

Electronic Supplementary Material (ESI) for Dalton Transaction

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SUPPLEMENTARY INFORMATION

Copper Hydride-Mediated Electrophilic Amidation of Vinylarenes with Dioxazolones – A Computational Mechanistic Study

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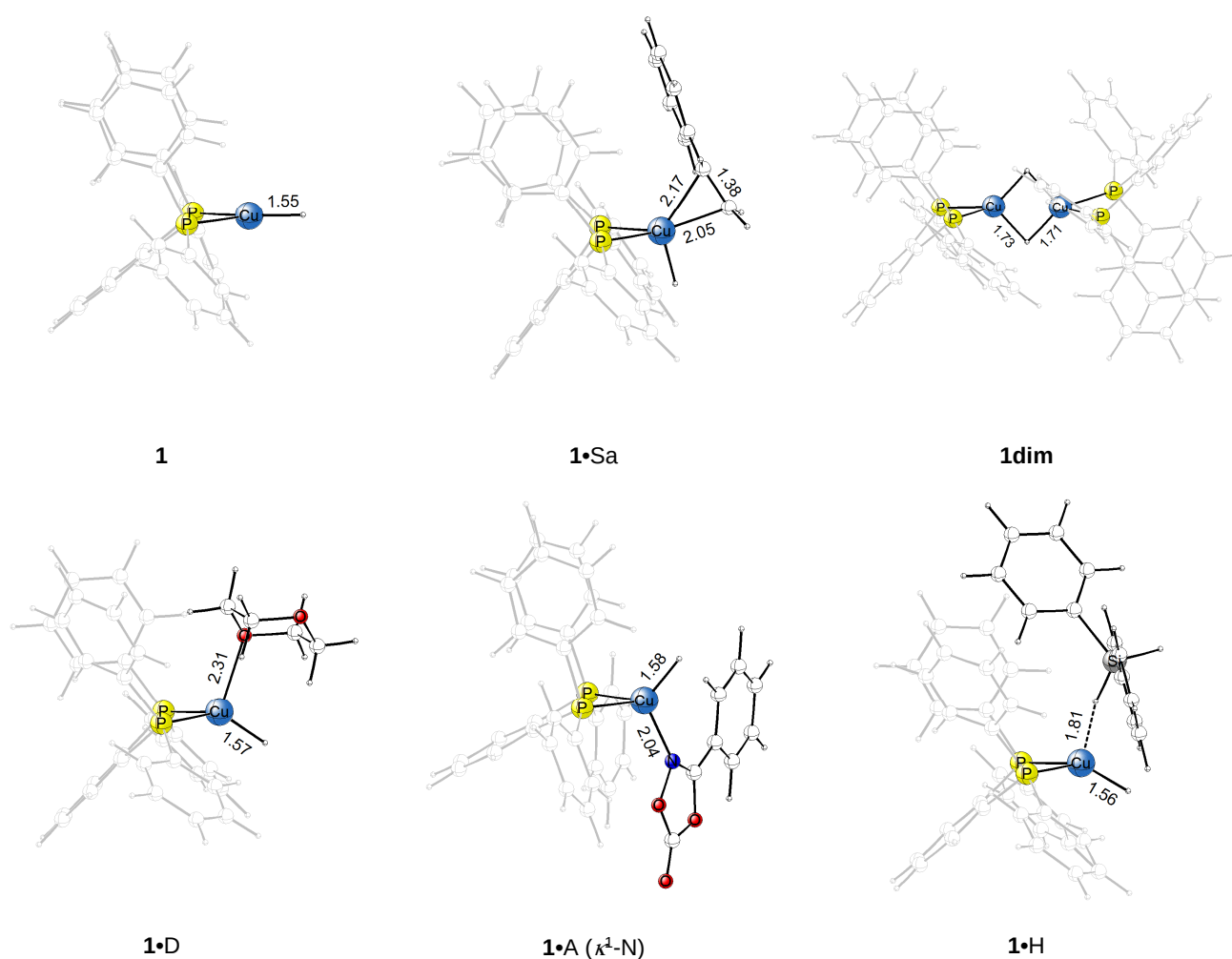


Fig. S1a. Selected structural parameter (angstrom) of the optimised structures of various forms of the catalytically competent $\{P^iP^j\}Cu^I$ hydride **1**.

The aryl groups at the $\{P^iP^j\}$ ligand are greyed out to enhance the visualisation of crucial structural aspects.

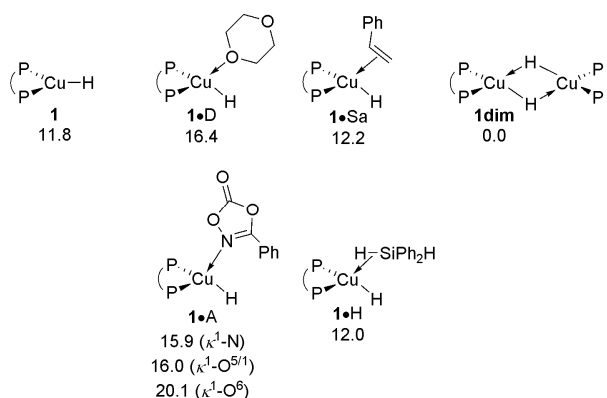


Fig. S1b. Various forms of the catalytically competent $\{\text{P}^{\text{P}}\}\text{Cu}^{\text{I}}$ hydride **1**.

