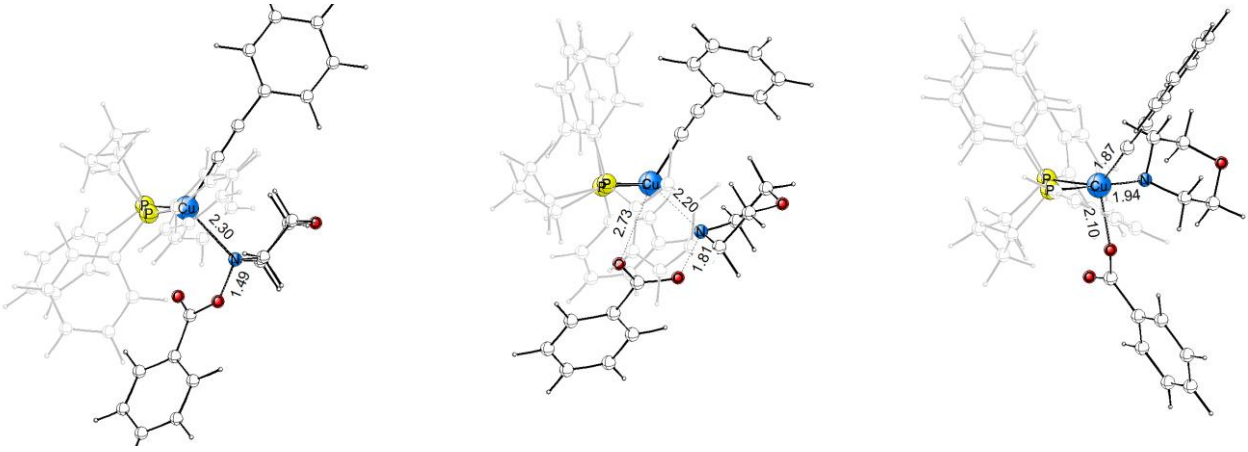
The backbone of the {P^P} ligand is greyed out to enhance the visualisation of crucial structural aspects.



4•S TS[**4**•S$_2$–**1**•HOBz] **1**•HOBz

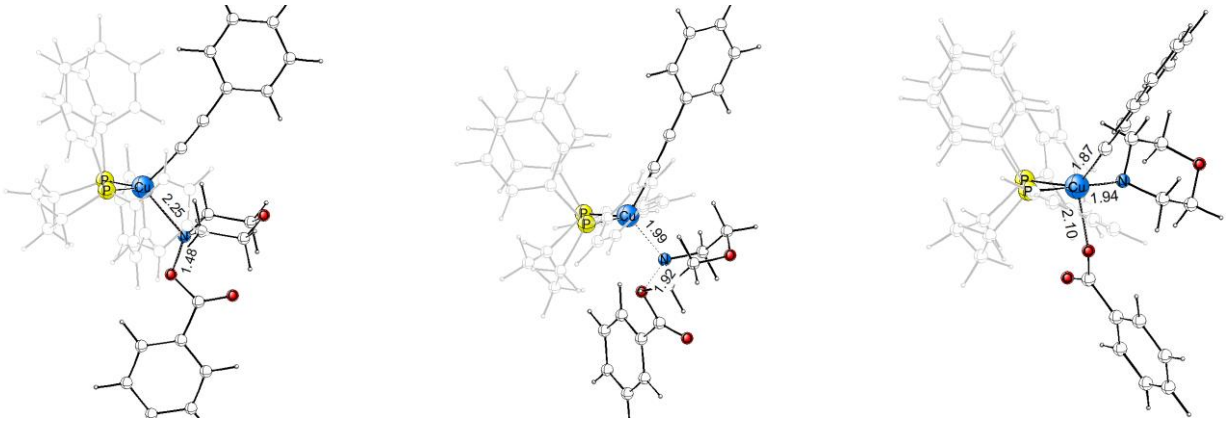
Fig. S11 Selected structural parameter (angstrom) of the optimised structures of key stationary points for alkynolysis of {P^P}Cu^{I} benzoate **4** by acetylene S.

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



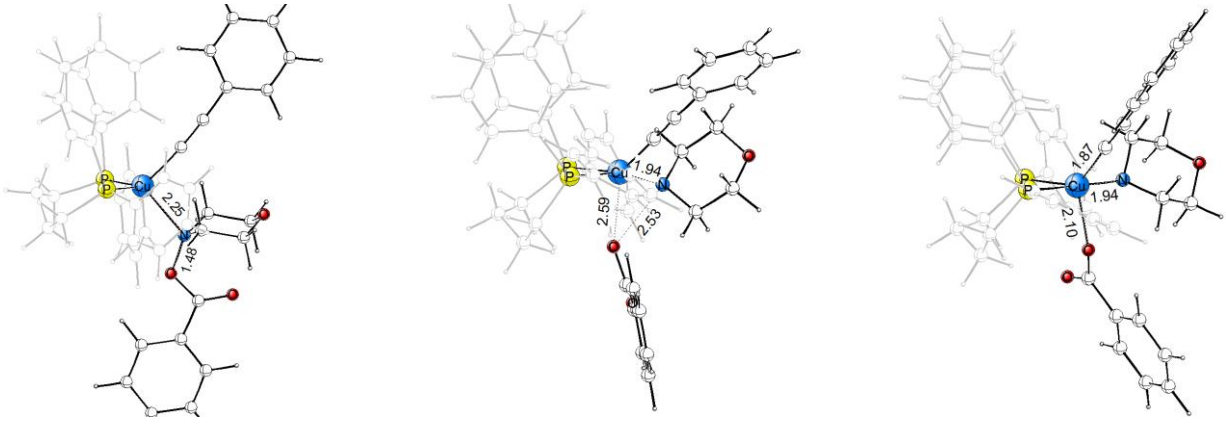
1$_1$•A TS[**1**$_1$•A–**5**] **5**

Fig. S12 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 multicentre TS structure at amine adduct **1**•A of the alkynylcopper.



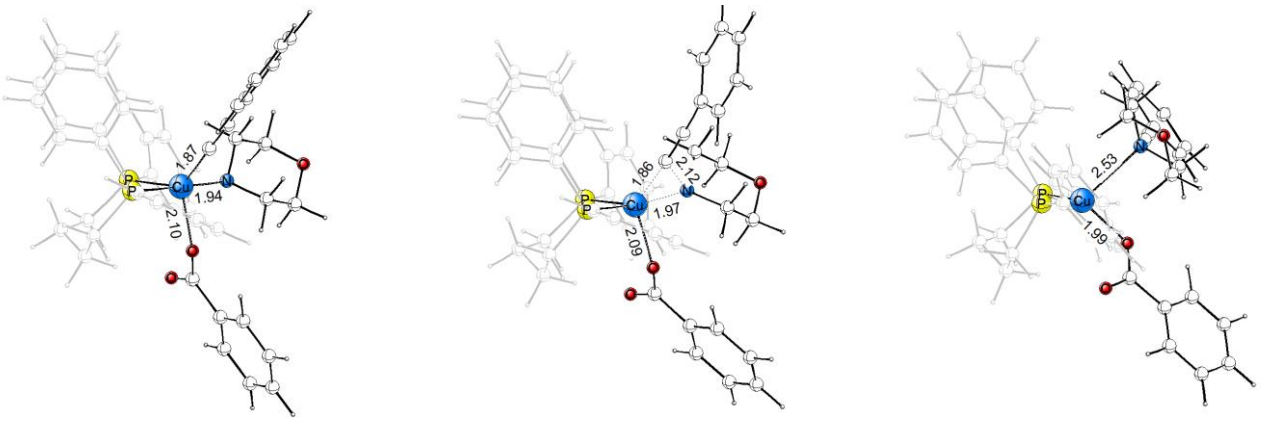
1$_2$•A TS[**1**$_2$•A–**5**] **5**

Fig. S13 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 classic TS structure at amine adduct **1**•A of the alkynylcopper.



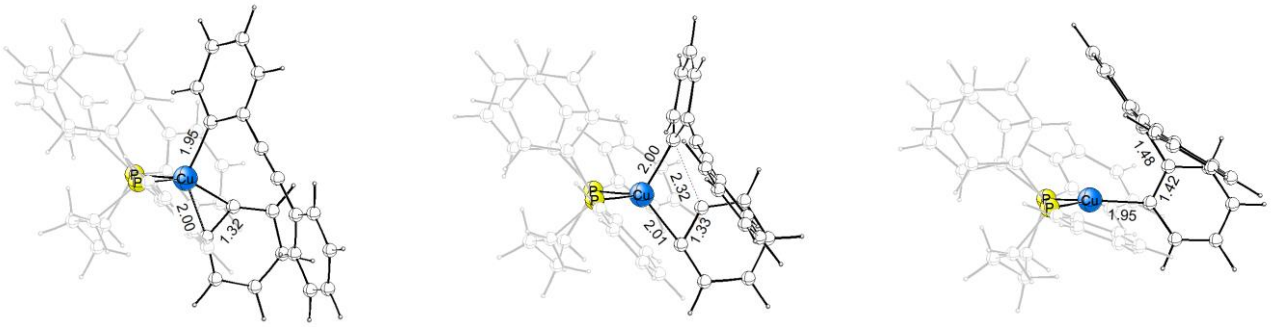
1$_2$•A TS$_{OA}$[**1**$_2$•A–**5**] **5**

Fig. S14 Selected structural parameter (angstrom) of the optimised structures of key stationary points for oxidative addition of O-benzoylhydroxylamine at amine adduct **1**•A of the alkynylcopper.



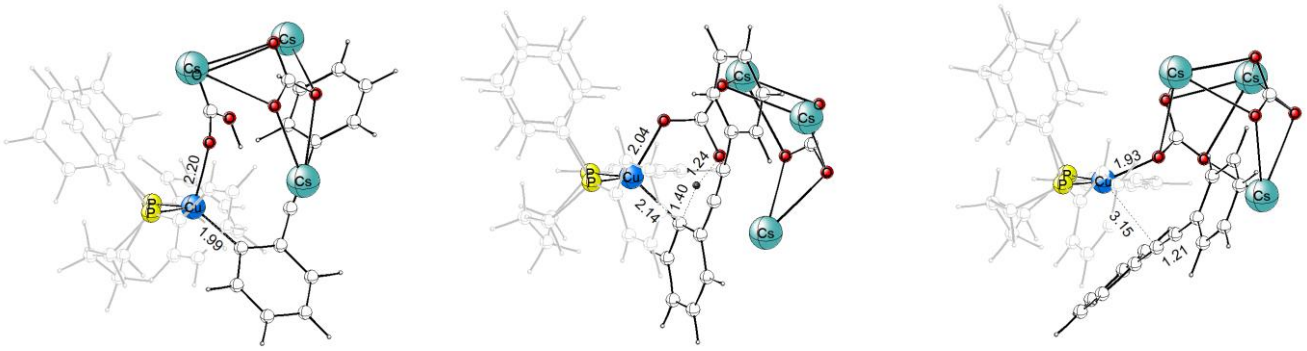
5 TS[**5**–**4**•PP] **4**•PP

Fig. S15 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 **5**.



2•B TS[**2**•B–**6**] **6**

Fig. S16 Selected structural parameter (angstrom) of the optimised structures of key stationary points for benzyne insertion into the Cu–C_{aryl} linkage at benzyne adduct **2**•B of the {P^P}Cu^{I} aryl.



2•{Cs'} TS[**2**•{Cs'}–**7**•PP•($CsCO_3$)•(Cs_2CO_3)$_2$] **7**•PP•($CsCO_3$)•(Cs_2CO_3)$_2$

Fig. S17 Selected structural parameter (angstrom) of the optimised structures of key stationary points for protonolytic release of diphenyl acetylene from {P^P}Cu^{I} aryl **2** by caesium bicarbonate.

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

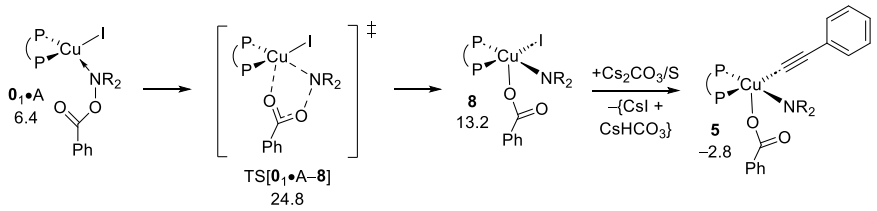


Fig. S18 Alternative avenue for alkynylcupration to involve formal {P^P}Cu^{III} species – oxidative S_N2-type oxidative addition of the hydroxylamine ester electrophile A, thus affording {P^P}Cu^{III} carboxylate amido iodide **8**, to be followed by facile transmetalation by alkyne S to deliver {P^P}Cu^{III} intermediate **5**. Free energies are given in kcal mol^{-1} relative to {½×**0dim** + A + S}.

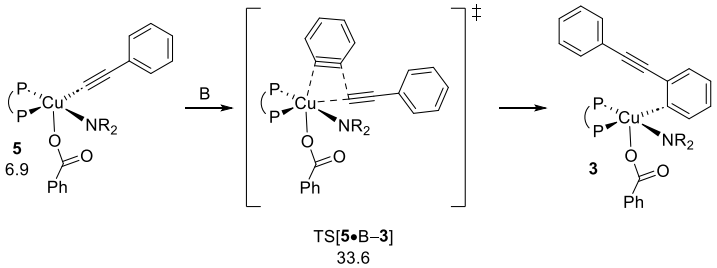


Fig. S19 Alternative avenue for alkynylcupration to involve formal {P^P}Cu^{III} species – benzyne insertion into the Cu–$C_{alkynyl}$ linkage commencing at {P^P}Cu^{III} carboxylate amido alkynyl **5**. Free energies are given in kcal mol^{-1} relative to {½×**1dim** + A + B}.

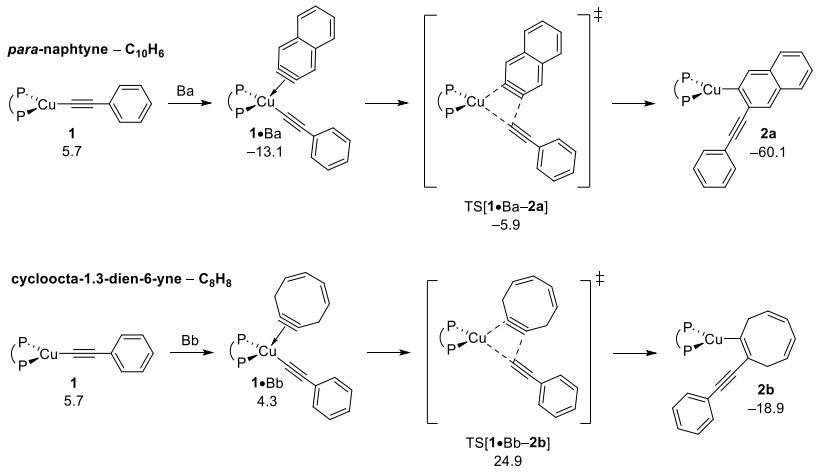


Fig. S20 Insertion of various arynes into the Cu–$C_{alkynyl}$ linkage at substrate adduct **1**•Bx of the {P^P}Cu^{I} alkynyl.

Free energies are given in kcal mol^{-1} relative to {½×**1dim** + Bx + A}.

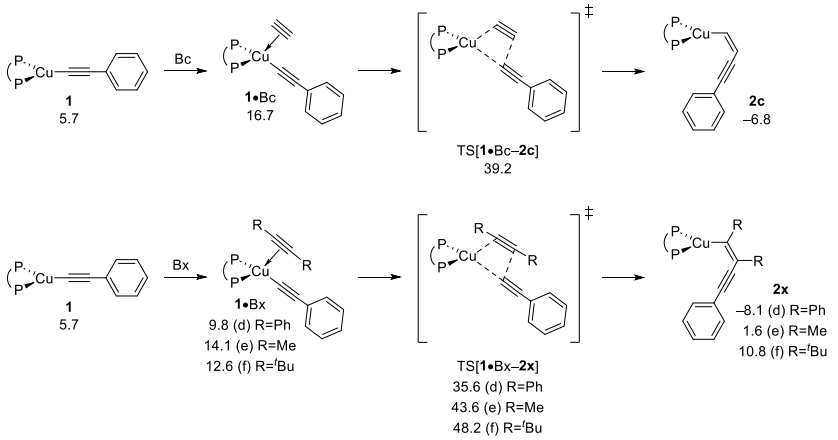


Fig. S21 Insertion of various acetylenes into the Cu–$C_{alkynyl}$ linkage at substrate adduct **1**•Bx of the {P^P}Cu^{I} alkynyl.

Free energies are given in kcal mol^{-1} relative to {½×**1dim** + Bx + A}.

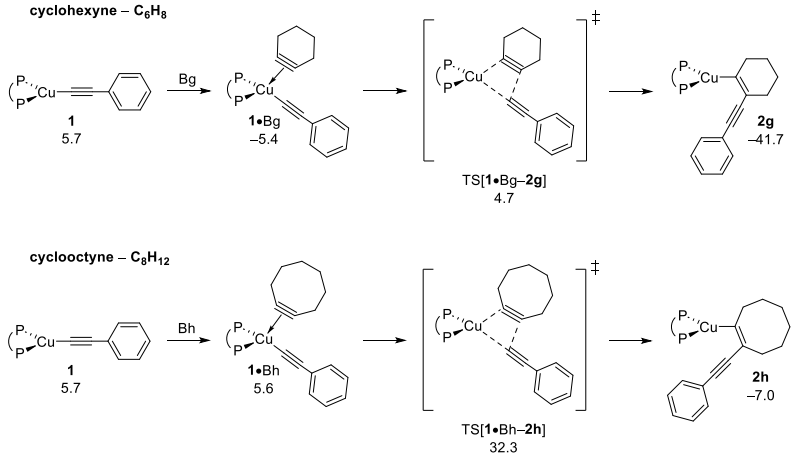


Fig. S22 Insertion of various cycloalkynes into the Cu–$C_{alkynyl}$ linkage at substrate adduct **1**•Bx of the {P^P}Cu^{I} alkynyl.

Free energies are given in kcal mol^{-1} relative to {½×**1dim** + Bx + A}.

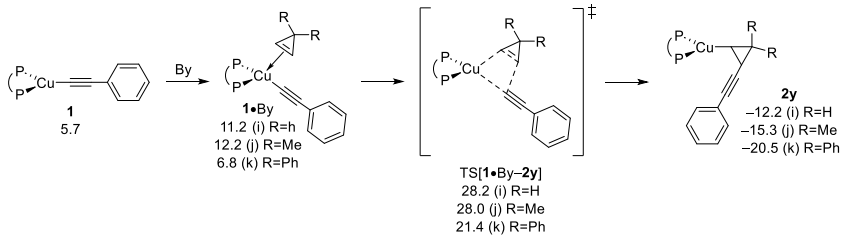


Fig. S23 Insertion of various cyclopropenes into the Cu–$C_{alkynyl}$ linkage at substrate adduct **1**•Bx of the {P^P}Cu^{I} alkynyl.

Free energies are given in kcal mol^{-1} relative to {½×**1dim** + Bx + A}.

Table S1 NBO analysis of aryne and acetylene bonding at {P°P}Cu^{I} alkynyl complex **1** exemplified for adducts **1**•B and **1**•Bc, respectively.

species	bond	ON[a]	δE^2 [kcalmol^{-1}][a]		WBI[a]
benzyne	C–C σ	1.99			2.33
	C–C π	1.92			
	C–C π	1.67			
1•B	Cu–C		C–C π→Cu	Cu→C–C π*	0.51
	Cu–C'		181.7 kcal mol^{-1}	46.0 kcal mol^{-1}	0.50
	C–C σ	1.95			1.72
	C–C σ	1.68			
	C–C π	1.64			
acetylene	C–C σ	2.00			2.99
	C–C π	2.00			
	C–C π	1.99			
1•Ac	Cu–C		C–C π→Cu	Cu→C–C π*	0.42
	Cu–C'		131.5 kcal mol^{-1}	18.7 kcal mol^{-1}	0.40
	C–C σ	1.99			2.51
	C–C σ	1.98			
	C–C π	1.75			

[a] ON and WBI represent occupation number and Wiberg bond index, respectively, whilst the second-order perturbation energy quantifies the electron transfer taking place due to substrate binding.

Cartesian coordinates (in Å) of located key structures

0

E_t = -3704.314919 a.u.

Cu	1.540452	-0.784828	0.007429
P	0.125057	-0.854134	1.756064
P	0.406947	-0.539733	-1.921532
C	-1.435923	-1.846017	1.539506
C	-1.951533	-1.798721	0.094656
C	-1.120651	-2.664838	-0.873847
C	-0.750403	-1.980856	-2.193114
C	-0.446297	0.872083	2.014370
C	0.690045	-1.358896	3.426883
C	1.263153	-0.402334	-3.540425
C	-0.609365	0.991837	-1.851933
H	-0.187249	-2.969757	-0.382448
H	-0.191918	-2.679284	-2.827721
H	-1.639016	-1.689038	-2.765807
H	-2.193482	-1.502522	2.254934
H	-1.190461	-2.877178	1.822717
H	-1.966263	-0.759142	-0.250861
H	-2.998249	-2.127833	0.081084
H	-1.660107	-3.594387	-1.095692
C	0.539389	1.815278	2.335938
C	-1.115318	3.568427	2.348788
C	-1.764797	1.299962	1.846524
C	-2.094312	2.642521	2.010962
H	-3.123963	2.962191	1.872380
H	-2.549090	0.596639	1.582431
C	0.203393	3.150204	2.511619
H	1.574431	1.497059	2.448927
H	-1.376399	4.615608	2.479674
H	0.976789	3.868774	2.770303
C	2.580674	-0.858711	-3.626042
C	2.617892	-0.316301	-5.975699
C	0.631997	0.110478	-4.677318
C	1.308363	0.150636	-5.890412
H	0.814861	0.553873	-6.771121
H	-0.383492	0.494974	-4.611927
C	3.252066	-0.817436	-4.844265
H	3.087755	-1.215685	-2.731937
H	3.146509	-0.279249	-6.924951
H	4.279635	-1.166252	-4.902061
C	-1.939590	1.093585	-2.264900
C	-1.979698	3.423525	-1.642518
C	0.025142	2.125390	-1.328366
C	-0.653162	3.332260	-1.231647
H	-0.148497	4.199330	-0.815030
H	1.055843	2.055377	-0.984961
C	-2.621130	2.302799	-2.156663
H	-2.462585	0.232138	-2.671435
H	-2.514347	4.366063	-1.556147
H	-3.657268	2.366600	-2.479615
C	-0.082321	-1.108328	4.565688
C	1.569941	-2.210239	5.930966
C	1.909510	-2.026749	3.550466
C	2.345103	-2.451676	4.802741
H	3.299603	-2.963046	4.893652
H	2.529351	-2.184034	2.670530
C	0.356716	-1.534890	5.812247
H	-1.018627	-0.560141	4.480106
H	1.913911	-2.538963	6.908474
H	-0.244743	-1.335051	6.695464
I	4.025728	-0.691361	0.274873

0•S

E_t = -4012.611945 a.u.

Cu	1.028375	-0.912479	0.414290
P	-0.431664	-1.025556	2.186147
P	-0.229126	-0.824548	-1.490069
C	-1.816859	-2.255171	2.041821
C	-2.416905	-2.281717	0.628296
C	-1.544731	-3.079773	-0.360013
C	-1.248422	-2.381819	-1.685334
C	-1.296677	0.565678	2.512396
C	0.288943	-1.422528	3.830485
C	0.586932	-0.712986	-3.135994
C	-1.427745	0.571578	-1.529662
H	-0.582579	-3.324150	0.102654
H	-0.650841	-3.049345	-2.315207
H	-2.166643	-2.157653	-2.241308
H	-2.564978	-2.042556	2.815707
H	-1.387055	-3.233976	2.285751
H	-2.561773	-1.257006	0.262526
H	-3.423030	-2.716630	0.680698
H	-2.023134	-4.042743	-0.579448
C	-0.506664	1.677884	2.834169
C	-2.465862	3.077315	2.956965
C	-2.678722	0.737809	2.404789
C	-3.256780	1.985491	2.623269
H	-4.333802	2.099474	2.531083
H	-3.323391	-0.095993	2.145995
C	-1.085768	2.918000	3.064124
H	0.572342	1.568570	2.913707
H	-2.919970	4.049266	3.132482
H	-0.456732	3.765189	3.325626
C	0.408632	0.372896	-3.995360
C	1.891971	-0.636296	-5.609453
C	1.454128	-1.747371	-3.513367
C	2.094433	-1.708792	-4.745107
H	2.760088	-2.521026	-5.026137
H	1.650318	-2.570658	-2.829319
C	1.057196	0.406408	-5.225842
H	-0.235928	1.198486	-3.708920
H	2.392459	-0.609365	-6.574424
H	0.907364	1.257384	-5.885858
C	-2.553151	0.600767	-2.360199
C	-3.139495	2.785362	-1.522472
C	-1.168151	1.669512	-0.706900
C	-2.015610	2.772374	-0.705009
H	-1.803623	3.611461	-0.048351
H	-0.301527	1.650004	-0.051069
C	-3.405597	1.698312	-2.351907
H	-2.760228	-0.226752	-3.034138
H	-3.809202	3.641785	-1.516907
H	-4.279173	1.707660	-2.998906
C	-0.289348	-0.981126	5.025182
C	1.397874	-2.156504	6.285483
C	1.427652	-2.232899	3.874163
C	1.974438	-2.599779	5.099943
H	2.858725	-3.231159	5.122806
H	1.881735	-2.580267	2.947071
C	0.265699	-1.346942	6.245852
H	-1.168902	-0.342271	5.001882
H	1.829584	-2.440670	7.241926
H	-0.188009	-0.998112	7.170156
I	2.404928	-3.196616	0.092732
C	2.489478	0.275540	1.324615
C	2.579931	0.752999	0.194090
C	2.832365	1.311136	-1.086527
C	2.371955	2.594103	-1.423000
C	2.676992	3.136676	-2.662667
C	3.585170	0.577813	-2.020530
C	3.887694	1.135892	-3.251533
C	3.437942	2.413308	-3.576663
H	3.674184	2.841790	-4.547143
H	4.465130	0.562231	-3.970723
H	3.912807	-0.424685	-1.760855
H	1.788671	3.158214	-0.700950
H	2.320996	4.132005	-2.915651
H	2.760666	0.087551	2.344036

0dim

E_t = -7408.686921 a.u.

Cu	1.542643	0.039760	-0.092151
P	2.851459	0.084496	1.787410
P	2.915998	0.248073	-1.914661
C	4.126914	1.447166	1.798822
C	4.780518	1.688005	0.431479
C	3.878545	2.500562	-0.519813
C	3.716648	1.931198	-1.931309
C	3.849569	-1.447176	1.978341
C	2.155291	0.311894	3.479333
C	2.328870	0.030115	-3.649270
C	4.304798	-0.976380	-1.904179
H	2.878062	2.587266	-0.084975
H	3.030959	2.575392	-2.496275
H	4.670956	1.930347	-2.470794
H	4.864297	1.226127	2.581013
H	3.597739	2.350700	2.126407
H	5.050462	0.729359	-0.025616
H	5.731326	2.214610	0.584715
H	4.258612	3.527100	-0.602168
C	3.146853	-2.648065	2.142849
C	5.217438	-3.877998	2.248903
C	5.244983	-1.486230	1.932915
C	5.922485	-2.694979	2.065686
H	7.008587	-2.707771	2.020816
H	5.821910	-0.578727	1.783453
C	3.825306	-3.850054	2.289285
H	2.059443	-2.640164	2.141905
H	5.749079	-4.820999	2.350849
H	3.262981	-4.770502	2.425586
C	1.307093	-0.894453	-3.881471
C	1.493514	-0.534143	-6.256766
C	2.919915	0.678921	-4.737033
C	2.499566	0.400548	-6.033442
H	2.967221	0.910674	-6.872419
H	3.719224	1.399868	-4.584339
C	0.900309	-1.180804	-5.178846
H	0.827898	-1.389915	-3.040506
H	1.166461	-0.750892	-7.270862
H	0.096838	-1.893886	-5.344065
C	5.573054	-0.723295	-2.433146
C	6.279534	-2.960821	-1.873617
C	4.034972	-2.240552	-1.372406
C	5.014606	-3.226646	-1.362212
H	4.789357	-4.198418	-0.931594
H	3.051997	-2.452009	-0.958995
C	6.556440	-1.706344	-2.408880
H	5.807469	0.239970	-2.878528
H	7.049563	-3.728395	-1.857025
H	7.541931	-1.491532	-2.815309
C	2.784774	-0.198238	4.618501
C	1.145275	0.879882	6.021957
C	1.007219	1.095016	3.626149
C	0.510332	1.382503	4.891993
H	-0.394917	1.976026	4.992295
H	0.499545	1.473937	2.742386
C	2.277923	0.083234	5.882692
H	3.670377	-0.821291	4.518437
H	0.753242	1.101732	7.011623
H	2.770293	-0.324064	6.762707
I	- 0.069960	2.214587	-0.027564
I	0.079125	-2.195641	-0.295158
Cu	-1.534907	-0.026918	-0.111532
P	-2.862458	-0.306684	1.734431
P	-2.893843	-0.004646	-1.955591
C	-4.136020	-1.660502	1.564040
C	-4.776289	-1.732207	0.171626
C	-3.861747	-2.416488	-0.864971
C	-3.689989	-1.673219	-2.191894
C	-3.865101	1.189229	2.103205
C	-2.187192	-0.741653	3.393876
C	-2.298744	0.434133	-3.644975
C	-4.285056	1.206609	-1.795692
H	-2.864785	-2.553589	-0.434744
H	-2.998471	-2.239559	-2.828627

1dim (cont)

H	-4.640119	-1.605219	-2.734603
H	-4.881344	-1.537666	2.360246
H	-3.608679	-2.597311	1.783292
H	-5.047973	-0.725614	-0.165211
H	-5.725208	-2.278290	0.249891
H	-4.236377	-3.425738	-1.079451
C	-3.165704	2.360307	2.422964
C	-5.238150	3.572470	2.640023
C	-5.259836	1.234170	2.045596
C	-5.939954	2.419310	2.311511
H	-7.025627	2.437123	2.258406
H	-5.833979	0.351340	1.781731
C	-3.846668	3.538499	2.696257
H	-2.078505	2.348893	2.446007
H	-5.771583	4.498190	2.841955
H	-2.078505	2.348893	2.446007
H	-5.771583	4.498190	2.841955
H	-3.286697	4.437156	2.942895
C	-1.272678	1.376732	-3.751540
C	-1.443296	1.320350	-6.154486
C	-2.887017	-0.066537	-4.809809
C	-2.453400	0.368447	-6.057877
H	-2.911363	-0.035311	-6.957900
H	-3.697478	-0.789136	-4.754486
C	-0.853881	1.821154	-4.999571
H	-0.802519	1.764731	-2.851308
H	-1.111476	1.665522	-7.130762
H	-0.042501	2.541078	-5.068064
C	-5.549940	1.021886	-2.359808
C	-6.261915	3.171055	-1.527609
C	-4.020639	2.392631	-1.105066
C	-4.999813	3.371270	-0.980645
H	-4.775269	4.285021	-0.437355
H	-3.044882	2.544666	-0.650719
C	-6.534686	1.993441	-2.217359
H	-5.781898	0.120742	-2.921447
H	-7.033594	3.929088	-1.416719
H	-7.517676	1.831057	-2.653110
C	-2.835935	-0.381382	4.578498
C	-1.214671	-1.626598	5.858970
C	-1.038397	-1.534431	3.457865
C	-0.561127	-1.981065	4.684426
H	0.342041	-2.584946	4.722329
H	-0.514478	-1.794807	2.541281
C	-2.349355	-0.822742	5.804207
H	-3.718965	0.252378	4.544965
H	-0.833749	-1.967063	6.818849
H	-2.861362	-0.538039	6.720478

0•S•{Cs}

E_t = -4620.852020 a.u.

Cu	0.861326	0.050092	0.049792
P	-0.510972	-0.156200	1.889023
P	-0.350353	0.106109	-1.938815
C	-1.833266	-1.455517	1.657112
C	-2.379218	-1.406370	0.225816
C	-1.483927	-2.171290	-0.763365
C	-1.285310	-1.500500	-2.123646
C	-1.569446	1.326958	2.173036
C	0.158643	-0.497556	3.561040
C	0.611677	0.212243	-3.507955
C	-1.562485	1.466113	-2.209333
H	-0.491510	-2.302061	-0.317532
H	-0.657987	-2.141133	-2.754471
H	-2.232921	-1.363253	-2.657412
H	-2.630341	-1.279032	2.387999
H	-1.397681	-2.440754	1.865017
H	-2.487197	-0.356079	-0.073848
H	-3.395388	-1.819343	0.205702
H	-1.883122	-3.182912	-0.915223
C	-2.361300	1.438708	3.320839
C	-3.273472	3.516002	2.503107
C	-1.623633	2.330923	1.206930
C	-2.478788	3.417633	1.367701
H	-2.512649	4.186875	0.600934
H	-0.980877	2.276062	0.335104
C	-3.208113	2.527255	3.483360
H	-2.301287	0.681198	4.099566
H	-3.939121	4.366082	2.632254
H	-3.815756	2.608653	4.381217
C	1.881971	0.792267	-3.494490
C	2.077092	0.459420	-5.875678
C	0.075958	-0.230994	-4.721782
C	0.807822	-0.113318	-5.896619
H	0.382405	-0.461950	-6.834229
H	-0.923005	-0.659420	-4.757122
C	2.608281	0.917576	-4.675854
H	2.292543	1.170022	-2.560009
H	2.645844	0.555156	-6.797031
H	3.592918	1.377223	-4.653573
C	-1.037629	2.756537	-2.364244
C	-3.265049	3.672570	-2.495566
C	-2.948720	1.299807	-2.194521
C	-3.793118	2.397679	-2.336994
H	-4.869880	2.249951	-2.323253
H	-3.391754	0.316376	-2.070875
C	-1.883262	3.847402	-2.509060
H	0.039072	2.909422	-2.355230
H	-3.926482	4.528020	-2.606119
H	-1.458604	4.840721	-2.628885
C	-0.419926	-1.425870	4.432469
C	1.196114	-0.859505	6.130004
C	1.274145	0.233173	3.985132
C	1.784438	0.058600	5.266319
H	2.667055	0.619360	5.556959
H	1.776302	0.923907	3.310544
C	0.100581	-1.605556	5.709972
H	-1.274020	-2.022765	4.127172
H	1.608476	-1.005762	7.125342
H	-0.352336	-2.338133	6.374225
I	2.210370	2.391628	0.138070
C	2.361870	-1.258707	-0.647487
C	2.233136	-1.898502	0.396833
C	2.119950	-2.674747	1.577483
C	1.287709	-3.809986	1.603487
C	1.203231	-4.578019	2.754338
C	2.867546	-2.335443	2.717290
C	2.781567	-3.121421	3.855950
C	1.947623	-4.234995	3.882492
H	0.561258	-5.455297	2.769297
H	0.728783	-4.085759	0.713515
H	3.524440	-1.468346	2.738914
H	1.876413	-4.841067	4.782268
H	3.369989	-2.834757	4.722648
H	2.793181	-1.044666	-1.604853
Cs	5.654531	0.695678	1.253855
Cs	6.247919	2.999974	6.104034
Cs	4.331440	3.923608	2.868411
Cs	7.983120	-0.801608	4.711700

0•S•{Cs} (cont)

O	8.331279	2.089639	4.549122
O	8.107354	1.145426	2.527122
O	6.929185	3.000684	3.035848
C	7.811127	2.087804	3.360124
O	5.422793	0.331596	5.785999
O	4.366928	1.470017	4.154216
C	4.984936	0.394558	4.571333
O	5.191538	-0.588829	3.752624
H	2.264694	3.435098	2.531194
C	3.249175	-0.156937	3.523623
H	3.280094	-0.579032	1.426402
H	3.125066	0.538041	5.549801
H	3.497326	-1.171982	3.800289

1•{CsI}•{Cs'}

E_t = -4620.901204 a.u.