Free energies are given in kcal mol^{-1} relative to $\{\frac{1}{2}\times\mathbf{1dim} + \text{reactant}\}$

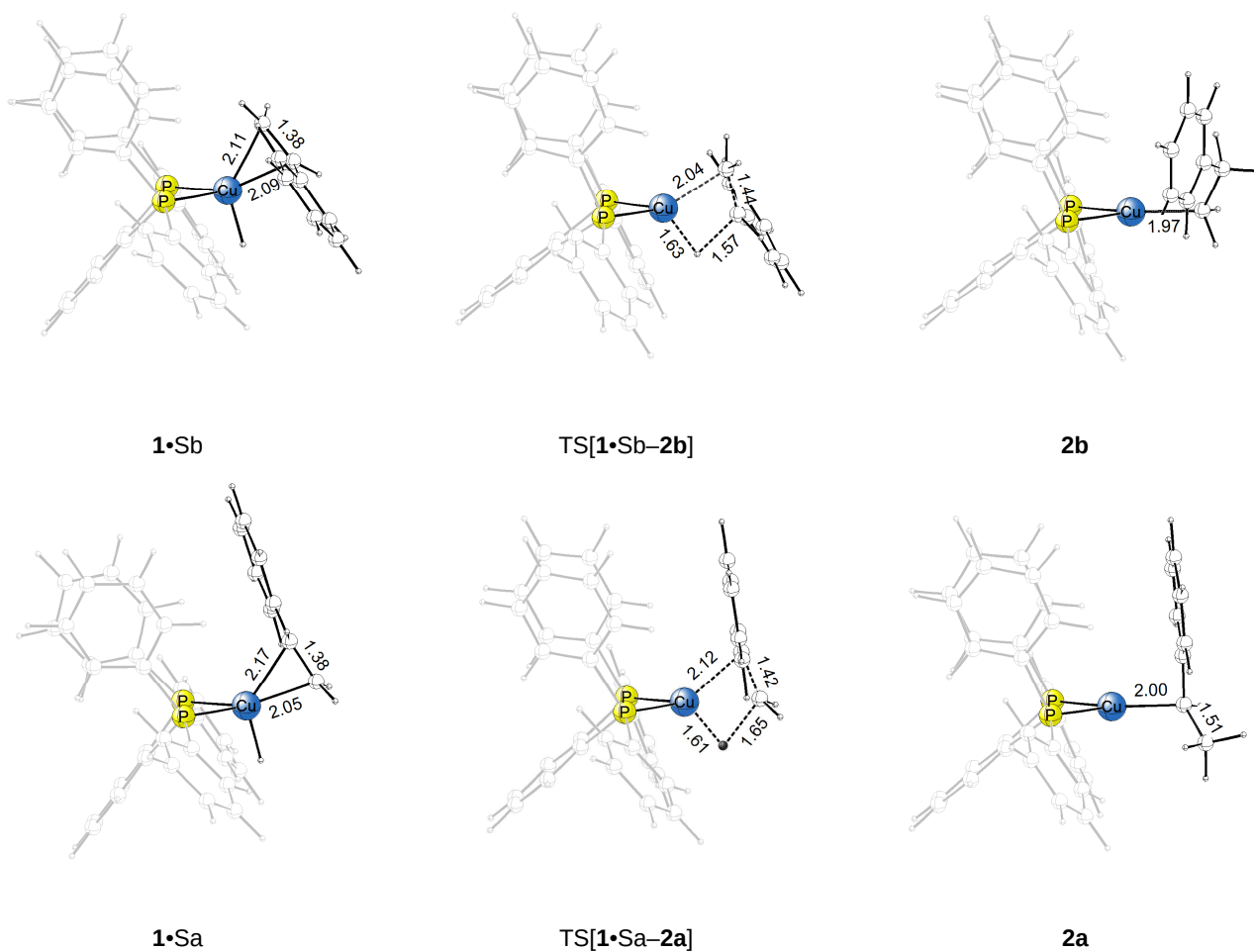


Fig. S2. Selected structural parameter (angstrom) of the optimised structures of key stationary points for olefin C=C bond insertion into the Cu-H linkage at styrene adduct **2•S** of the $\{\text{P}^{\text{P}}\}\text{Cu}^{\text{I}}$ hydride through regioisomeric pathways for 1,2-insertion (top) and 2,1-insertion (bottom).

The aryl groups at the $\{\text{P}^{\text{P}}\}$ ligand are greyed out to enhance the visualisation of crucial structural aspects.

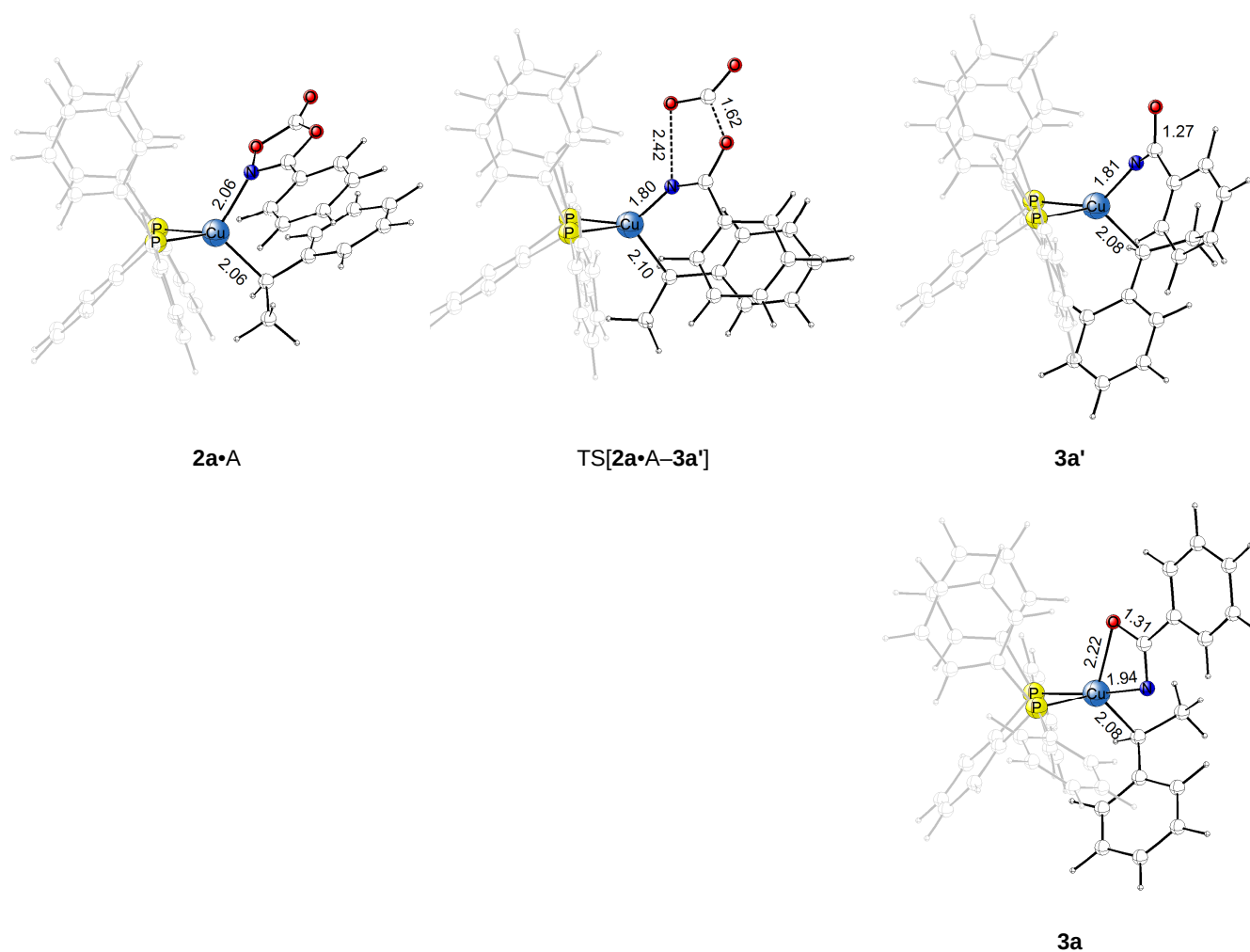


Fig. S3. Selected structural parameter (angstrom) of the optimised structures of key stationary points for oxidative Cu=N between benzylcopper **2a** and dioxazolone A with simultaneously occurring CO₂ extrusion at amine adduct **2a•A** of the benzylcopper.

The aryl groups at the {P[^]P} ligand are greyed out to enhance the visualisation of crucial structural aspects.

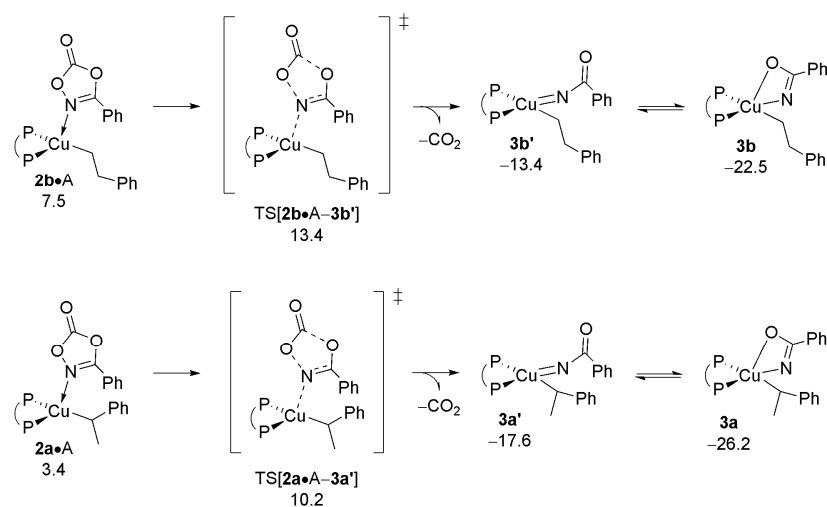


Fig. S4. Oxidative Cu=N coupling between {P[^]P}Cu^I alkyl/benzyl **2b/2a** and dioxazolone with concurrent CO₂ extrusion. Free energies are given in kcal mol⁻¹ relative to {½×**1dim** + reactant}.