Cu	-0.315378	0.408956	0.315924
P	-1.742780	0.207040	2.075174
P	-1.506255	0.490575	-1.630392
C	-2.953136	-1.188445	1.838404
C	-3.574035	-1.168666	0.433140
C	-2.691145	-1.856419	-0.629644
C	-2.542189	-1.051033	-1.921766
C	-2.800697	1.638668	2.523441
C	-0.925556	-0.284421	3.651800
C	-0.337482	0.523189	-3.044479
C	-2.678353	1.857506	-1.999178
H	-1.688772	-2.033485	-0.222380
H	-2.060937	-1.657252	-2.695926
H	-3.521008	-0.751086	-2.314302
H	-3.708545	-1.155137	2.632618
H	-2.394884	-2.119666	1.987211
H	-3.778511	-0.131673	0.133623
H	-4.555927	-1.657481	0.469613
H	-3.106901	-2.844354	-0.867545
C	-4.198730	1.604102	2.513696
C	-4.292817	3.965618	3.002835
C	-2.161015	2.862989	2.766141
C	-2.901181	4.011737	3.013309
H	-2.384749	4.950695	3.194902
H	-1.076673	2.924134	2.722418
C	-4.937039	2.760465	2.747839
H	-4.730615	0.679918	2.311005
H	-4.872354	4.867434	3.183956
H	-6.023055	2.715435	2.728534
C	0.335777	-0.643241	-3.434839
C	1.713166	0.624270	-4.960969
C	0.052709	1.744161	-3.608551
C	1.067033	1.790428	-4.559819
H	1.357127	2.747322	-4.986244
H	-0.433946	2.663612	-3.294950
C	1.342326	-0.592770	-4.393672
H	0.095557	-1.594757	-2.967233
H	2.512176	0.663746	-5.696203
H	1.850528	-1.507216	-4.690884
C	-2.940729	2.797323	-1.001541
C	-4.550763	3.884635	-2.428236
C	-3.353026	1.948825	-3.221932
C	-4.282824	2.958394	-3.435124
H	-4.802204	3.023708	-4.388119
H	-3.142284	1.232020	-4.013497
C	-3.878061	3.804586	-1.214780
H	-2.399020	2.746507	-0.061457
H	-5.281718	4.671925	-2.596312
H	-4.074959	4.526440	-0.426505
C	-0.113945	-1.429417	3.616797
C	0.489731	-1.102395	5.931384
C	-1.014058	0.443317	4.841364
C	-0.304944	0.038451	5.969746
H	-0.384456	0.615754	6.887615
H	-1.641866	1.328379	4.890818
C	0.577612	-1.838199	4.750709
H	0.003870	-1.979746	2.684593
H	1.035146	-1.419882	6.816491
H	1.192846	-2.734290	4.710424
I	0.840190	2.866478	0.376758
C	0.890512	-1.088045	0.198122
C	1.575245	-2.105006	0.047059
C	2.339680	-3.277942	-0.165237
C	2.551172	-3.779948	-1.466129
C	3.272159	-4.948549	-1.675472
C	2.909772	-3.988570	0.910627
C	3.625499	-5.157416	0.695737
C	3.809665	-5.649878	-0.597083
H	3.409908	-5.319374	-2.688731
H	2.127602	-3.239363	-2.308331
H	2.781530	-3.600035	1.916474
H	4.359154	-6.573492	-0.760905
H	4.043623	-5.693386	1.545126
H	6.284907	2.078252	-3.761272
Cs	2.805722	0.488781	2.540036
Cs	7.995105	1.831331	0.230192
Cs	3.362457	0.611963	-1.473306
Cs	6.263353	-2.820701	-0.625761

1•{CsI}•{Cs'} (cont)

O	5.977843	-0.647805	-2.548264
O	5.731514	1.299101	-3.601440
O	7.658437	0.882298	-2.492769
C	6.536073	0.435772	-2.821373
O	6.799220	-0.561703	1.085611
O	5.300234	1.126636	0.977261
C	5.578657	-0.148616	0.979792
O	4.604689	-1.002008	0.844230

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E_t = -3714.363400 a.u.

Cu	0.526219	-0.287030	-0.017819
P	-0.905603	-0.519573	1.704856
P	-0.704456	-0.306539	-1.907598
C	-1.981983	-2.034620	1.570169
C	-2.467537	-2.281406	0.133087
C	-1.359048	-2.815239	-0.801125
C	-1.240722	-2.080986	-2.142866
C	-2.090014	0.867584	1.904137
C	-0.187072	-0.687284	3.384558
C	0.122946	0.079080	-3.500442
C	-2.211502	0.743081	-1.949645
H	-0.385303	-2.745960	-0.294932
H	-0.445598	-2.535405	-2.745996
H	-2.161420	-2.154788	-2.734460
H	-2.817218	-1.947920	2.276858
H	-1.367467	-2.876696	1.913045
H	-2.883134	-1.352914	-0.276562
H	-3.302010	-2.993321	0.161969
H	-1.520760	-3.882956	-0.995444
C	-3.464211	0.761494	1.677876
C	-3.745026	3.116323	2.125676
C	-1.552511	2.119273	2.232888
C	-2.374750	3.231430	2.350740
H	-1.944361	4.192473	2.617787
H	-0.482603	2.215745	2.406441
C	-4.284325	1.881381	1.786529
H	-3.910812	-0.191138	1.411529
H	-4.387852	3.987613	2.212963
H	-5.350323	1.783720	1.601840
C	-0.582629	0.433867	-4.653502
C	1.488381	0.556288	-5.883718
C	1.517236	-0.020176	-3.540805
C	2.193669	0.212469	-4.734420
H	3.276957	0.137276	-4.759151
H	2.066317	-0.260516	-2.630972
C	0.100858	0.670755	-5.841065
H	-1.664441	0.536730	-4.620717
H	2.019894	0.745383	-6.812190
H	-0.450625	0.949413	-6.734659
C	-3.468633	0.328867	-2.395891
C	-4.389841	2.502352	-1.895410
C	-2.062182	2.050420	-1.470370
C	-3.139753	2.925131	-1.451548
H	-3.007594	3.932502	-1.068527
H	-1.093786	2.376986	-1.097333
C	-4.552073	1.203660	-2.364416
H	-3.617853	-0.678841	-2.772319
H	-5.236603	3.182268	-1.869177
H	-5.524693	0.866697	-2.712016
C	-0.978717	-0.617899	4.535858
C	0.968092	-1.026911	5.897785
C	1.186366	-0.915413	3.497199
C	1.758581	-1.087931	4.755285
H	2.827764	-1.260349	4.838045
H	1.802590	-0.939247	2.599123
C	-0.401108	-0.788824	5.787753
H	-2.043911	-0.414376	4.452051
H	1.417960	-1.156429	6.878234
H	-1.017538	-0.731546	6.680500
C	2.399629	-0.371115	0.072606
C	3.628233	-0.426258	0.131908
C	5.041737	-0.489702	0.200133
C	5.720660	-1.711835	0.028119
C	7.105300	-1.769246	0.096729
C	5.807743	0.667175	0.442323
C	7.191985	0.599201	0.508371
C	7.850604	-0.616705	0.336771
H	8.934219	-0.665528	0.389419
H	5.139071	-2.609186	-0.159185
H	7.609096	-2.722708	-0.038725
H	5.293490	1.613762	0.575953
H	7.764004	1.504113	0.695888

1•S

E_t = -4022.653249 a.u.

Cu	0.471886	-0.980420	-0.516210
P	-0.934808	-1.331131	1.404829
P	-0.972422	-1.015542	-2.280229
C	-2.244552	-2.658999	1.353464
C	-2.967135	-2.573919	-0.002861
C	-2.186526	-3.296862	-1.121323
C	-2.050915	-2.536144	-2.445767
C	-1.945423	0.119168	1.919893
C	0.043079	-1.662924	2.916466
C	-0.132942	-0.926214	-3.912566
C	-2.091761	0.436743	-2.379439
H	-1.174597	-3.511412	-0.757929
H	-1.545642	-3.172517	-3.182594
H	-3.028400	-2.283359	-2.874005
H	-2.938798	-2.529427	2.192070
H	-1.772702	-3.643759	1.457515
H	-3.119512	-1.515929	-0.255241
H	-3.972149	-3.002814	0.089277
H	-2.653827	-4.269477	-1.322609
C	-2.644785	0.118274	3.132495
C	-3.506801	2.316340	2.646270
C	-2.019273	1.234546	1.086025
C	-2.801679	2.328772	1.449157
H	-2.846789	3.191868	0.791392
H	-1.435455	1.262263	0.171787
C	-3.422882	1.210567	3.492229
H	-2.563272	-0.731717	3.806706
H	-4.113116	3.171872	2.931166
H	-3.959122	1.204890	4.437171
C	-0.858108	-0.963764	-5.108308
C	1.191887	-0.782294	-6.363647
C	1.256422	-0.804198	-3.952868
C	1.915717	-0.731203	-5.177882
H	2.996866	-0.630340	-5.201837
H	1.814259	-0.750940	-3.020352
C	-0.197045	-0.897414	-6.327977
H	-1.943496	-1.030001	-5.084072
H	1.706689	-0.725053	-7.318582
H	-0.765012	-0.926489	-7.253578
C	-1.473115	1.687302	-2.517465
C	-3.615534	2.785362	-2.367857
C	-3.479342	0.380059	-2.236478
C	-4.235960	1.549399	-2.232116
H	-5.314243	1.489416	-2.115806
H	-3.989551	-0.571090	-2.121750
C	-2.231125	2.849919	-2.512693
H	-0.390701	1.744643	-2.593745
H	-4.206808	3.696597	-2.357456
H	-1.736091	3.812181	-2.608767
C	0.971649	-0.677334	3.281826
C	1.719410	-2.039512	5.124641
C	-0.026561	-2.840645	3.663110
C	0.810803	-3.026095	4.762125
H	0.745753	-3.945714	5.337265
H	-0.736408	-3.619931	3.402554
C	1.795763	-0.862834	4.381282
H	1.053485	0.228051	2.682872
H	2.372494	-2.187315	5.980080
H	2.516753	-0.095426	4.647138
C	1.062962	0.837996	-0.348482
C	1.354359	2.027686	-0.232020
C	1.662198	3.401842	-0.073215
C	2.111400	3.901673	1.164866
C	2.401814	5.249109	1.323266
C	1.521176	4.308585	-1.141074
C	1.812823	5.655029	-0.973955
C	2.254046	6.134632	0.257419
H	2.482376	7.188650	0.384817
H	2.221207	3.210938	1.995588
H	2.745276	5.613562	2.287806
H	1.187331	3.932281	-2.103780
H	1.698922	6.337302	-1.812259
C	1.448410	-2.781747	-0.806752
C	2.185325	-2.176841	-0.014108
C	3.183071	-1.829872	0.945966
C	3.585344	-2.802756	1.877077
C	4.561573	-2.504011	2.815425
C	3.770494	-0.556279	0.979138

1•S (cont)

C	4.752184	-0.274738	1.917724
C	5.150729	-1.242263	2.837976
H	4.858648	-3.258406	3.538321
H	3.112709	-3.779754	1.860534
H	3.417684	0.201584	0.286836
H	5.914323	-1.011918	3.575540
H	5.203384	0.713342	1.935901
H	1.201702	-3.563705	-1.495354

1dim

E_t = -7428.800485 a.u.

Cu	-1.212304	0.026702	-0.169381
P	-2.614313	0.170538	-1.971146
P	-2.593677	-0.175279	1.640534
C	-3.699535	1.692136	-1.944367
C	-3.748568	2.344435	-0.556768
C	-4.533970	1.555440	0.515263
C	-3.735107	1.287239	1.798163
C	-3.726678	-1.288661	-2.153793
C	-1.900765	0.195622	-3.670909
C	-1.917909	-0.216192	3.352527
C	-3.730406	-1.617855	1.586848
H	-4.877630	0.595705	0.110011
H	-4.392184	1.132783	2.662993
H	-3.093159	2.143250	2.044038
H	-3.230075	2.389188	-2.649736
H	-4.704496	1.478995	-2.330411
H	-2.716235	2.496019	-0.217101
H	-4.187644	3.344256	-0.664980
H	-5.446662	2.103619	0.779147
C	-3.112738	-2.491867	-2.524644
C	-5.217581	-3.652901	-2.369018
C	-5.097620	-1.288194	-1.891976
C	-5.836288	-2.464813	-1.998776
H	-6.901754	-2.447269	-1.787123
H	-5.610590	-0.374763	-1.608208
C	-3.849942	-3.661985	-2.633248
H	-2.045389	-2.513456	-2.720250
H	-5.796876	-4.568685	-2.446543
H	-3.345909	-4.583413	-2.913904
C	-0.706850	0.438929	3.594371
C	-0.837758	-0.151188	5.928823
C	-2.579408	-0.845242	4.410075
C	-2.040126	-0.810874	5.692124
H	-2.557529	-1.310122	6.506907
H	-3.509184	-1.378851	4.232216
C	-0.173155	0.472859	4.877758
H	-0.178936	0.904524	2.765201
H	-0.411416	-0.137476	6.928087
H	0.780393	0.965782	5.048851
C	-5.042302	-1.618507	2.070973
C	-5.298065	-3.931912	1.434498
C	-3.222594	-2.785354	1.005705
C	-3.997252	-3.937262	0.939864
H	-3.588582	-4.829339	0.473227
H	-2.223171	-2.774653	0.574113
C	-5.821231	-2.769354	1.992499
H	-5.468044	-0.721547	2.512043
H	-5.910108	-4.827330	1.369918
H	-6.840748	-2.756206	2.368206
C	-2.628607	0.666329	-4.768094
C	-0.774770	0.171616	-6.229135
C	-0.610853	-0.299762	-3.869135
C	-0.055469	-0.317582	-5.145219
H	0.954664	-0.692164	-5.286855
H	-0.042900	-0.660211	-3.013955
C	-2.064208	0.663305	-6.038493
H	-3.644739	1.029915	-4.637614
H	-0.333011	0.173113	-7.221677
H	-2.634992	1.038530	-6.883438
C	0.066454	-1.536390	-0.653238
C	0.007132	-2.730677	-0.974669
C	-0.148337	-4.087718	-1.339203
C	-0.449596	-5.065631	-0.369067
C	-0.663003	-6.386041	-0.737626
C	-0.051962	-4.493474	-2.686223
C	-0.264047	-5.817066	-3.044038
C	-0.575282	-6.769878	-2.075033
H	-0.742517	-7.804490	-2.359339
H	-0.511556	-4.766844	0.673731
H	-0.896070	-7.124537	0.024815
H	0.182647	-3.748022	-3.441310
H	-0.188863	-6.109093	-4.088033
Cu	1.214034	0.071467	-0.142592
P	2.633609	0.977451	-1.690733
P	2.577324	-0.800254	1.471836
C	3.722899	-0.290577	-2.526944
C	3.760583	-1.618348	-1.759520
C	4.533353	-1.584875	-0.421488

1dim (cont)

C	3.721400	-2.094571	0.777212
C	3.743424	2.276558	-0.997467
C	1.936350	1.929148	-3.107443
C	1.884950	-1.741986	2.894159
C	3.710310	0.411145	2.262353
H	4.878046	-0.566599	-0.203051
H	4.369647	-2.463561	1.581673
H	3.079582	-2.935721	0.484217
H	3.262174	-0.458893	-3.508383
H	4.730868	0.101688	-2.712769
H	2.725498	-1.933544	-1.577012
H	4.203597	-2.378864	-2.414878
H	5.445080	-2.188393	-0.509031
C	3.129573	3.478164	-0.621318
C	5.229569	4.336605	0.188417
C	5.111852	2.122683	-0.769965
C	5.848145	3.147738	-0.179536
H	6.911632	3.009381	-0.005825
H	5.624754	1.209096	-1.053349
C	3.864443	4.498926	-0.036126
H	2.064057	3.610725	-0.779640
H	5.806967	5.131226	0.652575
H	3.360453	5.417333	0.254335
C	0.673534	-2.414146	2.707050
C	0.780158	-3.262840	4.961687
C	2.534361	-1.831367	4.127838
C	1.982823	-2.589849	5.155538
H	2.490871	-2.646753	6.114430
H	3.464246	-1.294624	4.295397
C	0.127565	-3.173044	3.736155
H	0.155016	-2.321364	1.755457
H	0.344224	-3.843267	5.770113
H	-0.826147	-3.672443	3.586041
C	5.017404	0.131098	2.672877
C	5.272423	2.392780	3.474191
C	3.204704	1.702987	2.447171
C	3.976491	2.683716	3.058594
H	3.569708	3.683755	3.181118
H	2.209561	1.943794	2.077132
C	5.793613	1.118178	3.273301
H	5.441482	-0.858432	2.526850
H	5.882372	3.162767	3.938547
H	6.809444	0.889633	3.584102
C	2.675962	2.166621	-4.270075
C	0.834667	3.412325	-5.204924
C	0.646950	2.452987	-2.999682
C	0.103673	3.197595	-4.042545
H	-0.906152	3.589083	-3.954620
H	0.069851	2.262624	-2.097160
C	2.123660	2.895865	-5.316801
H	3.691860	1.790513	-4.360826
H	0.402371	3.978908	-6.024924
H	2.703541	3.068252	-6.219321
C	-0.064728	1.634916	0.340139
C	-0.005915	2.798818	0.758509
C	0.148933	4.120674	1.235303
C	0.437947	4.368970	2.592894
C	0.650881	5.662875	3.046029
C	0.064234	5.222999	0.360035
C	0.275734	6.513389	0.823794
C	0.574798	6.741691	2.166228
H	0.741624	7.752978	2.524962
H	0.490837	3.528227	3.279111
H	0.874411	5.833345	4.095785
H	-0.160878	5.042623	-0.687670
H	0.209665	7.349303	0.132607

1•T

E_t = -3946.753344 a.u.