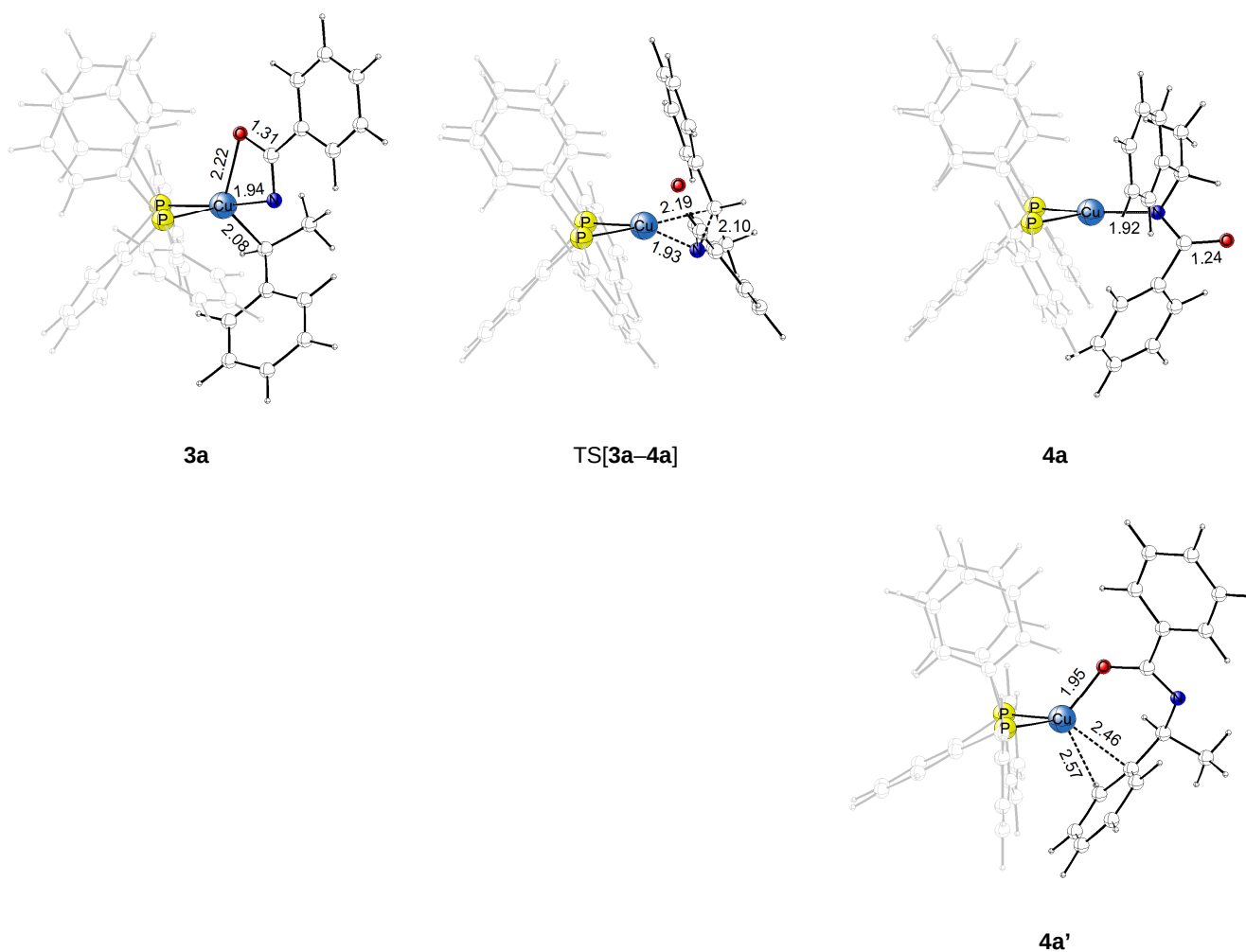


Fig. S5. Selected structural parameter (angstrom) of the optimised structures of key stationary points for C–N bond forming reductive elimination at $\{P^{\wedge}P\}Cu^{III}$ intermediate **3a**.

The aryl groups at the $\{P^{\wedge}P\}$ ligand are greyed out to enhance the visualisation of crucial structural aspects.