Cu	0.050814	-0.502143	-0.167186
P	-1.304493	-0.639965	1.639094
P	-1.278832	-0.419052	-1.982063
C	-2.857869	-1.661132	1.595319
C	-3.484677	-1.631138	0.189914
C	-2.729727	-2.524057	-0.819104
C	-2.443512	-1.864807	-2.174874
C	-1.905546	1.074818	1.938936
C	-0.525387	-1.061594	3.252073
C	-0.496705	-0.266874	-3.641720
C	-2.316330	1.103575	-1.925608
H	-1.767362	-2.829247	-0.393291
H	-1.924441	-2.579209	-2.826303
H	-3.372412	-1.585737	-2.686894
H	-3.568462	-1.320433	2.358216
H	-2.575685	-2.688598	1.859831
H	-3.517158	-0.595408	-0.171217
H	-4.532091	-1.950535	0.261065
H	-3.299220	-3.446576	-0.990982
C	-3.252007	1.443593	1.949369
C	-2.640465	3.747243	2.327535
C	-0.927221	2.063895	2.106656
C	-1.294693	3.386763	2.311386
H	-0.524831	4.141364	2.446471
H	0.125681	1.794462	2.053082
C	-3.614851	2.774815	2.138386
H	-4.033392	0.704856	1.801758
H	-2.926892	4.784325	2.478675
H	-4.666065	3.048866	2.134986
C	-1.174443	-0.543771	-4.832421
C	0.791016	0.046023	-6.099259
C	0.829151	0.172641	-3.690388
C	1.466758	0.332287	-4.917404
H	2.496457	0.677056	-4.947181
H	1.354320	0.384612	-2.759107
C	-0.530341	-0.392885	-6.055277
H	-2.210062	-0.874013	-4.810563
H	1.291405	0.165488	-7.056102
H	-1.061684	-0.613385	-6.976948
C	-1.729683	2.232161	-1.342286
C	-3.725605	3.514576	-1.768113
C	-3.613694	1.198307	-2.433890
C	-4.316185	2.396658	-2.349039
H	-5.327365	2.456256	-2.742021
H	-4.092069	0.341066	-2.898555
C	-2.429071	3.430716	-1.270620
H	-0.724408	2.161282	-0.931326
H	-4.276788	4.448353	-1.701043
H	-1.963776	4.294372	-0.805438
C	-1.251587	-1.515895	4.356920
C	0.779496	-1.649915	5.652443
C	0.860103	-0.901694	3.360663
C	1.506116	-1.188484	4.559173
H	2.582173	-1.057898	4.632841
H	1.425178	-0.549860	2.497580
C	-0.599391	-1.814125	5.548596
H	-2.329829	-1.633736	4.296950
H	1.285187	-1.881278	6.585699
H	-1.170858	-2.170191	6.401268
C	1.722149	0.365767	0.064573
C	2.801873	0.918331	0.282949
C	4.059063	1.517774	0.547426
C	4.334677	2.097930	1.801109
C	5.570194	2.672711	2.062307
C	5.073571	1.540021	-0.429096
C	6.307517	2.114392	-0.158923
C	6.564524	2.684462	1.086109
H	7.530860	3.134405	1.293691
H	3.558988	2.087043	2.561457
H	5.761050	3.115403	3.036361
H	4.871014	1.097921	-1.400049
H	7.076504	2.119656	-0.926884
O	0.706875	-2.843189	-0.483303
C	1.647022	-2.980891	-1.565755
H	1.591624	-4.010649	-1.955494
H	1.347721	-2.281863	-2.351993
C	3.023765	-2.684871	-0.957523
H	3.288374	-1.635879	-1.111947

1•T (cont)

H	3.798288	-3.317639	-1.400770
C	2.827424	-2.954276	0.555810
H	2.974756	-2.026725	1.115149
H	3.514271	-3.712069	0.943991
C	1.369604	-3.414278	0.659551
H	0.852079	-3.057513	1.554816
H	1.289522	-4.512765	0.607771

1•A

E_t = -4421.549549 a.u.

Cu	0.099385	0.035261	0.321366
P	-1.215996	-0.203640	2.166758
P	-1.180893	0.143060	-1.549794
C	-2.857353	-1.065604	1.979931
C	-3.524877	-0.742202	0.630800
C	-3.064922	-1.675302	-0.510082
C	-2.692460	-0.945414	-1.803159
C	-1.694191	1.516670	2.614006
C	-0.625970	-0.913151	3.764220
C	-0.164774	-0.112308	-3.056552
C	-1.857720	1.834627	-1.810134
H	-2.196571	-2.249272	-0.173866
H	-2.482812	-1.668636	-2.598590
H	-3.518403	-0.314739	-2.153276
H	-3.493655	-0.808823	2.835482
H	-2.656190	-2.140771	2.053985
H	-3.324202	0.303614	0.359987
H	-4.614055	-0.807118	0.745569
H	-3.853549	-2.407245	-0.729317
C	-3.017150	1.958803	2.700499
C	-2.266784	4.214566	3.119979
C	-0.659779	2.447217	2.786891
C	-0.944781	3.782042	3.046345
H	-0.126988	4.486741	3.168796
H	0.373213	2.131704	2.673397
C	-3.299804	3.300178	2.946495
H	-3.844017	1.269594	2.564819
H	-2.490180	5.261131	3.308317
H	-4.334034	3.628626	2.998162
C	0.642039	0.943330	-3.503752
C	1.696491	-0.511826	-5.116690
C	-0.012946	-1.372078	-3.645307
C	0.907342	-1.567522	-4.670634
H	1.004642	-2.551773	-5.121465
H	-0.595667	-2.220998	-3.298296
C	1.560020	0.743276	-4.527090
H	0.561666	1.918985	-3.031836
H	2.414738	-0.665334	-5.916858
H	2.177192	1.572557	-4.860877
C	-1.716014	2.795768	-0.808944
C	-2.953050	4.381890	-2.141558
C	-2.540686	2.162303	-2.987342
C	-3.083195	3.430243	-3.152395
H	-3.607071	3.678735	-4.071158
H	-2.635994	1.426581	-3.783100
C	-2.269320	4.063725	-0.974081
H	-1.150123	2.558144	0.086933
H	-3.381145	5.372109	-2.271024
H	-2.159692	4.799139	-0.181844
C	-0.330368	-2.282840	3.809575
C	0.343309	-2.088302	6.119085
C	-0.428474	-0.142922	4.913473
C	0.055487	-0.728623	6.079908
H	0.202989	-0.114697	6.964080
H	-0.656681	0.918166	4.903078
C	0.143890	-2.863617	4.979795
H	-0.466700	-2.895233	2.923330
H	0.719816	-2.542188	7.031311
H	0.362568	-3.927893	4.999283
C	1.285539	1.549351	0.379272
C	1.930521	2.599575	0.378060
C	2.598589	3.848994	0.392207
C	1.882032	5.040685	0.160518
C	2.523868	6.270502	0.179935
C	3.981181	3.945188	0.640744
C	4.614796	5.179950	0.657103
C	3.893145	6.349669	0.428259
H	4.393044	7.313685	0.442087
H	0.816157	4.973866	-0.039034
H	1.952367	7.176808	-0.003016
H	4.543413	3.034077	0.822192
H	5.682911	5.231484	0.851391
C	-1.575378	-6.311626	-1.906813
C	-0.871758	-6.541083	-3.086607
C	0.244826	-5.767403	-3.394736
C	0.659808	-4.763793	-2.529369
C	-0.046013	-4.532686	-1.343231
C	-1.164113	-5.312717	-1.035163

1•A (cont)

H	-2.445549	-6.914821	-1.665976
H	-1.193139	-7.324529	-3.766884
H	0.794554	-5.948377	-4.313719
H	1.523373	-4.153800	-2.770727
H	-1.697278	-5.118376	-0.109906
C	0.329822	-3.460040	-0.384559
O	1.408822	-2.784332	-0.820499
O	-0.262500	-3.229280	0.649747
N	1.732547	-1.528020	-0.103606
C	2.406905	-1.869699	1.178196
C	2.729560	-0.912253	-1.020594
H	2.612840	-0.892291	1.633692
C	3.696223	-2.651572	0.985209
H	1.698647	-2.404089	1.816547
C	4.011035	-1.722411	-1.140791
H	2.924358	0.077848	-0.594074
H	2.252662	-0.772086	-1.995790
H	4.198315	-2.774877	1.950370
H	3.484109	-3.654811	0.575589
H	4.742487	-1.155986	-1.726246
H	3.827872	-2.682640	-1.652101
O	4.603850	-1.956801	0.135688

1•P

E_t = -4540.163259 a.u.

Cu	-0.094576	-0.483852	0.307898
P	-1.767264	-0.714930	1.990842
P	-1.391924	-0.399554	-1.591047
C	-3.185990	-1.901331	1.733197
C	-3.676168	-1.932077	0.279496
C	-2.693598	-2.686562	-0.642894
C	-2.307544	-1.974746	-1.943822
C	-2.575044	0.902647	2.295573
C	-1.221902	-1.235188	3.670440
C	-0.637610	0.079991	-3.200955
C	-2.666999	0.935973	-1.501509
H	-1.764641	-2.872722	-0.089502
H	-1.603957	-2.618815	-2.486051
H	-3.172210	-1.816802	-2.598869
H	-3.987697	-1.661833	2.441977
H	-2.811282	-2.891338	2.021740
H	-3.835113	-0.908151	-0.077643
H	-4.661838	-2.412817	0.247775
H	-3.101782	-3.673771	-0.894635
C	-3.955635	1.109602	2.261874
C	-3.642140	3.447453	2.771057
C	-1.731205	1.994128	2.544746
C	-2.263167	3.251904	2.796497
H	-1.594985	4.084169	3.000376
H	-0.652837	1.858979	2.512038
C	-4.483668	2.376993	2.491564
H	-4.635545	0.292007	2.045416
H	-4.058027	4.433799	2.957308
H	-5.559052	2.524643	2.450676
C	0.008046	1.322193	-3.251503
C	0.450271	1.017962	-5.603852
C	-0.718997	-0.691795	-4.361581
C	-0.175207	-0.223162	-5.556062
H	-0.247766	-0.832878	-6.452507
H	-1.202792	-1.662978	-4.351020
C	0.542634	1.787558	-4.445728
H	0.100081	1.920103	-2.347389
H	0.867189	1.383768	-6.537911
H	1.039161	2.753650	-4.467859
C	-2.342055	2.099750	-0.799395
C	-4.452493	3.088159	-1.424041
C	-3.890898	0.865264	-2.173333
C	-4.782166	1.931317	-2.125082
H	-5.732470	1.861283	-2.647033
H	-4.159546	-0.017048	-2.746349
C	-3.228849	3.171107	-0.770057
H	-1.390359	2.162896	-0.276419
H	-5.147808	3.922370	-1.392151
H	-2.962734	4.066934	-0.217139
C	-0.607894	-2.487986	3.788072
C	-0.248712	-2.121341	6.141853
C	-1.346455	-0.434559	4.807523
C	-0.859476	-0.877206	6.034177
H	-0.960858	-0.242342	6.909974
H	-1.822011	0.538808	4.738900
C	-0.129388	-2.928915	5.014257
H	-0.475035	-3.111804	2.906474
H	0.138030	-2.460075	7.098641
H	0.358607	-3.896681	5.084151
C	0.816431	1.224575	0.363478
C	1.352871	2.325484	0.228473
C	1.957715	3.589850	0.009096
C	3.279263	3.689889	-0.468852
C	3.852805	4.932731	-0.699676
C	1.242178	4.780071	0.243857
C	1.825410	6.017433	0.010391
C	3.133426	6.102305	-0.462292
H	3.588020	7.071766	-0.644002
H	3.843823	2.781227	-0.659467
H	4.873582	4.988407	-1.068452
H	0.221069	4.710159	0.608884
H	1.255606	6.923928	0.197078
C	1.074255	-2.446131	0.011938
C	1.342136	-1.837240	1.059541
C	2.082356	-1.669981	2.278693
C	2.811737	-2.767551	2.769893
C	3.522740	-2.659664	3.955250
C	2.092560	-0.466682	2.993129

1•P (cont)

C	2.807336	-0.369391	4.179027
C	3.517595	-1.461995	4.667839
H	4.068314	-1.382018	5.600673
C	1.039612	-3.132975	-1.227200
C	1.754876	-2.595721	-2.341445
C	0.275556	-4.298245	-1.393741
C	1.560868	-3.183990	-3.597185
C	0.129199	-4.884531	-2.642377
C	0.752027	-4.304940	-3.746525
N	2.571105	-1.488473	-2.141094
C	2.951118	-0.659283	-3.280857
C	3.710095	-1.632871	-1.217182
C	3.407613	0.694866	-2.748124
C	4.147779	-0.259968	-0.741851
O	4.514030	0.562786	-1.855458
H	2.798669	-3.701471	2.214589
H	1.543989	0.379321	2.589850
H	-0.473755	-5.780019	-2.756458
H	-0.232612	-4.712932	-0.528460
H	0.634630	-4.748240	-4.731526
H	2.068822	-2.772635	-4.463101
H	2.805760	0.567517	4.728402
H	3.744384	1.333230	-3.571914
H	4.080924	-3.514049	4.327972
H	3.432045	-2.250201	-0.361539
H	4.548193	-2.126465	-1.744778
H	2.084383	-0.513917	-3.933246
H	3.769327	-1.117634	-3.869801
H	3.329838	0.211624	-0.173296
H	5.038097	-0.339998	-0.109495
H	2.565549	1.179893	-2.229833

1•B

E_t = -3945.242077 a.u.

Cu	0.883249	-0.991022	-0.319863
P	-0.760042	-1.025981	1.612167
P	-0.702612	-0.785681	-1.966558
C	-2.239154	-2.165192	1.556938
C	-2.887342	-2.240029	0.166508
C	-2.033453	-3.040445	-0.842200
C	-1.720218	-2.333797	-2.164849
C	-1.478671	0.623706	1.949428
C	-0.019378	-1.520701	3.219289
C	0.020012	-0.581991	-3.640469
C	-1.869917	0.623983	-1.827295
H	-1.076150	-3.297703	-0.375227
H	-1.092977	-2.986550	-2.785271
H	-2.625032	-2.129103	-2.750368
H	-2.954928	-1.861151	2.331278
H	-1.866363	-3.155252	1.848693
H	-3.068916	-1.226998	-0.209188
H	-3.878052	-2.700911	0.266360
H	-2.528757	-3.991755	-1.073848
C	-0.589389	1.664381	2.253021
C	-2.424462	3.226607	2.371412
C	-2.842856	0.909705	1.844748
C	-3.310260	2.204557	2.050221
H	-4.372779	2.411098	1.957455
H	-3.556451	0.130068	1.597962
C	-1.062927	2.951014	2.475814
H	0.477275	1.465418	2.303686
H	-2.792111	4.235380	2.537995
H	-0.360006	3.741812	2.722474
C	1.293375	-1.108288	-3.876102
C	1.168591	-0.395031	-6.175898
C	-0.668463	0.051608	-4.677836
C	-0.093664	0.142500	-5.941054
H	-0.631631	0.640620	-6.742607
H	-1.647541	0.486476	-4.495399
C	1.860829	-1.019064	-5.142317
H	1.842983	-1.575225	-3.061783
H	1.617269	-0.317526	-7.162170
H	2.852627	-1.425835	-5.316656
C	-1.339018	1.840979	-1.383218
C	-3.505764	2.880971	-1.598612
C	-3.227411	0.550993	-2.154141
C	-4.040873	1.674229	-2.036178
H	-5.094649	1.603307	-2.290639
H	-3.666834	-0.378532	-2.502945
C	-2.154610	2.960519	-1.276281
H	-0.289327	1.896800	-1.102797
H	-4.142216	3.756414	-1.504280
H	-1.733646	3.897015	-0.922478
C	0.864543	-2.606328	3.214124
C	1.122799	-2.427305	5.604973
C	-0.322538	-0.892146	4.429995
C	0.249180	-1.343897	5.615066
H	0.008753	-0.846790	6.550698
H	-1.002250	-0.044948	4.445527
C	1.426350	-3.058956	4.402557
H	1.124638	-3.092125	2.276906
H	1.569486	-2.775488	6.531993
H	2.113677	-3.899947	4.383860
C	1.639574	0.728225	-0.117349
C	2.122926	1.844773	0.029246
C	2.609852	3.164385	0.209638
C	1.716415	4.248940	0.299068
C	2.185456	5.542072	0.482252
C	3.988168	3.428046	0.309025
C	4.448843	4.724460	0.490675
C	3.553290	5.788115	0.579125
H	3.918610	6.800897	0.721146
H	0.650637	4.052452	0.226841
H	1.479485	6.365852	0.547807
H	4.683884	2.597765	0.239684
H	5.517309	4.908197	0.564299
C	1.460702	-2.871231	-0.456873
C	2.396731	-2.130536	0.080906
C	1.597149	-4.241815	-0.621997
C	3.620694	-2.554139	0.547445
C	2.821156	-4.759768	-0.162488
C	3.802818	-3.942236	0.405612

1•B (cont)

H	0.844202	-4.891844	-1.061959
H	4.376199	-1.913922	0.991203
H	3.011250	-5.826541	-0.253389
H	4.732649	-4.390615	0.747464

TS[**1**•B–**2**]

E_t = -3945.233702 a.u.

Cu	0.376469	-0.940875	-0.138826
P	-0.979970	-1.057068	1.711465
P	-1.105330	-0.748419	-1.886091
C	-2.368843	-2.293508	1.659526
C	-3.072323	-2.333966	0.292624
C	-2.253645	-3.078857	-0.785865
C	-2.084126	-2.321859	-2.107591
C	-1.800438	0.541551	2.071791
C	-0.157324	-1.463781	3.300009
C	-0.385107	-0.478863	-3.551981
C	-2.300857	0.631638	-1.709914
H	-1.248501	-3.289591	-0.399764
H	-1.487818	-2.925688	-2.802752
H	-3.044035	-2.132274	-2.602955
H	-3.068654	-2.080869	2.477926
H	-1.915589	-3.267980	1.881239
H	-3.287463	-1.310401	-0.038128
H	-4.050775	-2.814702	0.416511
H	-2.717265	-4.050829	-0.996340
C	-3.184480	0.729270	2.082828
C	-2.883687	3.075920	2.558567
C	-0.962100	1.643308	2.291109
C	-1.501712	2.897086	2.543342
H	-0.838568	3.740270	2.715778
H	0.116523	1.515156	2.243409
C	-3.721002	1.992225	2.321398
H	-3.859175	-0.101420	1.901410
H	-3.305145	4.059461	2.746885
H	-4.799125	2.125404	2.318893
C	-0.991714	0.323719	-4.521191
C	0.807084	-0.155652	-6.057012
C	0.832020	-1.107149	-3.840604
C	1.419195	-0.950012	-5.090790
H	2.365821	-1.438101	-5.304067
H	1.325535	-1.705544	-3.077672
C	-0.395677	0.482314	-5.768707
H	-1.925362	0.832897	-4.298464
H	1.272003	-0.026431	-7.030310
H	-0.872450	1.110096	-6.516316
C	-1.789375	1.823075	-1.180070
C	-3.962006	2.854440	-1.358060
C	-3.652861	0.566355	-2.057147
C	-4.479828	1.671920	-1.876296
H	-5.530514	1.607354	-2.145138
H	-4.074830	-0.344245	-2.471772
C	-2.614839	2.928178	-1.015092
H	-0.744171	1.870485	-0.879870
H	-4.609231	3.715303	-1.215116
H	-2.206567	3.842264	-0.594767
C	-0.711419	-1.101555	4.531901
C	1.116209	-2.180575	5.677580
C	1.042758	-2.178915	3.266352
C	1.672981	-2.538985	4.453998
H	2.607862	-3.090871	4.419512
H	1.485358	-2.443367	2.308853
C	-0.075484	-1.459767	5.714954
H	-1.632946	-0.525392	4.562838
H	1.613632	-2.455445	6.603500
H	-0.508451	-1.171936	6.668866
C	1.497008	0.589413	-0.001861
C	2.160063	1.620221	0.102773
C	2.878461	2.830125	0.227823
C	3.163897	3.620455	-0.903739
C	3.880184	4.801394	-0.776357
C	3.336005	3.271701	1.485762
C	4.050622	4.455157	1.601011
C	4.327538	5.226337	0.473553
H	4.890049	6.150438	0.567896
H	2.815921	3.284630	-1.875714
H	4.093914	5.396380	-1.660104
H	3.125734	2.664558	2.361176
H	4.398734	4.778265	2.578332
C	1.613676	-2.489715	-0.393961
C	2.328841	-1.374347	-0.301921
C	2.282935	-3.696957	-0.586103
C	3.694274	-1.225164	-0.370112
C	3.682549	-3.647474	-0.669677
C	4.373211	-2.438518	-0.563922

TS[**1**•B–**2**] (cont)

H	1.764241	-4.650303	-0.669660
H	4.204479	-0.271523	-0.284060
H	4.243827	-4.567169	-0.819431
H	5.457991	-2.429542	-0.631901

2

E_t = -3945.319780 a.u.

Cu	0.941283	-1.120241	0.215201
P	-0.376413	-1.226693	2.026568
P	-0.464291	-0.962628	-1.552894
C	-1.507751	-2.707254	1.959838
C	-2.107711	-2.929923	0.562612
C	-1.087190	-3.480312	-0.460641
C	-1.032172	-2.725977	-1.796832
C	-1.489353	0.207361	2.288683
C	0.410178	-1.422553	3.675847
C	0.244576	-0.503801	-3.185771
C	-1.973354	0.085192	-1.474195
H	-0.078273	-3.452615	-0.022340
H	-0.275053	-3.181288	-2.446718
H	-1.983486	-2.780784	-2.339333
H	-2.284866	-2.605129	2.728225
H	-0.893603	-3.568816	2.252030
H	-2.535737	-1.988876	0.197191
H	-2.951670	-3.625510	0.652403
H	-1.298383	-4.538261	-0.661438
C	-0.872510	1.452563	2.471135
C	-3.026034	2.526235	2.607674
C	-2.883727	0.143467	2.250717
C	-3.645494	1.298475	2.407501
H	-4.729186	1.234613	2.368159
H	-3.391146	-0.803259	2.093085
C	-1.634919	2.599891	2.638804
H	0.214081	1.516608	2.482903
H	-3.623383	3.425077	2.731405
H	-1.142199	3.556623	2.787911
C	-0.497274	0.115837	-4.194848
C	1.468046	0.210007	-5.592491
C	1.606102	-0.755164	-3.386145
C	2.211123	-0.405322	-4.588027
H	3.271013	-0.595840	-4.729939
H	2.193176	-1.196700	-2.582763
C	0.114683	0.469761	-5.393402
H	-1.548895	0.339373	-4.037724
H	1.945267	0.494998	-6.525997
H	-0.467199	0.955315	-6.172056
C	-3.252043	-0.321637	-1.864939
C	-4.140446	1.851442	-1.305941
C	-1.797605	1.386206	-0.989242
C	-2.869706	2.265421	-0.917273
H	-2.706398	3.270677	-0.541325
H	-0.814670	1.713272	-0.662246
C	-4.329969	0.555411	-1.774082
H	-3.422314	-1.323176	-2.248238
H	-4.982269	2.535026	-1.239359
H	-5.318878	0.224084	-2.078782
C	-0.316466	-1.289593	4.863429
C	1.663859	-1.811414	6.136587
C	1.769423	-1.738496	3.727861
C	2.391532	-1.935991	4.957939
H	3.450204	-2.176859	4.991262
H	2.336325	-1.813278	2.801513
C	0.309603	-1.484968	6.088486
H	-1.368870	-1.016820	4.828461
H	2.151845	-1.959511	7.095932
H	-0.257427	-1.377507	7.008958
C	2.976148	0.887191	-0.527465
C	2.305216	1.859050	-0.818466
C	1.464040	2.925798	-1.222377
C	0.962274	3.849632	-0.289138
C	0.078288	4.842512	-0.689586
C	1.064659	3.035237	-2.566620
C	0.179013	4.029751	-2.955074
C	-0.319733	4.935297	-2.021336
H	-1.015326	5.710253	-2.330152
H	1.271918	3.768645	0.748330
H	-0.302651	5.549688	0.042415
H	1.442767	2.316996	-3.287737
H	-0.129608	4.093538	-3.994726
C	2.858526	-1.444390	0.119333
C	3.662172	-0.321836	-0.220534
C	3.565557	-2.631729	0.372448
C	5.063116	-0.385991	-0.288178
C	4.955892	-2.711902	0.302162
C	5.709440	-1.585561	-0.025445

2 (cont)

H	3.013245	-3.533369	0.638866
H	5.630641	0.503721	-0.549183
H	5.457305	-3.655713	0.505757
H	6.793113	-1.643554	-0.076634

2$_1$•A

E_t = -4652.507320 a.u.

Cu	0.276379	0.394241	0.733283
P	-0.948759	0.029364	2.679989
P	-1.200042	0.341521	-0.982328
C	-2.759004	-0.199534	2.318756
C	-3.270275	0.972331	1.453609
C	-3.849156	0.552200	0.100776
C	-2.934599	-0.317903	-0.772668
C	-1.023352	1.525403	3.756490
C	-0.589382	-1.290562	3.904323
C	-0.588189	-0.634744	-2.418274
C	-1.581511	1.977269	-1.737560
H	-1.255612	-4.562266	4.567571
C	0.209754	-3.376360	5.605484
H	0.519971	-4.183830	6.262317
C	0.799043	-2.118449	5.712870
H	1.568902	-1.938818	6.458182
C	0.403559	-1.085860	4.872183
H	0.863020	-0.105833	4.974401
C	-1.181363	-2.555654	3.809223
C	-0.432694	2.712145	3.319708
H	0.120330	2.715903	2.383075
C	-0.522095	3.867788	4.092487
H	-0.051408	4.783168	3.745388
C	-1.199247	3.845322	5.305903
H	-1.265258	4.745492	5.910751
C	-1.788894	2.662631	5.750356
H	-2.314664	2.639891	6.700893
C	-1.702762	1.509967	4.980298
H	-2.153427	0.587101	5.338227
H	-2.861624	-1.151883	1.788633
H	-3.316741	-0.283644	3.258615
H	-4.032399	1.530784	2.008064
H	-2.461320	1.694305	1.273505
H	-1.937488	-2.750220	3.056168
C	0.694542	-0.322378	-2.887991
H	1.252598	0.482112	-2.411716
C	1.248225	-1.020866	-3.952825
H	2.238432	-0.753603	-4.312728
C	0.539763	-2.060444	-4.553673
H	0.976007	-2.613158	-5.381044
C	-0.726108	-2.388101	-4.084439
H	-1.280586	-3.208062	-4.532669
C	-1.289805	-1.679233	-3.025500
H	-2.274518	-1.967336	-2.672956
C	-0.784606	-3.587031	4.655504
C	-2.276775	2.081584	-2.945994
H	-2.551960	1.182239	-3.493403
C	-2.593481	3.330433	-3.465989
H	-3.117918	3.405035	-4.414460
C	-2.217371	4.485332	-2.784324
H	-2.448196	5.461294	-3.201601
C	-1.525914	4.387428	-1.582069
H	-1.213881	5.285706	-1.057221
C	-1.207037	3.137309	-1.060197
H	-0.632082	3.052383	-0.140378
H	-3.398170	-0.410652	-1.762906
H	-2.832594	-1.328707	-0.360030
H	-4.784933	-0.002260	0.257518
H	-4.112182	1.459581	-0.457529
C	2.181836	2.655172	-1.084143
C	1.843404	3.082971	-2.171847
C	1.424794	3.687208	-3.383596
C	0.777437	2.958953	-4.395296
C	0.362662	3.589264	-5.559969
C	1.647045	5.063405	-3.583494
C	1.227141	5.683868	-4.750108
C	0.581428	4.951253	-5.744506
H	0.254412	5.439692	-6.657821
H	0.590634	1.900278	-4.253359
H	-0.141126	3.009939	-6.328941
H	2.146914	5.630645	-2.804434
H	1.404536	6.747164	-4.885983
C	1.948433	1.416852	1.067403
C	2.672379	2.282362	0.198347
C	2.562846	1.223682	2.322859
C	3.909318	2.858041	0.565832
C	3.785103	1.776224	2.695547
C	4.470827	2.598172	1.803959

2$_1$•A (cont)

H	2.051452	0.606897	3.062764
H	4.416479	3.510424	-0.140621
H	4.200285	1.571855	3.680105
H	5.426048	3.039327	2.075122
C	-0.292315	-5.888356	-2.818065
C	-1.631606	-6.268466	-2.788941
C	-2.514570	-5.641699	-1.912376
C	-2.059393	-4.638315	-1.068332
C	-0.718648	-4.248170	-1.103155
C	0.166709	-4.880113	-1.980876
H	0.396827	-6.377176	-3.500418
H	-1.987103	-7.055997	-3.447354
H	-3.558489	-5.939826	-1.885372
H	-2.730187	-4.139041	-0.376026
H	1.204930	-4.570465	-2.016354
C	-0.297880	-3.144222	-0.198632
O	1.005751	-2.854437	-0.375226
O	-1.030822	-2.599980	0.602324
N	1.523407	-1.739710	0.446839
C	1.831492	-2.306589	1.783866
C	2.793658	-1.399445	-0.235436
H	2.197757	-1.454329	2.368125
C	2.884166	-3.403249	1.749374
H	0.901240	-2.657085	2.238999
C	3.822130	-2.521720	-0.206221
H	3.171529	-0.520252	0.297689
H	2.558447	-1.101680	-1.261865
H	3.146808	-3.689734	2.773143
H	2.499582	-4.296828	1.227776
H	4.772516	-2.156776	-0.609307
H	3.490676	-3.376861	-0.819521
O	4.084626	-2.951604	1.127780

TS[**2**$_1$•A–**3**]

E_t = -4652.486221 a.u.

Cu	0.317882	0.382332	0.722169
P	-1.021986	-0.149859	2.746292
P	-1.310170	0.118844	-0.930777
C	-2.528529	-1.250673	2.585529
C	-3.777438	-0.553900	2.038295
C	-3.569762	0.227483	0.739804
C	-2.939663	-0.598967	-0.400367
C	-1.737282	1.278328	3.664010
C	-0.089329	-1.056247	4.044150
C	-0.858660	-0.892689	-2.395221
C	-1.914379	1.679492	-1.705364
H	-2.954311	1.110724	0.956529
H	-3.609342	-0.626023	-1.267332
H	-2.752848	-1.635271	-0.095620
H	-2.221007	-2.077495	1.937320
H	-2.748205	-1.671933	3.574485
H	-4.548224	-1.322262	1.884152
H	-4.169112	0.134942	2.797135
H	-4.535571	0.626691	0.410581
C	-1.769603	2.524198	3.033278
C	-2.931209	3.476410	4.916491
C	-2.311283	1.144332	4.933065
C	-2.901377	2.238228	5.556069
H	-3.340006	2.126101	6.543589
H	-2.286764	0.182035	5.439063
C	-2.365523	3.617648	3.654208
H	-1.301543	2.637496	2.059284
H	-3.391724	4.330210	5.405646
H	-2.377524	4.580751	3.152066
C	-1.675213	-1.874036	-2.966379
C	-0.023895	-2.276739	-4.680910
C	0.388276	-0.637400	-2.970329
C	0.801892	-1.314489	-4.109312
H	1.767402	-1.082097	-4.548812
H	1.026046	0.117562	-2.525073
C	-1.256819	-2.560036	-4.102417
H	-2.634071	-2.126818	-2.525571
H	0.299500	-2.817557	-5.565979
H	-1.891513	-3.333172	-4.525461
C	-1.564549	2.897822	-1.124262
C	-2.830236	4.081784	-2.798921
C	-2.729545	1.671266	-2.841662
C	-3.186953	2.866918	-3.383711
H	-3.810710	2.854036	-4.273251
H	-2.982696	0.728342	-3.321457
C	-2.019648	4.095326	-1.669105
H	-0.903227	2.902900	-0.261423
H	-3.175497	5.016067	-3.232573
H	-1.722995	5.037656	-1.217578
C	0.046596	-2.449302	3.957918
C	1.631704	-2.438997	5.780204
C	0.636666	-0.372396	5.027041
C	1.489229	-1.057856	5.885217
H	2.045545	-0.508282	6.639327
H	0.531282	0.704087	5.129876
C	0.899893	-3.130711	4.819819
H	-0.478044	-3.000309	3.184543
H	2.305086	-2.972018	6.445122
H	1.001559	-4.208600	4.728198
C	1.696066	2.755676	-1.204558
C	1.660978	2.593500	-2.409047
C	1.575451	2.311248	-3.797244
C	2.696538	1.842981	-4.504214
C	2.584253	1.487200	-5.841986
C	0.347986	2.424711	-4.472015
C	0.244980	2.058179	-5.806061
C	1.358464	1.585712	-6.496506
H	1.272069	1.295158	-7.539508
H	3.646605	1.752926	-3.986175
H	3.457888	1.123630	-6.375978
H	-0.520577	2.780044	-3.929627
H	-0.715763	2.133205	-6.308004
C	1.241631	2.091549	1.140658
C	1.801571	2.991171	0.195728
C	1.483935	2.398391	2.486431
C	2.525985	4.129211	0.607032
C	2.204962	3.514427	2.901510
C	2.724722	4.391490	1.953006

TS[**2**$_1$•A–**3**] (cont)

H	1.094500	1.735200	3.256389
H	2.934761	4.792555	-0.150280
H	2.360829	3.696264	3.962525
H	3.289295	5.266834	2.260347
C	0.063226	-5.000374	-2.982551
C	-1.217095	-5.503587	-2.772152
C	-1.966846	-5.065953	-1.681511
C	-1.431318	-4.137417	-0.800962
C	-0.143849	-3.637134	-1.006325
C	0.601053	-4.069058	-2.102753
H	0.643472	-5.328727	-3.840092
H	-1.632698	-6.236147	-3.458067
H	-2.968622	-5.452823	-1.517232
H	-1.994994	-3.778626	0.055039
H	1.590926	-3.655511	-2.263397
C	0.405179	-2.652151	-0.018675
O	1.660200	-2.367617	-0.199055
O	-0.317297	-2.198980	0.876800
N	2.012456	-0.679092	0.589540
C	2.584732	-1.028939	1.904242
C	3.070771	-0.166785	-0.302180
H	2.718658	-0.074387	2.435563
C	3.919437	-1.762114	1.853969
H	1.845522	-1.624577	2.444733
C	4.384648	-0.939723	-0.266645
H	3.266843	0.860908	0.029812
H	2.676497	-0.119596	-1.320662
H	4.330909	-1.824513	2.866848
H	3.775340	-2.782062	1.465327
H	5.138988	-0.378128	-0.828692
H	4.264619	-1.932119	-0.726486
O	4.874891	-1.065489	1.062193

3

E_t = -4652.529785 a.u.