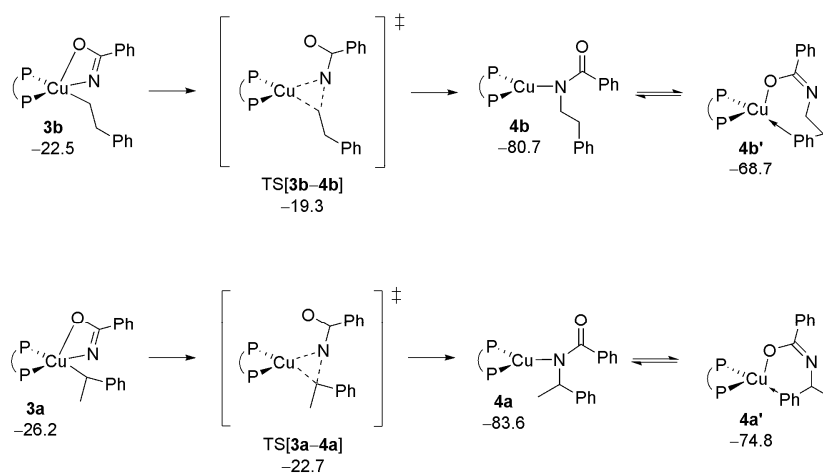


Fig. S6. C–N bond generating reductive elimination at $\{P^{\wedge}P\}Cu^{III}$ intermediates **3b/3a**.

Free energies are given in kcal mol⁻¹ relative to $\{1/2 \times \mathbf{1dim} + \text{reactant}\}$.

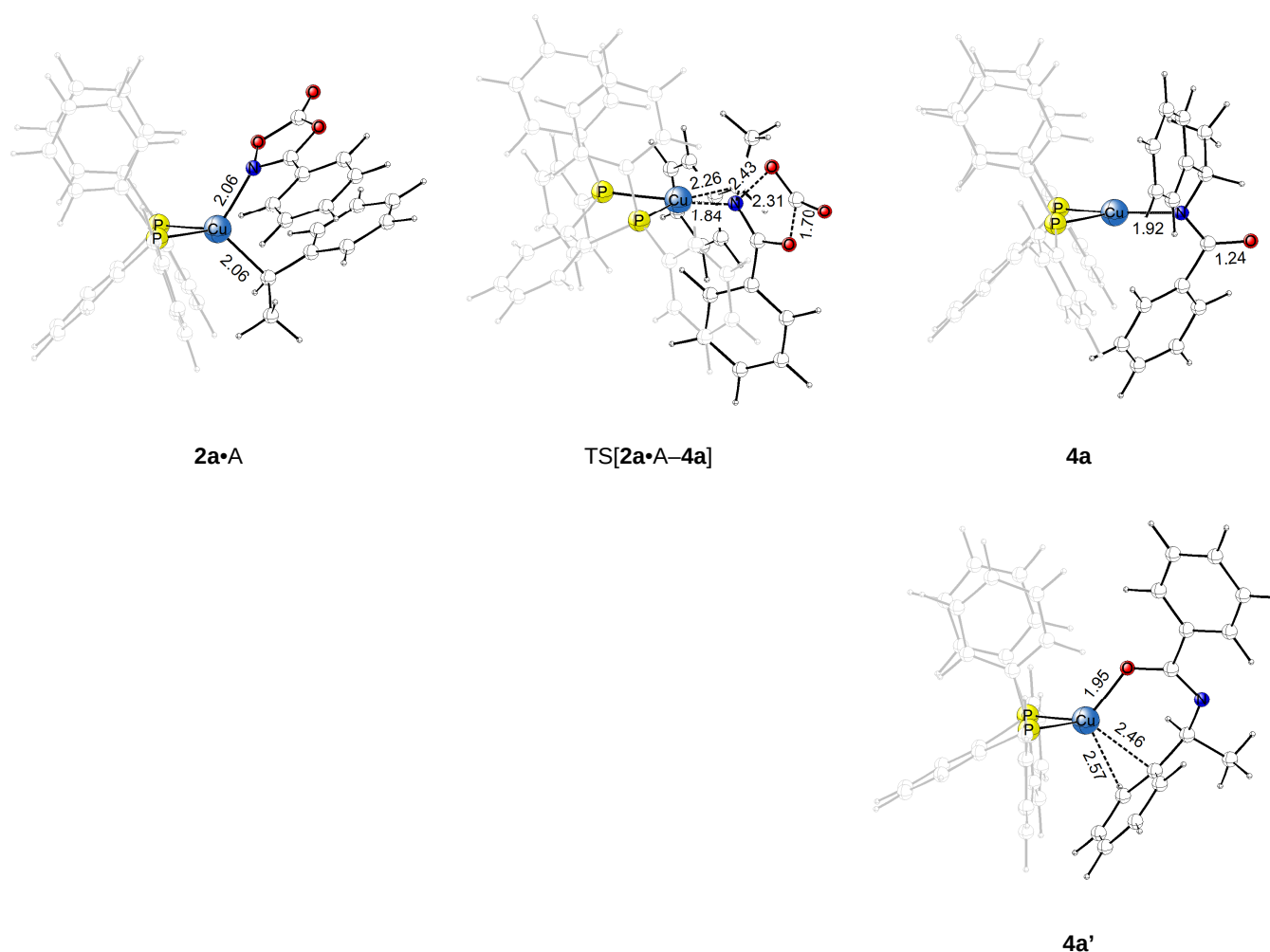


Fig. S7. Selected structural parameter (angstrom) of the optimised structures of key stationary points for S_N2 -type attack of the Cu–C linkage at dioxazolone A with simultaneous C–N bond formation and CO_2 cleavage at amine adduct **2a•A** of the benzylcopper.

The aryl groups at the {P^{Ar}P} ligand are greyed out to enhance the visualisation of crucial structural aspects.

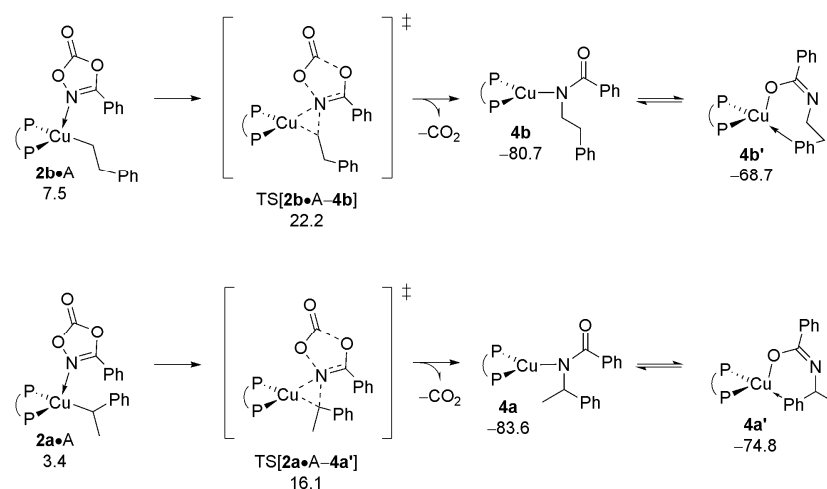


Fig. S8. S_N2 -type attack of the Cu–C linkage of {P^{Ar}P}Cu^I alkyl/benzyl **2b/2a** at dioxazolone A with concurrent C–N bond formation and CO_2 release.

Free energies are given in kcal mol⁻¹ relative to { $\frac{1}{2}$ ×**1dim** + reactant}.

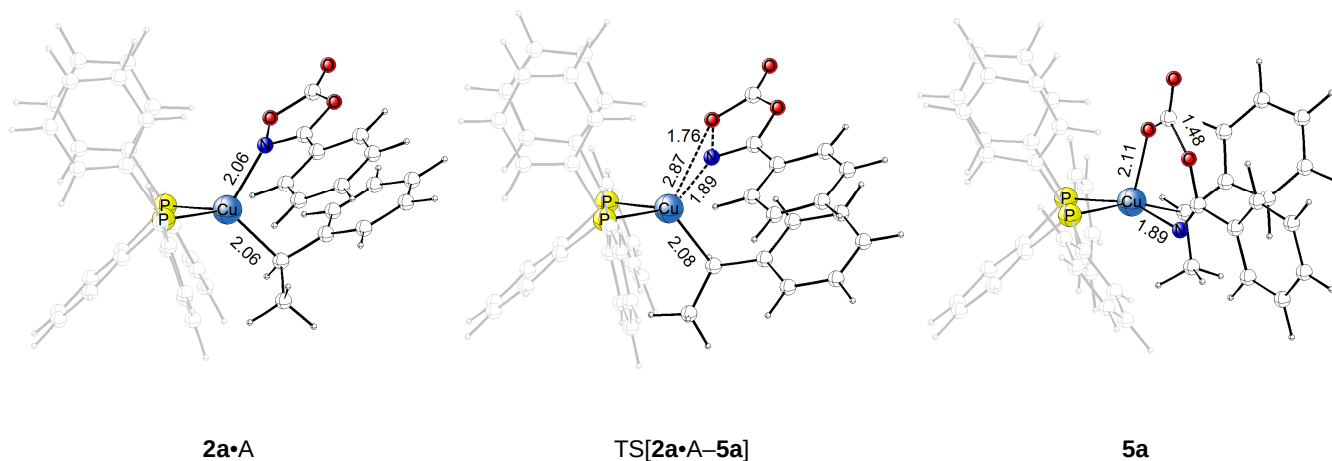


Fig. S9. Selected structural parameter (angstrom) of the optimised structures of key stationary points for oxidative insertion of benzylcopper **2a** into the N–O linkage of dioxazolone A.

The aryl groups at the {P[^]P} ligand are greyed out to enhance the visualisation of crucial structural aspects.

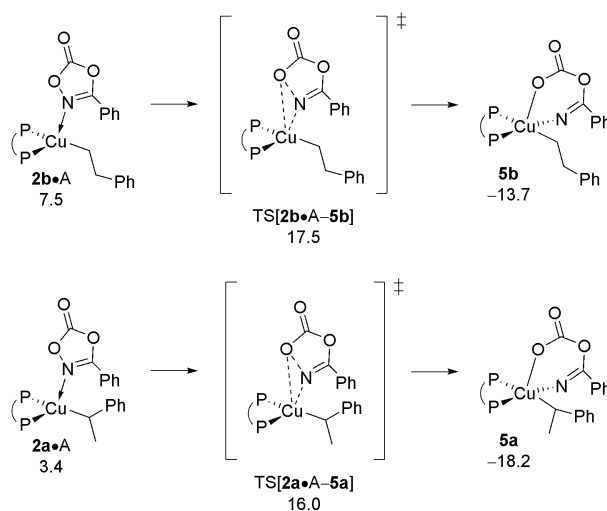


Fig. S10. Oxidative addition of {P[^]P}Cu^I alkyl/benzyl **2b/2a** into the dioxazolone's N–O bond.