Cu	0.628161	-0.243360	-0.088599
P	-0.880187	-0.419348	1.783416
P	-0.988412	-0.102656	-1.791046
C	-2.647271	-0.930023	1.547199
C	-3.398224	-0.029661	0.544700
C	-3.658857	-0.659070	-0.825043
C	-2.446097	-1.240125	-1.555038
C	-0.998734	1.155299	2.719930
C	-0.294893	-1.611519	3.054805
C	-0.265139	-0.686326	-3.363911
C	-1.802562	1.477446	-2.245411
H	0.758333	-1.879683	6.274617
C	0.585447	-3.525155	4.898145
H	0.934161	-4.265437	5.612584
C	0.234510	-3.908157	3.606885
H	0.307050	-4.947804	3.300033
C	-0.202244	-2.959599	2.690271
H	-0.441417	-3.259481	1.676116
C	0.050925	-1.233514	4.355034
C	-2.207262	1.740644	3.109781
H	-3.155725	1.289152	2.839991
C	-2.211771	2.909733	3.867885
H	-3.159687	3.349393	4.165351
C	-1.015163	3.501392	4.257173
H	-1.022211	4.405941	4.858581
C	0.193008	2.931273	3.864201
H	1.134025	3.392183	4.150579
C	0.201318	1.776612	3.092873
H	1.137761	1.320708	2.790424
H	-2.617529	-1.970657	1.204003
H	-3.134793	-0.946966	2.529179
H	-4.368070	0.253732	0.971694
H	-2.859494	0.915527	0.403749
H	-0.019882	-0.196156	4.664624
C	-0.168770	-2.055000	-3.627377
H	-0.577555	-2.778863	-2.930290
C	0.485293	-2.500036	-4.770832
H	0.565736	-3.566807	-4.956466
C	1.046204	-1.587348	-5.657267
H	1.562778	-1.938154	-6.546172
C	0.953381	-0.222852	-5.396848
H	1.400410	0.495825	-6.077494
C	0.307410	0.228182	-4.253970
H	0.263029	1.293221	-4.046092
C	0.488855	-2.188076	5.268462
C	-2.527242	1.577883	-3.439860
H	-2.535492	0.747521	-4.141277
C	-3.224313	2.741690	-3.737846
H	-3.780144	2.812864	-4.668425
C	-3.208150	3.814185	-2.848190
H	-3.749375	4.725573	-3.085978
C	-2.495134	3.719475	-1.658738
H	-2.465766	4.554639	-0.964992
C	-1.796628	2.553194	-1.359128
H	-1.227160	2.483629	-0.437445
H	-2.753798	-1.568006	-2.555636
H	-2.034613	-2.111351	-1.037632
H	-4.383608	-1.477303	-0.709900
H	-4.139140	0.096090	-1.459443
C	1.597115	2.718311	-1.064846
C	1.108347	3.719790	-0.578277
C	0.473778	4.880273	-0.079863
C	-0.431890	4.806866	0.993240
C	-1.079503	5.948007	1.444098
C	0.712732	6.131477	-0.679011
C	0.059362	7.265255	-0.219875
C	-0.840599	7.180703	0.841210
H	-1.349927	8.071494	1.196558
H	-0.619223	3.849655	1.467293
H	-1.776166	5.869885	2.274163
H	1.409877	6.192582	-1.508571
H	0.252273	8.223536	-0.693598
C	1.970830	0.282062	-1.385007
C	2.234708	1.628501	-1.702258
C	2.660826	-0.733431	-2.030713
C	3.196910	1.917889	-2.696381
C	3.613118	-0.427162	-3.001473
C	3.878874	0.898726	-3.336647

3 (cont)

H	2.451286	-1.775985	-1.787044
H	3.392469	2.958834	-2.937917
H	4.141986	-1.236715	-3.497426
H	4.620184	1.137509	-4.094044
C	-2.093307	-6.096777	-0.076905
C	-1.438356	-7.297655	-0.332992
C	-0.099470	-7.284256	-0.718638
C	0.578662	-6.078510	-0.847641
C	-0.067558	-4.866502	-0.588431
C	-1.409514	-4.891534	-0.203043
H	-3.137835	-6.099620	0.222947
H	-1.968919	-8.240636	-0.233044
H	0.415980	-8.219546	-0.919800
H	1.620514	-6.042945	-1.150076
H	-1.917987	-3.954715	0.001311
C	0.714980	-3.569300	-0.734837
O	1.879492	-3.650881	-1.149934
O	0.087592	-2.493829	-0.408662
N	2.094340	-0.230548	1.188308
C	2.759384	-1.528289	1.213772
C	3.120883	0.803078	1.219523
H	2.025323	-2.337279	1.174962
C	3.544657	-1.641096	2.527234
H	3.460747	-1.664924	0.371946
C	3.893976	0.665580	2.541243
H	2.669767	1.802031	1.167114
H	3.853465	0.717994	0.397171
H	2.844705	-1.601382	3.379135
H	4.092701	-2.588878	2.550577
H	3.213997	0.818961	3.399463
H	4.693724	1.413847	2.582432
O	4.515410	-0.604971	2.637309

TS[**3**–**4**•P]

E_t = -4652.531372 a.u.

Cu	0.497444	-0.361509	0.039295
P	-1.001992	-0.484841	1.972724
P	-1.166937	-0.103504	-1.552138
C	-2.815678	-0.866667	1.840514
C	-3.563985	0.009527	0.814855
C	-3.837194	-0.629212	-0.548465
C	-2.640371	-1.221278	-1.300101
C	-1.001687	1.112792	2.901746
C	-0.401978	-1.592201	3.314486
C	-0.530738	-0.628496	-3.180675
C	-1.926999	1.537747	-1.843029
H	1.728187	-4.193360	3.795995
C	0.541867	-3.271948	5.338450
H	0.909725	-3.925125	6.124822
C	-0.389875	-2.279814	5.633865
H	-0.749611	-2.154857	6.651188
C	-0.856574	-1.440312	4.628476
H	-1.565023	-0.652769	4.873560
C	0.533327	-2.585641	3.026105
C	0.222352	1.497926	3.462861
H	1.081994	0.851041	3.323484
C	0.335080	2.655082	4.220438
H	1.293481	2.923097	4.657068
C	-0.781379	3.463629	4.426733
H	-0.699770	4.365990	5.026313
C	-1.999793	3.102262	3.863420
H	-2.877550	3.723671	4.018813
C	-2.113769	1.935171	3.108893
H	-3.085432	1.669569	2.707745
H	-2.874754	-1.929081	1.587855
H	-3.242495	-0.743112	2.843645
H	-4.536293	0.292447	1.239178
H	-3.035238	0.953972	0.652825
H	0.880498	-2.707051	2.007254
C	0.014611	0.297916	-4.073848
H	-0.018967	1.359356	-3.846398
C	0.616513	-0.136761	-5.248735
H	1.045631	0.591967	-5.930322
C	0.692077	-1.495472	-5.539314
H	1.175630	-1.831423	-6.452355
C	0.156176	-2.422097	-4.650163
H	0.217579	-3.487075	-4.856656
C	-0.451619	-1.993578	-3.476204
H	-0.836790	-2.733860	-2.783011
C	1.001775	-3.421380	4.034602
C	-2.702597	1.784758	-2.981471
H	-2.786167	1.027075	-3.756452
C	-3.357223	3.002323	-3.128792
H	-3.949776	3.190995	-4.019349
C	-3.257580	3.975289	-2.136286
H	-3.771632	4.925398	-2.251227
C	-2.493060	3.734034	-1.000476
H	-2.398596	4.491485	-0.227806
C	-1.823386	2.522634	-0.860060
H	-1.209893	2.343880	0.019372
H	-2.969322	-1.540559	-2.296423
H	-2.274126	-2.104821	-0.768557
H	-4.559643	-1.447134	-0.421254
H	-4.325278	0.125550	-1.178050
C	1.617048	2.569871	-1.108961
C	1.163078	3.609377	-0.672367
C	0.539536	4.759325	-0.139728
C	0.063794	4.749871	1.183817
C	-0.621405	5.845283	1.688229
C	0.320167	5.899363	-0.933673
C	-0.368418	6.988066	-0.418235
C	-0.845141	6.966360	0.891424
H	-1.388306	7.818531	1.289036
H	0.223188	3.870479	1.800473
H	-0.989618	5.815658	2.709201
H	0.676283	5.905705	-1.958851
H	-0.541859	7.858757	-1.044204
C	1.963303	0.105042	-1.217053
C	2.187747	1.418332	-1.693766
C	2.513646	-0.969619	-1.915985
C	2.985746	1.600594	-2.846565
C	3.282914	-0.765918	-3.054346
C	3.538789	0.525122	-3.514134

TS[**3**–**4**•P] (cont)

H	2.308297	-1.979747	-1.580231
H	3.145466	2.616256	-3.197156
H	3.678575	-1.627070	-3.586021
H	4.151413	0.686467	-4.396041
C	0.564842	-6.107198	-2.656094
C	-0.538782	-6.953627	-2.572926
C	-1.563488	-6.667688	-1.673952
C	-1.483394	-5.542461	-0.861956
C	-0.386557	-4.681209	-0.948798
C	0.637184	-4.972999	-1.853415
H	1.368867	-6.332889	-3.351707
H	-0.600294	-7.834075	-3.206989
H	-2.426828	-7.324328	-1.607049
H	-2.266920	-5.302851	-0.149969
H	1.482493	-4.295098	-1.923465
C	-0.369012	-3.425064	-0.102104
O	-1.258552	-3.295079	0.762502
O	0.540320	-2.566131	-0.372547
N	2.244193	-0.149799	0.915883
C	3.178556	-1.268342	0.915735
C	2.962465	1.087043	1.193478
H	2.644305	-2.205342	0.727698
C	3.872658	-1.333797	2.277485
H	3.963703	-1.156087	0.145852
C	3.734575	0.968171	2.515279
H	2.262675	1.925483	1.271857
H	3.695772	1.332988	0.403607
H	3.130434	-1.486629	3.078772
H	4.590601	-2.161056	2.288002
H	3.042472	0.886831	3.369941
H	4.348925	1.865896	2.648742
O	4.615959	-0.142378	2.514322

4●P

E_t = -4652.613180 a.u.

Cu	0.167202	-0.991753	-0.127322
P	-1.042933	-1.116756	1.777714
P	-1.224905	-0.802899	-1.920495
C	-1.857400	-2.795054	1.807200
C	-2.041029	-3.350165	0.392072
C	-2.990039	-2.536357	-0.515942
C	-2.392537	-2.255047	-1.905749
C	-2.411198	0.109750	1.905441
C	-0.267368	-0.967510	3.443007
C	-0.488809	-0.957836	-3.601058
C	-2.337058	0.649188	-2.062264
H	-3.262289	-1.591028	-0.028709
H	-3.162891	-2.086007	-2.668524
H	-1.805437	-3.117964	-2.243405
H	-1.174430	-3.446023	2.362072
H	-2.806388	-2.754444	2.355008
H	-1.047461	-3.411409	-0.064845
H	-2.402470	-4.383413	0.470248
H	-3.934653	-3.079126	-0.647042
C	-3.550743	-0.099774	2.690515
C	-4.371801	2.096675	2.121078
C	-2.265919	1.329385	1.240948
C	-3.236433	2.320675	1.352108
H	-3.100872	3.263748	0.831525
H	-1.389644	1.502817	0.621001
C	-4.527589	0.884118	2.790129
H	-3.672642	-1.026099	3.244695
H	-5.133369	2.867019	2.204387
H	-5.409036	0.707619	3.400434
C	-0.797178	-0.112863	-4.668426
C	0.760085	-1.300929	-6.081339
C	0.453797	-1.978403	-3.785386
C	1.064207	-2.152394	-5.021167
H	1.787654	-2.952738	-5.153316
H	0.725422	-2.616099	-2.946685
C	-0.169189	-0.282375	-5.899784
H	-1.525650	0.682383	-4.542922
H	1.244266	-1.432832	-7.044973
H	-0.415328	0.383483	-6.722354
C	-1.735311	1.907470	-2.188463
C	-3.892883	2.979935	-2.151521
C	-3.729389	0.577191	-1.973862
C	-4.499366	1.736914	-2.014084
H	-5.580183	1.664135	-1.933573
H	-4.229963	-0.378867	-1.862109
C	-2.505117	3.061068	-2.242855
H	-0.653333	1.981678	-2.249349
H	-4.497222	3.882259	-2.180985
H	-2.015809	4.025943	-2.344643
C	0.723447	-1.890753	3.806770
C	1.150031	-0.654848	5.839529
C	-0.531048	0.116172	4.287876
C	0.175356	0.268697	5.477936
H	-0.042501	1.113442	6.126016
H	-1.290139	0.845186	4.018896
C	1.417936	-1.733803	5.000475
H	0.968414	-2.710473	3.135757
H	1.701703	-0.532993	6.767276
H	2.183375	-2.456146	5.270012
C	0.961722	3.197585	-0.286322
C	0.295524	3.940690	0.408443
C	-0.532837	4.672036	1.289310
C	-1.298494	5.758526	0.829883
C	-2.159723	6.421582	1.692001
C	-0.646530	4.282096	2.636928
C	-1.511292	4.951674	3.488448
C	-2.273312	6.020325	3.021506
H	-2.950353	6.540969	3.691955
H	-1.210269	6.064957	-0.207723
H	-2.747640	7.257887	1.324809
H	-0.062527	3.440404	2.997465
H	-1.596356	4.634300	4.523668
C	2.067914	1.040965	-1.019666
C	1.639863	2.386070	-1.224710
C	2.511027	0.331013	-2.151842
C	1.780318	2.959804	-2.511985
C	2.608231	0.910715	-3.401220
C	2.268306	2.250488	-3.587393

4●P (cont)

H	2.723529	-0.726839	-2.055821
H	1.461184	3.990884	-2.629681
H	2.926423	0.300861	-4.241264
H	2.353348	2.718782	-4.562454
C	4.106292	-6.391811	-0.148537
C	4.706439	-6.181152	-1.387898
C	4.318893	-5.095270	-2.168721
C	3.334441	-4.225663	-1.712250
C	2.729291	-4.430649	-0.469816
C	3.124995	-5.520458	0.308447
H	4.406795	-7.238530	0.462575
H	5.474971	-6.861692	-1.744140
H	4.786345	-4.927145	-3.135255
H	3.021970	-3.376621	-2.313126
H	2.645972	-5.662935	1.272053
C	1.670688	-3.488290	0.051764
O	1.203278	-3.675497	1.186955
O	1.338942	-2.537369	-0.748845
N	1.999986	0.327620	0.216540
C	3.173596	-0.566068	0.490944
C	1.800964	1.089462	1.477936
H	2.879069	-1.220885	1.319351
C	4.393787	0.258921	0.872428
H	3.390921	-1.210401	-0.358411
C	3.033864	1.903645	1.844345
H	1.631675	0.343968	2.260965
H	0.909364	1.709251	1.412831
H	5.231580	-0.404838	1.110439
H	4.687646	0.906409	0.026394
H	2.869000	2.422515	2.795102
H	3.255064	2.656892	1.070338
O	4.160174	1.049047	2.036285

4

E_t = -3826.819468 a.u.

Cu	0.183651	-0.778893	-0.199414
P	-1.020855	-0.897228	1.664725
P	-1.061275	-0.604500	-2.016741
C	-2.340914	-2.223594	1.650216
C	-2.523701	-2.827483	0.251310
C	-3.209564	-1.901971	-0.778210
C	-2.464134	-1.820904	-2.121463
C	-1.841976	0.720078	1.940916
C	-0.163461	-1.175682	3.263854
C	-0.296839	-0.710888	-3.681538
C	-1.913815	1.024752	-1.983501
H	-3.309640	-0.887679	-0.370352
H	-3.133916	-1.551322	-2.946674
H	-2.027140	-2.792274	-2.384747
H	-1.981227	-2.995028	2.341246
H	-3.287263	-1.852035	2.062162
H	-1.531334	-3.113931	-0.121429
H	-3.096660	-3.758775	0.343805
H	-4.234457	-2.248805	-0.958271
C	-0.993705	1.802628	2.214606
C	-2.880269	3.305316	2.215322
C	-3.210201	0.952660	1.793295
C	-3.724349	2.240604	1.926052
H	-4.790677	2.407112	1.802617
H	-3.892204	0.137037	1.573290
C	-1.512914	3.080681	2.361893
H	0.078628	1.638932	2.292967
H	-3.283776	4.308466	2.319502
H	-0.843983	3.908729	2.578897
C	1.003782	-1.214606	-3.765835
C	0.948126	-0.967195	-6.164012
C	-0.965168	-0.322331	-4.846082
C	-0.343903	-0.451500	-6.082418
H	-0.865175	-0.143979	-6.984618
H	-1.965705	0.099340	-4.785700
C	1.620589	-1.345970	-5.006986
H	1.532440	-1.488310	-2.854106
H	1.433006	-1.063737	-7.131408
H	2.632873	-1.735117	-5.066358
C	-3.221370	1.241694	-2.427481
C	-3.074955	3.562426	-1.788532
C	-1.196288	2.092807	-1.430682
C	-1.773545	3.353656	-1.342554
H	-1.208433	4.171006	-0.904507
H	-0.189342	1.926338	-1.051856
C	-3.798227	2.504316	-2.328543
H	-3.808814	0.428341	-2.843504
H	-3.528931	4.546051	-1.706622
H	-4.817396	2.658785	-2.671926
C	-0.790999	-0.949847	4.493107
C	1.203557	-1.664461	5.644015
C	1.154246	-1.637465	3.232664
C	1.833600	-1.882169	4.423723
H	2.860787	-2.233858	4.394026
H	1.646786	-1.791416	2.274211
C	-0.109345	-1.196955	5.678119
H	-1.808234	-0.565871	4.520105
H	1.736428	-1.850787	6.572260
H	-0.598987	-1.018637	6.631440
C	5.792321	1.765261	0.552769
C	6.727697	0.737594	0.454400
C	6.303562	-0.566944	0.212263
C	4.949338	-0.844123	0.068890
C	4.008568	0.183843	0.167178
C	4.437900	1.490484	0.409913
H	6.122176	2.783212	0.741079
H	7.786819	0.953326	0.566124
H	7.032360	-1.369106	0.134919
H	4.598582	-1.853605	-0.120413
H	3.692000	2.275540	0.482123
C	2.550312	-0.109141	0.019609
O	2.188176	-1.313396	-0.198237
O	1.708675	0.827986	0.122669

4●S

E_t = -4135.109114 a.u.