Free energies are given in kcal mol⁻¹ relative to {½×**1dim** + reactant}.

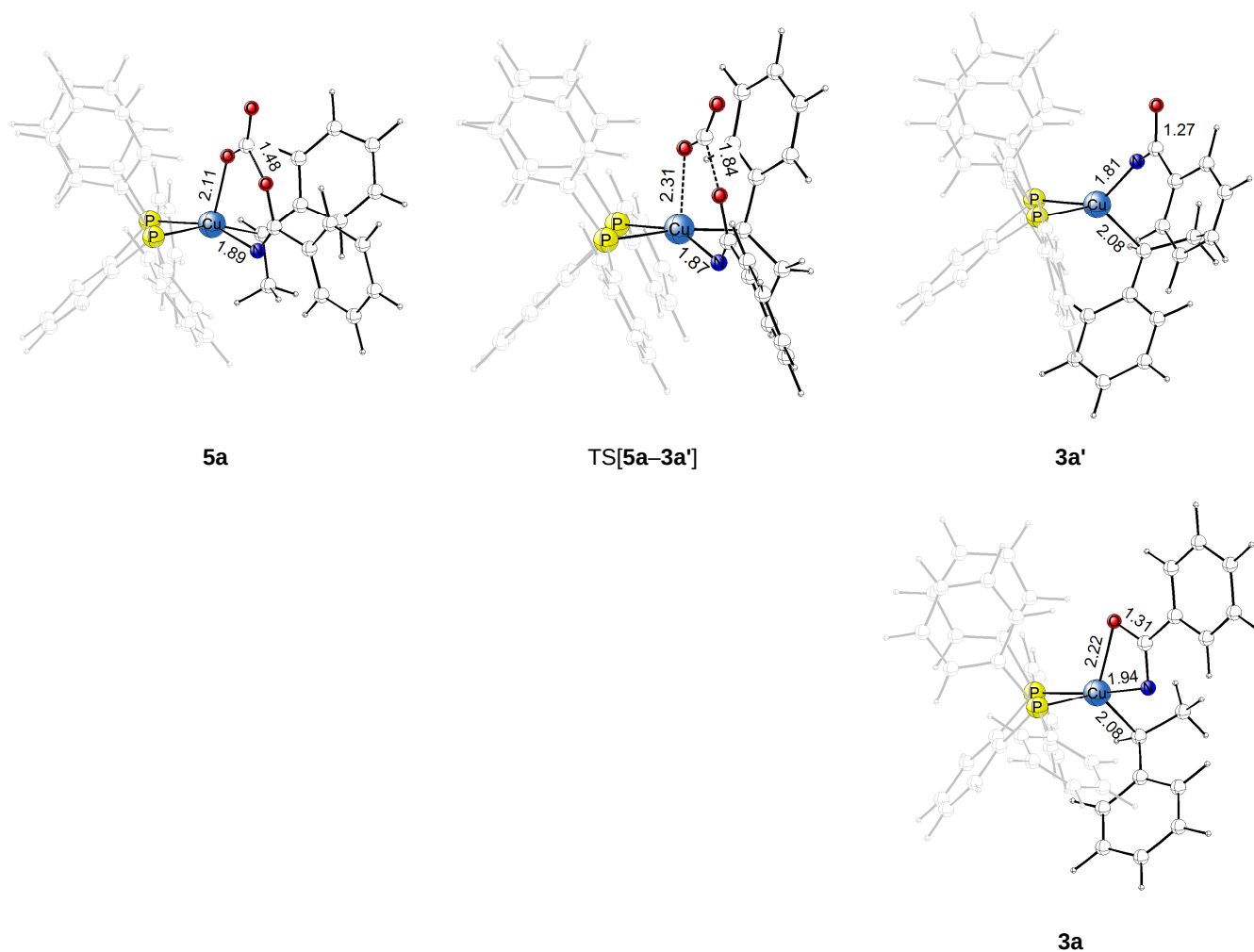


Fig. S11. Selected structural parameter (angstrom) of the optimised structures of key stationary points for CO₂ extrusion at cyclic {P[^]P}Cu^{III} intermediate **5a**.

The aryl groups at the {P[^]P} ligand are greyed out to enhance the visualisation of crucial structural aspects.