Cu	0.050232	-1.060474	-0.263276
P	-1.316408	-1.190953	1.662686
P	-1.303762	-0.937247	-2.097870
C	-2.555827	-2.600644	1.638860
C	-2.769638	-3.104134	0.209998
C	-3.472205	-2.080214	-0.702593
C	-2.839227	-1.993904	-2.100200
C	-2.329593	0.303440	1.999014
C	-0.421738	-1.452428	3.241949
C	-0.578749	-1.300536	-3.744941
C	-1.969139	0.761835	-2.321183
H	-3.452394	-1.090278	-0.227676
H	-3.546415	-1.605988	-2.842893
H	-2.540301	-2.991643	-2.445577
H	-2.167938	-3.403223	2.275047
H	-3.501404	-2.267655	2.083398
H	-1.788475	-3.351595	-0.214331
H	-3.345364	-4.038446	0.232529
H	-4.534265	-2.338799	-0.798948
C	-2.119857	1.442266	1.217649
C	-3.860646	2.599938	2.422781
C	-3.301006	0.329124	3.007440
C	-4.063630	1.471003	3.215934
H	-4.815265	1.483478	4.000353
H	-3.451933	-0.540655	3.642577
C	-2.887511	2.585400	1.430876
H	-1.345488	1.437586	0.455368
H	-4.460192	3.491327	2.585878
H	-2.719949	3.461075	0.810679
C	0.766254	-1.660400	-3.833490
C	0.547394	-1.906979	-6.223871
C	-1.353286	-1.226672	-4.907851
C	-0.792633	-1.532806	-6.141252
H	-1.398399	-1.471415	-7.040984
H	-2.392340	-0.910854	-4.852619
C	1.324617	-1.964036	-5.072584
H	1.376869	-1.659580	-2.935667
H	0.986118	-2.141568	-7.189754
H	2.374729	-2.234180	-5.136628
C	-1.041322	1.775088	-2.596119
C	-2.803369	3.424448	-2.537343
C	-3.315169	1.097761	-2.154893
C	-3.727911	2.423401	-2.263750
H	-4.777230	2.670316	-2.128202
H	-4.057544	0.338101	-1.931826
C	-1.459975	3.094511	-2.706397
H	0.010043	1.522140	-2.714513
H	-3.126847	4.458433	-2.619582
H	-0.729366	3.869627	-2.919646
C	0.123891	-2.710052	3.533811
C	1.220262	-1.815174	5.487311
C	-0.112289	-0.374629	4.079095
C	0.701281	-0.557831	5.192070
H	0.929746	0.289474	5.832558
H	-0.506085	0.612540	3.855066
C	0.928376	-2.890763	4.652818
H	-0.056428	-3.553488	2.871972
H	1.854317	-1.955560	6.357748
H	1.341081	-3.873045	4.864329
C	3.346392	3.821829	1.400923
C	4.298429	4.332398	0.521905
C	4.398372	3.815341	-0.768247
C	3.554529	2.788343	-1.173648
C	2.599494	2.272345	-0.295860
C	2.498685	2.797883	0.993447
H	3.268041	4.222308	2.408274
H	4.961330	5.132387	0.841019
H	5.139158	4.213462	-1.456689
H	3.622893	2.358210	-2.168320
H	1.758898	2.378341	1.667812
C	1.735275	1.118236	-0.730407
O	1.936612	0.587493	-1.838142
O	0.842333	0.746980	0.116799
C	1.132133	-2.837611	-0.392878
C	2.000973	-2.146143	0.144694
C	3.057251	-1.377678	0.699955
C	4.097784	-0.931583	-0.132383
C	5.118536	-0.154111	0.393289

4●S (cont)

C	3.059269	-1.025424	2.059612
C	4.086058	-0.247351	2.570107
C	5.115501	0.193071	1.741367
H	5.908242	0.204829	-0.259632
H	4.067801	-1.169137	-1.189758
H	2.246174	-1.352902	2.696982
H	5.906272	0.820595	2.141519
H	4.072503	0.029592	3.620333
H	0.744366	-3.746168	-0.805409

4●T

E_t = -4059.203352 a.u.

Cu	0.361697	0.070080	0.199284
P	-1.070938	-0.002413	1.922972
P	-0.800841	0.303195	-1.723447
C	-2.020629	-1.610609	1.781103
C	-1.899632	-2.294005	0.413731
C	-2.633426	-1.611195	-0.765007
C	-1.721984	-1.293773	-1.963366
C	-2.280301	1.380393	1.851539
C	-0.657756	-0.005303	3.724113
C	0.132928	0.446545	-3.301003
C	-2.096136	1.591437	-1.886827
H	-3.122417	-0.687264	-0.430412
H	-2.274625	-1.259325	-2.909872
H	-0.952941	-2.068400	-2.076770
H	-1.548243	-2.251938	2.534971
H	-3.063655	-1.478393	2.096553
H	-0.832350	-2.384692	0.178020
H	-2.274325	-3.319519	0.522228
H	-3.447270	-2.258593	-1.113343
C	-3.636426	1.245818	1.552440
C	-3.954130	3.628236	1.772938
C	-1.770332	2.662305	2.098742
C	-2.602006	3.772582	2.077025
H	-2.192716	4.756914	2.287469
H	-0.711709	2.783111	2.321055
C	-4.464988	2.365308	1.502189
H	-4.065979	0.267450	1.362330
H	-4.603657	4.498366	1.741282
H	-5.516102	2.242620	1.256913
C	-0.217465	1.319911	-4.333785
C	1.686613	0.579225	-5.621585
C	1.277019	-0.351678	-3.433878
C	2.041855	-0.289938	-4.592050
H	2.926267	-0.914335	-4.685432
H	1.569526	-1.003012	-2.612078
C	0.560274	1.384434	-5.487152
H	-1.095407	1.952354	-4.237018
H	2.290555	0.633280	-6.522891
H	0.281533	2.068459	-6.283954
C	-3.320818	1.390087	-2.529991
C	-3.934416	3.688118	-2.126339
C	-1.811063	2.852110	-1.354576
C	-2.717879	3.896853	-1.483934
H	-2.482116	4.869810	-1.063366
H	-0.874355	3.006661	-0.822990
C	-4.236389	2.431940	-2.642075
H	-3.570488	0.421339	-2.951841
H	-4.650104	4.500363	-2.217232
H	-5.186893	2.260911	-3.139813
C	-1.466870	0.605861	4.686996
C	0.018374	-0.152141	6.431725
C	0.492298	-0.693486	4.125692
C	0.821683	-0.766734	5.475594
H	1.716220	-1.304438	5.777393
H	1.120056	-1.175355	3.378131
C	-1.126159	0.532643	6.034003
H	-2.362632	1.142554	4.388410
H	0.282124	-0.206270	7.484361
H	-1.760961	1.010883	6.774981
C	3.433012	-4.890323	-1.907383
C	4.204074	-5.679098	-1.057257
C	4.282408	-5.363594	0.297215
C	3.594065	-4.265409	0.798701
C	2.824324	-3.465398	-0.049026
C	2.749390	-3.788549	-1.405604
H	3.364701	-5.136067	-2.963768
H	4.740933	-6.538978	-1.448678
H	4.881578	-5.978313	0.963529
H	3.635519	-4.002920	1.851121
H	2.142436	-3.168782	-2.057788
C	2.097657	-2.269176	0.520537
O	2.124633	-2.083841	1.748020
O	1.509065	-1.516464	-0.340485
O	1.969347	1.520652	0.454906
C	2.690322	1.922394	-0.729146
H	3.096152	2.935090	-0.571730
H	1.981766	1.938664	-1.562489
C	3.797822	0.886330	-0.871480

4●T (cont)

H	3.405254	0.000112	-1.376306
H	4.650050	1.268157	-1.441155
C	4.153845	0.544386	0.593482
H	4.242431	-0.535229	0.735067
H	5.097116	1.007257	0.898830
C	2.980775	1.111661	1.414732
H	2.520842	0.370282	2.071905
H	3.280986	1.997813	1.992099
C	2.608231	0.910715	-3.401220
C	2.268306	2.250488	-3.587393

4●A

E_t = -4534.011139 a.u.

Cu	0.033178	-0.305977	0.383866
P	-1.339847	-0.413953	2.217702
P	-1.185476	-0.109290	-1.566011
C	-2.738795	-1.643375	2.039833
C	-2.933040	-2.103993	0.592052
C	-3.492716	-1.048570	-0.382929
C	-2.763673	-1.078420	-1.737636
C	-2.111751	1.230938	2.527922
C	-0.683940	-0.799695	3.900916
C	-0.249783	-0.399284	-3.115664
C	-1.806705	1.605187	-1.845158
H	-3.408277	-0.039404	0.042715
H	-3.375709	-0.642185	-2.536158
H	-2.518241	-2.112034	-2.009728
H	-2.438036	-2.507597	2.644583
H	-3.667351	-1.261215	2.481480
H	-1.963213	-2.452059	0.221510
H	-3.592927	-2.981593	0.590730
H	-4.565804	-1.212692	-0.540175
C	-3.464701	1.515084	2.335117
C	-3.069388	3.845546	2.824631
C	-1.241285	2.271868	2.880086
C	-1.718647	3.567740	3.025035
H	-1.025584	4.363743	3.282780
H	-0.181537	2.071804	3.022838
C	-3.939164	2.816415	2.484840
H	-4.164996	0.733318	2.058783
H	-3.440543	4.861010	2.931009
H	-4.993870	3.022828	2.326169
C	1.006425	0.216567	-3.206331
C	1.315436	-0.711133	-5.411698
C	-0.704908	-1.179590	-4.180025
C	0.077422	-1.335647	-5.321926
H	-0.281364	-1.954291	-6.139676
H	-1.669731	-1.675483	-4.125013
C	1.777388	0.066672	-4.351155
H	1.367441	0.814587	-2.370346
H	1.924921	-0.837312	-6.302020
H	2.746506	0.554024	-4.414589
C	-1.787679	2.527063	-0.798780
C	-2.793124	4.191750	-2.224230
C	-2.314875	1.992953	-3.090489
C	-2.805801	3.278495	-3.278047
H	-3.192520	3.572494	-4.249912
H	-2.308376	1.292018	-3.922391
C	-2.282709	3.815279	-0.988009
H	-1.358005	2.248576	0.157445
H	-3.172513	5.198879	-2.374113
H	-2.249760	4.522115	-0.164152
C	-1.497755	-1.312355	4.917118
C	0.379332	-1.328630	6.432377
C	0.661649	-0.536406	4.169956
C	1.187101	-0.798498	5.432712
H	2.233970	-0.585439	5.628875
H	1.287166	-0.087051	3.400464
C	-0.966007	-1.580257	6.173249
H	-2.554108	-1.494217	4.739491
H	0.792105	-1.538727	7.415135
H	-1.606312	-1.979445	6.954985
C	1.420103	5.475491	-0.538382
C	1.934132	6.289615	0.467869
C	2.368870	5.721861	1.663917
C	2.287079	4.347191	1.852752
C	1.769659	3.525872	0.848264
C	1.338599	4.100282	-0.349453
H	1.077591	5.913905	-1.472011
H	1.996720	7.364614	0.320763
H	2.772262	6.354640	2.450062
H	2.616512	3.882729	2.777269
H	0.927706	3.455657	-1.119601
C	1.637709	2.041045	1.090515
O	2.015867	1.579367	2.185274
O	1.107311	1.370056	0.134938
C	2.983655	-3.849085	-4.676454
C	2.122633	-4.701854	-5.360355
C	0.878525	-5.018169	-4.818492
C	0.497368	-4.482652	-3.597311
C	1.361993	-3.628544	-2.907155

4●Â (cont)

H	3.255064	2.656892	1.070338
O	4.160174	1.049047	2.036285
C	2.609462	-3.312602	-3.451013
H	3.950622	-3.596765	-5.101530
H	2.420961	-5.121417	-6.316991
H	0.206317	-5.684938	-5.350488
H	-0.468581	-4.712375	-3.158859
H	3.273545	-2.636858	-2.924311
C	0.894800	-3.090424	-1.602975
O	1.902711	-2.462114	-0.960373
O	-0.226886	-3.234695	-1.163356
N	1.580573	-1.817648	0.339104
C	1.392151	-2.900677	1.347231
C	2.850447	-1.100691	0.635977
H	1.186786	-2.371632	2.285753
C	2.621224	-3.779030	1.516012
H	0.506972	-3.480556	1.071746
C	4.032051	-2.034200	0.849321
H	2.646904	-0.501880	1.531511
H	3.031199	-0.393042	-0.178950
H	2.455628	-4.482242	2.338805
H	2.818767	-4.359806	0.598541
H	4.891010	-1.450885	1.195788
H	4.312030	-2.543810	-0.087555
O	3.761094	-3.001011	1.863970

4●S

E_t = -4135.109114 a.u.

Cu	0.050232	-1.060474	-0.263276
P	-1.316408	-1.190953	1.662686
P	-1.303762	-0.937247	-2.097870
C	-2.555827	-2.600644	1.638860
C	-2.769638	-3.104134	0.209998
C	-3.472205	-2.080214	-0.702593
C	-2.839227	-1.993904	-2.100200
C	-2.329593	0.303440	1.999014
C	-0.421738	-1.452428	3.241949
C	-0.578749	-1.300536	-3.744941
C	-1.969139	0.761835	-2.321183
H	-3.452394	-1.090278	-0.227676
H	-3.546415	-1.605988	-2.842893
H	-2.540301	-2.991643	-2.445577
H	-2.167938	-3.403223	2.275047
H	-3.501404	-2.267655	2.083398
H	-1.788475	-3.351595	-0.214331
H	-3.345364	-4.038446	0.232529
H	-4.534265	-2.338799	-0.798948
C	-2.119857	1.442266	1.217649
C	-3.860646	2.599938	2.422781
C	-3.301006	0.329124	3.007440
C	-4.063630	1.471003	3.215934
H	-4.815265	1.483478	4.000353
H	-3.451933	-0.540655	3.642577
C	-2.887511	2.585400	1.430876
H	-1.345488	1.437586	0.455368
H	-4.460192	3.491327	2.585878
H	-2.719949	3.461075	0.810679
C	0.766254	-1.660400	-3.833490
C	0.547394	-1.906979	-6.223871
C	-1.353286	-1.226672	-4.907851
C	-0.792633	-1.532806	-6.141252
H	-1.398399	-1.471415	-7.040984
H	-2.392340	-0.910854	-4.852619
C	1.324617	-1.964036	-5.072584
H	1.376869	-1.659580	-2.935667
H	0.986118	-2.141568	-7.189754
H	2.374729	-2.234180	-5.136628
C	-1.041322	1.775088	-2.596119
C	-2.803369	3.424448	-2.537343
C	-3.315169	1.097761	-2.154893
C	-3.727911	2.423401	-2.263750
H	-4.777230	2.670316	-2.128202
H	-4.057544	0.338101	-1.931826
C	-1.459975	3.094511	-2.706397
H	0.010043	1.522140	-2.714513
H	-3.126847	4.458433	-2.619582
H	-0.729366	3.869627	-2.919646
C	0.123891	-2.710052	3.533811
C	1.220262	-1.815174	5.487311
C	-0.112289	-0.374629	4.079095
C	0.701281	-0.557831	5.192070
H	0.929746	0.289474	5.832558
H	-0.506085	0.612540	3.855066
C	0.928376	-2.890763	4.652818
H	-0.056428	-3.553488	2.871972
H	1.854317	-1.955560	6.357748
H	1.341081	-3.873045	4.864329
C	3.346392	3.821829	1.400923
C	4.298429	4.332398	0.521905
C	4.398372	3.815341	-0.768247
C	3.554529	2.788343	-1.173648
C	2.599494	2.272345	-0.295860
C	2.498685	2.797883	0.993447
H	3.268041	4.222308	2.408274
H	4.961330	5.132387	0.841019
H	5.139158	4.213462	-1.456689
H	3.622893	2.358210	-2.168320
H	1.758898	2.378341	1.667812
C	1.735275	1.118236	-0.730407
O	1.936612	0.587493	-1.838142
O	0.842333	0.746980	0.116799
C	1.132133	-2.837611	-0.392878
C	2.000973	-2.146143	0.144694
C	3.057251	-1.377678	0.699955
C	4.097784	-0.931583	-0.132383
C	5.118536	-0.154111	0.393289

4●S (cont)

C	3.059269	-1.025424	2.059612
C	4.086058	-0.247351	2.570107
C	5.115501	0.193071	1.741367
H	5.908242	0.204829	-0.259632
H	4.067801	-1.169137	-1.189758
H	2.246174	-1.352902	2.696982
H	5.906272	0.820595	2.141519
H	4.072503	0.029592	3.620333
H	0.744366	-3.746168	-0.805409

TS[**4**●S_2–**1**●HOBz]

E_t = -4135.089781 a.u.

Cu	0.446370	-0.285257	-0.323306
P	-0.870880	-0.361055	1.507030
P	-0.809333	0.013214	-2.142717
C	-2.170217	-1.706163	1.418372
C	-2.270795	-2.326124	0.017658
C	-2.954547	-1.439806	-1.047278
C	-2.134659	-1.275409	-2.337663
C	-1.727879	1.227420	1.835445
C	-0.051881	-0.672446	3.122949
C	-0.032305	0.030326	-3.805982
C	-1.750255	1.589607	-2.050220
H	-3.167705	-0.444589	-0.636536
H	-2.768214	-1.021807	-3.196675
H	-1.623485	-2.212281	-2.594034
H	-1.841293	-2.470902	2.131974
H	-3.141830	-1.341546	1.774984
H	-1.257262	-2.582516	-0.312336
H	-2.809523	-3.278176	0.101305
H	-3.932239	-1.864857	-1.305213
C	-3.067188	1.475558	1.528321
C	-2.813350	3.790976	2.160238
C	-0.933021	2.286448	2.297387
C	-1.474513	3.552913	2.465796
H	-0.846413	4.359902	2.833232
H	0.117147	2.112663	2.520575
C	-3.604505	2.750414	1.689086
H	-3.707280	0.679984	1.159476
H	-3.234487	4.784526	2.284385
H	-4.646808	2.927101	1.439401
C	-0.632196	0.634990	-4.914163
C	1.221466	-0.047813	-6.298382
C	1.204189	-0.605672	-3.951499
C	1.824056	-0.647925	-5.196814
H	2.786931	-1.139601	-5.301764
H	1.678377	-1.058155	-3.082217
C	-0.005784	0.595350	-6.155049
H	-1.581261	1.153816	-4.804037
H	1.711616	-0.072087	-7.267636
H	-0.473663	1.072977	-7.011386
C	-3.061507	1.757747	-2.504956
C	-3.047348	4.053135	-1.763077
C	-1.100755	2.668394	-1.437804
C	-1.742770	3.893219	-1.305363
H	-1.229302	4.718438	-0.820852
H	-0.094661	2.535614	-1.045619
C	-3.706301	2.983016	-2.359236
H	-3.595889	0.933711	-2.969139
H	-3.553870	5.006995	-1.644843
H	-4.727441	3.099358	-2.711731
C	-0.764844	-0.629081	4.326501
C	1.252766	-1.133882	5.547514
C	1.316275	-0.948870	3.143628
C	1.966248	-1.175137	4.355024
H	3.032882	-1.380016	4.360975
H	1.869091	-0.994610	2.208791
C	-0.115407	-0.864323	5.531932
H	-1.827296	-0.395985	4.319187
H	1.760492	-1.307946	6.492100
H	-0.673895	-0.829867	6.463199
C	3.939045	4.525965	1.582568
C	5.285698	4.333728	1.884379
C	5.876375	3.090545	1.671455
C	5.125460	2.039345	1.158890
C	3.775064	2.229389	0.856620
C	3.185519	3.478148	1.070786
H	3.478136	5.495763	1.747280
H	5.874707	5.153694	2.285816
H	6.926045	2.940938	1.907225
H	5.571188	1.064934	0.989031
H	2.134602	3.606329	0.830062
C	2.943638	1.111999	0.322501
O	1.729561	1.317550	0.088460
O	3.537140	-0.019773	0.149999
C	1.750726	-1.847700	-0.366450
C	1.461531	-3.047341	-0.357745
C	0.987444	-4.380219	-0.295542
H	2.737465	-0.843893	-0.146745
C	1.037210	-5.233052	-1.413354

TS[**4**•S_2–**1**•HOBz] (cont)

C	0.510252	-6.515203	-1.343660
C	0.399998	-4.859453	0.892178
C	-0.131571	-6.139276	0.949124
C	-0.080259	-6.972477	-0.167189
H	-0.587149	-6.492175	1.870319
H	0.369552	-4.205069	1.758977
H	1.491046	-4.869056	-2.329930
H	0.556362	-7.163154	-2.214508
H	-0.496636	-7.974390	-0.119485

1•HOBz

E_t = -4135.100566 a.u.

Cu	0.163405	-0.514567	0.462213
P	-1.208368	-0.563531	2.243723
P	-1.112464	-0.277812	-1.397282
C	-2.186419	-2.161353	2.108126
C	-2.145990	-2.792410	0.709719
C	-2.977283	-2.074839	-0.378075
C	-2.183006	-1.774504	-1.660923
C	-2.422904	0.784449	2.529954
C	-0.443213	-0.741577	3.908113
C	-0.162867	-0.098446	-2.955097
C	-2.314888	1.111599	-1.432778
H	-3.385188	-1.131342	0.008641
H	-2.843500	-1.626996	-2.522477
H	-1.517327	-2.610609	-1.909431
H	-1.698774	-2.836831	2.820487
H	-3.213454	-2.019949	2.467475
H	-1.094690	-2.847135	0.397072
H	-2.489779	-3.830769	0.798136
H	-3.849823	-2.685932	-0.638691
C	-3.781813	0.696513	2.222125
C	-4.108139	3.004600	2.846675
C	-1.916409	2.008542	2.990339
C	-2.752447	3.103556	3.155742
H	-2.343771	4.040393	3.524401
H	-0.857673	2.097622	3.224514
C	-4.616900	1.800675	2.376445
H	-4.207502	-0.233174	1.858397
H	-4.761576	3.863480	2.970235
H	-5.670666	1.713767	2.127476
C	0.886352	-1.001615	-3.171638
C	1.484658	0.161009	-5.197818
C	-0.364416	0.945893	-3.861730
C	0.459385	1.073845	-4.975736
H	0.304917	1.899135	-5.664995
H	-1.153513	1.671814	-3.688715
C	1.694810	-0.878022	-4.294114
H	1.093866	-1.776225	-2.435415
H	2.130029	0.267401	-6.065295
H	2.506707	-1.582727	-4.449718
C	-2.066111	2.201843	-0.593622
C	-4.074393	3.286674	-1.368259
C	-3.455903	1.125097	-2.241560
C	-4.332725	2.204281	-2.205046
H	-5.218095	2.201001	-2.834760
H	-3.664794	0.297176	-2.913082
C	-2.937131	3.285746	-0.567755
H	-1.186703	2.190588	0.043769
H	-4.761951	4.127448	-1.339050
H	-2.735777	4.119746	0.097978
C	-1.165734	-0.542773	5.089103
C	0.772330	-1.160878	6.385116
C	0.891899	-1.148182	3.975032
C	1.493548	-1.360415	5.212491
H	2.532066	-1.675872	5.256164
H	1.452173	-1.300019	3.053846
C	-0.557676	-0.750539	6.321739
H	-2.201439	-0.215421	5.043578
H	1.245486	-1.321156	7.349929
H	-1.122950	-0.591737	7.235918
C	1.451792	4.555240	-2.939393
C	2.446969	4.449789	-3.909405
C	3.341147	3.383547	-3.878038
C	3.243332	2.419466	-2.882742
C	2.247348	2.524692	-1.908554
C	1.352538	3.597737	-1.940875
H	0.751703	5.385158	-2.965031
H	2.524157	5.199999	-4.691589
H	4.113265	3.298782	-4.637170
H	3.922700	1.574803	-2.861696
H	0.577349	3.656345	-1.183670
C	2.073501	1.485075	-0.865320
O	1.157871	1.525330	-0.042738
O	2.965001	0.506369	-0.922205
C	1.679516	-1.679463	0.450374
C	2.638503	-2.456017	0.445725
C	3.735451	-3.354464	0.449763
H	2.661091	-0.250167	-0.336616
C	5.002845	-2.951053	-0.011234

1•HOBz (cont)

C	6.071706	-3.835720	-0.002810
C	3.582667	-4.673998	0.916065
C	4.657621	-5.551161	0.918227
C	5.907392	-5.139440	0.460213
H	4.520205	-6.565863	1.282060
H	2.608699	-4.992231	1.274724
H	5.130868	-1.935060	-0.372949
H	7.042841	-3.505411	-0.361349
H	6.746433	-5.828821	0.464630

2•B

E_t = -4176.205843 a.u.

Cu	0.312899	-0.156961	-0.336777
P	-1.182521	-0.278124	1.417462
P	-1.291873	-0.024409	-2.291287
C	-2.589745	-1.487506	1.262561
C	-3.262486	-1.493048	-0.119218
C	-2.471920	-2.322806	-1.153513
C	-2.251818	-1.625452	-2.496987
C	-2.000981	1.314989	1.808490
C	-0.460729	-0.811434	3.016245
C	-0.287680	0.065707	-3.823958
C	-2.590185	1.254936	-2.570534
H	-1.486276	-2.561806	-0.740989
H	-1.675400	-2.274653	-3.165056
H	-3.203621	-1.406336	-2.995690
H	-3.298879	-1.285454	2.075176
H	-2.154906	-2.472447	1.473549
H	-3.389802	-0.462699	-0.477074
H	-4.278961	-1.892312	-0.015325
H	-2.981732	-3.278940	-1.328686
C	-3.386711	1.496084	1.781168
C	-3.114727	3.842789	2.272028
C	-1.178123	2.418196	2.073864
C	-1.732956	3.669645	2.307751
H	-1.078589	4.513193	2.506904
H	-0.098683	2.299700	2.085747
C	-3.938568	2.753631	2.010789
H	-4.051210	0.665530	1.566600
H	-3.546719	4.824043	2.447883
H	-5.017246	2.878793	1.979571
C	0.543248	-1.011746	-4.159203
C	1.473386	0.243858	-5.997694
C	-0.203519	1.241506	-4.577746
C	0.668058	1.326122	-5.658137
H	0.717089	2.245050	-6.235490
H	-0.825687	2.095199	-4.324902
C	1.409207	-0.922957	-5.242086
H	0.538031	-1.919064	-3.560601
H	2.153904	0.312236	-6.841488
H	2.046120	-1.768751	-5.484964
C	-2.796871	2.238074	-1.600821
C	-4.587733	3.185017	-2.908268
C	-3.394728	1.251697	-3.717215
C	-4.385120	2.210805	-3.885084
H	-5.000353	2.200933	-4.780496
H	-3.233279	0.503856	-4.490090
C	-3.793496	3.197260	-1.768114
H	-2.177969	2.256002	-0.708386
H	-5.363705	3.933720	-3.041173
H	-3.942320	3.950464	-0.999883
C	-0.865843	-0.275454	4.241110
C	0.609570	-1.795986	5.396464
C	0.486872	-1.838140	2.990819
C	1.013751	-2.332778	4.177806
H	1.765345	-3.116569	4.144890
H	0.828993	-2.233457	2.036634
C	-0.326565	-0.766538	5.425972
H	-1.594950	0.529369	4.269807
H	1.033668	-2.173214	6.322786
H	-0.639930	-0.340977	6.375194
C	2.719968	0.788202	1.475927
C	3.248895	-0.149435	2.038301
C	3.813828	-1.303161	2.627233
C	4.385664	-1.264402	3.910275
C	4.889617	-2.421132	4.487812
C	3.773482	-2.528649	1.935841
C	4.279615	-3.678516	2.524339
C	4.836252	-3.632981	3.801716
H	5.230618	-4.536082	4.258399
H	4.411985	-0.321084	4.446566
H	5.325163	-2.378785	5.482262
H	3.337787	-2.559524	0.941568
H	4.239788	-4.618231	1.980207
C	1.122292	1.616507	-0.197335
C	2.148986	1.862992	0.750622
C	0.685550	2.710436	-0.948079
C	2.624331	3.169346	0.978823
C	1.165740	4.002039	-0.734434
C	2.125760	4.235947	0.246780

2•B (cont)

H	-0.062334	2.565666	-1.723611
H	3.396093	3.324635	1.727818
H	0.786062	4.825434	-1.334707
H	2.499420	5.240345	0.425406
C	0.981565	-1.993513	-0.759380
C	1.836729	-1.040483	-1.077021
C	1.269062	-3.329447	-1.019424
C	3.071326	-1.189369	-1.667283
C	2.511158	-3.571130	-1.632241
C	3.389401	-2.529420	-1.948112
H	0.602169	-4.155861	-0.779141
H	3.746605	-0.373808	-1.906719
H	2.800586	-4.593853	-1.863722
H	4.341810	-2.761073	-2.419027

TS[**2**•B–**6**]

E_t = -4176.1950838 a.u.

Cu	0.401925	-0.506128	-0.783641
P	-1.081846	-0.675077	1.022764
P	-1.119190	-0.381983	-2.571571
C	-2.485052	-1.902727	0.852150
C	-3.143160	-1.984355	-0.528390
C	-2.271285	-2.733989	-1.558372
C	-2.051629	-1.970567	-2.864200
C	-1.940864	0.876019	1.503043
C	-0.415743	-1.326097	2.604765
C	-0.351690	-0.090458	-4.213641
C	-2.362372	0.966043	-2.427668
H	-1.283399	-2.934372	-1.124143
H	-1.416698	-2.556169	-3.539914
H	-2.993082	-1.785875	-3.395415
H	-3.210468	-1.675801	1.644080
H	-2.044743	-2.874217	1.108105
H	-3.377682	-0.978013	-0.895382
H	-4.111043	-2.490024	-0.419741
H	-2.718224	-3.709362	-1.787882
C	-3.307401	1.086839	1.297789
C	-3.108370	3.358507	2.089008
C	-1.166676	1.928677	2.009618
C	-1.746495	3.156395	2.301579
H	-1.128195	3.959616	2.692929
H	-0.105201	1.780078	2.182777
C	-3.885026	2.319355	1.589992
H	-3.935568	0.300134	0.893075
H	-3.559286	4.322251	2.308941
H	-4.946119	2.468120	1.411344
C	0.749843	-0.888496	-4.552856
C	1.031071	0.350208	-6.603426
C	-0.745203	0.935313	-5.076089
C	-0.053850	1.152383	-6.265148
H	-0.363597	1.956998	-6.926205
H	-1.582531	1.575022	-4.812313
C	1.429400	-0.672656	-5.744991
H	1.096069	-1.655797	-3.862496
H	1.573300	0.527910	-7.527673
H	2.286097	-1.292213	-5.993879
C	-1.984532	2.097018	-1.695166
C	-4.118507	3.127139	-2.130015
C	-3.635437	0.930121	-3.006266
C	-4.511231	2.000047	-2.847708
H	-5.501455	1.955274	-3.292181
H	-3.954012	0.069266	-3.586804
C	-2.850884	3.175469	-1.561163
H	-1.009624	2.128798	-1.219508
H	-4.803194	3.962122	-2.009505
H	-2.537204	4.040252	-0.984235
C	-0.930882	-0.958887	3.850076
C	0.436680	-2.637731	4.916131
C	0.539051	-2.343040	2.524736
C	0.955479	-2.999675	3.677272
H	1.704539	-3.782931	3.607572
H	0.961470	-2.608695	1.557295
C	-0.498882	-1.611016	5.000339
H	-1.669633	-0.165130	3.920723
H	0.776530	-3.140839	5.816548
H	-0.895948	-1.314885	5.967476
C	2.125917	1.163477	1.496354
C	2.452235	0.593990	2.518535
C	2.865008	-0.086592	3.688191
C	2.418020	0.326186	4.953847
C	2.824600	-0.349848	6.094976
C	3.732321	-1.189900	3.597922
C	4.137214	-1.854665	4.745973
C	3.683647	-1.441410	5.997098
H	3.996765	-1.969850	6.892960
H	1.738621	1.170021	5.022291
H	2.461172	-0.028123	7.066976
H	4.068259	-1.513299	2.616979
H	4.805983	-2.707064	4.664699
C	1.404057	1.217233	-0.863384
C	1.854336	1.878401	0.303989
C	1.410183	1.956746	-2.053000
C	2.070669	3.271740	0.293005
C	1.655210	3.326007	-2.067750
C	1.941933	3.997616	-0.880061

TS[**2**•B–**6**] (cont)

H	1.174437	1.464173	-2.991424
H	2.351723	3.763315	1.220346
H	1.598418	3.870323	-3.007200
H	2.093158	5.073329	-0.875502
C	1.643157	-2.078761	-0.965407
C	2.296830	-0.915509	-0.997809
C	2.390064	-3.255683	-1.033390
C	3.652584	-0.701516	-1.100057
C	3.784590	-3.135460	-1.137575
C	4.404524	-1.884759	-1.173444
H	1.933906	-4.244744	-1.004218
H	4.116713	0.280100	-1.116826
H	4.398746	-4.032125	-1.191859
H	5.486656	-1.821519	-1.257780

6

E_t = -4176.296160 a.u.

Cu	0.236422	-0.836444	-0.453888
P	-1.024227	-1.083303	1.377242
P	-1.131726	-0.798747	-2.277775
C	-2.200199	-2.530263	1.273660
C	-2.811394	-2.688666	-0.125364
C	-1.815201	-3.278562	-1.145655
C	-1.777243	-2.543167	-2.488699
C	-2.111522	0.337429	1.791984
C	-0.172987	-1.440595	2.963274
C	-0.331552	-0.475931	-3.897978
C	-2.585523	0.319990	-2.276953
H	-0.800300	-3.254540	-0.721879
H	-1.077442	-3.039682	-3.171035
H	-2.757782	-2.548630	-2.979594
H	-2.964701	-2.424888	2.053712
H	-1.612686	-3.419987	1.533201
H	-3.175649	-1.716213	-0.481009
H	-3.697481	-3.332742	-0.057468
H	-2.045666	-4.337276	-1.320769
C	-3.504772	0.303828	1.692743
C	-3.632546	2.632982	2.312015
C	-1.487350	1.540671	2.147024
C	-2.243113	2.675302	2.411065
H	-1.744537	3.598354	2.694787
H	-0.402214	1.581798	2.215314
C	-4.258428	1.445880	1.950674
H	-4.019067	-0.607921	1.406033
H	-4.222851	3.522058	2.515250
H	-5.340470	1.403844	1.863959
C	0.888373	-1.119473	-4.144799
C	1.089099	0.038776	-6.250688
C	-0.825565	0.435120	-4.833855
C	-0.115907	0.689698	-6.004083
H	-0.506853	1.402988	-6.724556
H	-1.757291	0.959792	-4.642879
C	1.587925	-0.868452	-5.318362
H	1.314992	-1.781701	-3.394381
H	1.643425	0.244214	-7.162105
H	2.538472	-1.365034	-5.490487
C	-2.458265	1.498713	-1.535979
C	-4.694413	2.152618	-2.148697
C	-3.781095	0.070874	-2.958325
C	-4.831855	0.979886	-2.887533
H	-5.758384	0.774865	-3.416612
H	-3.896609	-0.828011	-3.557745
C	-3.502905	2.414158	-1.479986
H	-1.536089	1.697429	-0.995309
H	-5.517183	2.860129	-2.095240
H	-3.387976	3.321436	-0.894129
C	-0.820805	-1.338798	4.198309
C	1.146873	-2.191226	5.300772
C	1.143608	-1.901327	2.908199
C	1.796231	-2.285946	4.075280
H	2.824979	-2.629545	4.028253
H	1.657745	-1.927608	1.948309
C	-0.159474	-1.710418	5.362823
H	-1.838806	-0.958952	4.247531
H	1.664882	-2.475193	6.212506
H	-0.663105	-1.623958	6.321730
C	1.908987	1.650588	0.924358
C	2.342857	1.356842	2.020181
C	2.914849	0.964445	3.250478
C	2.302208	1.279943	4.475087
C	2.884447	0.884031	5.669802
C	4.121943	0.241179	3.256929
C	4.697503	-0.142498	4.458757
C	4.083941	0.175976	5.668772
H	4.538937	-0.127041	6.607320
H	1.363775	1.825936	4.472860
H	2.397569	1.127631	6.609873
H	4.586745	-0.009176	2.308114
H	5.632817	-0.695484	4.452300
C	1.927764	1.472685	-1.531486
C	1.477943	2.106706	-0.345233
C	1.590436	2.049600	-2.757094
C	0.680742	3.263210	-0.429590
C	0.800540	3.192055	-2.829171
C	0.339396	3.797267	-1.662520

6 (cont)

H	1.930986	1.565764	-3.668687
H	0.357027	3.742268	0.489507
H	0.535990	3.602267	-3.799609
H	-0.279723	4.688393	-1.714020
C	2.137383	-0.926176	-0.882399
C	2.722985	0.221628	-1.469935
C	2.940433	-2.080043	-0.876505
C	4.004109	0.201847	-2.028157
C	4.227713	-2.108314	-1.414669
C	4.763485	-0.964039	-1.998447
H	2.546154	-3.003071	-0.448901
H	4.412409	1.107808	-2.472870
H	4.811703	-3.026080	-1.384742
H	5.764130	-0.975776	-2.422138