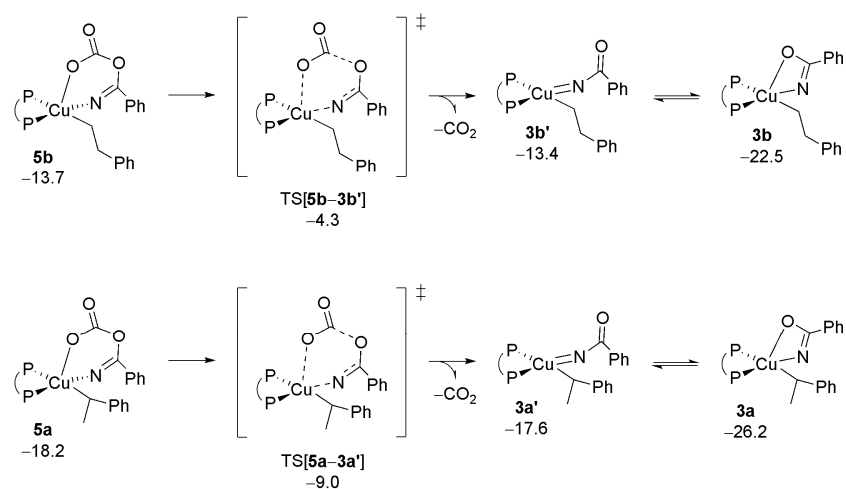


Fig. S12. Decarboxylation at cyclic {P[^]P}Cu^{III} intermediate **5b/5a**.

Free energies are given in kcal mol⁻¹ relative to {½×**1dim** + reactant}.

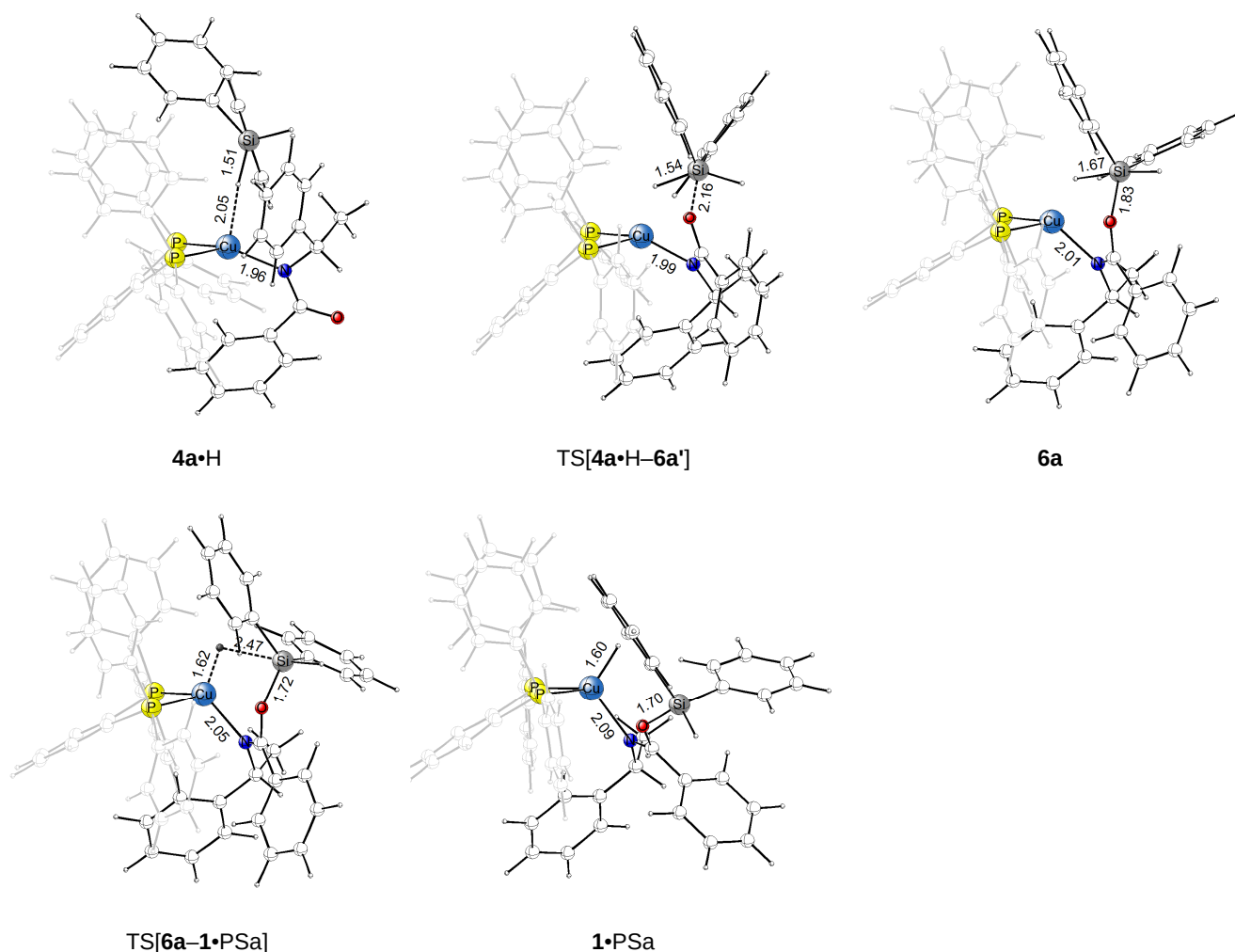


Fig S13. Selected structural parameter (angstrom) of the optimised structures of key stationary points for nucleophilic attack of amidate **4a** at Ph_2SiH_2 and hydrogen atom transfer at silicate **6a**.

The aryl groups at the $\{\text{P}^\wedge\text{P}\}$ ligand are greyed out to enhance the visualisation of crucial structural aspects.

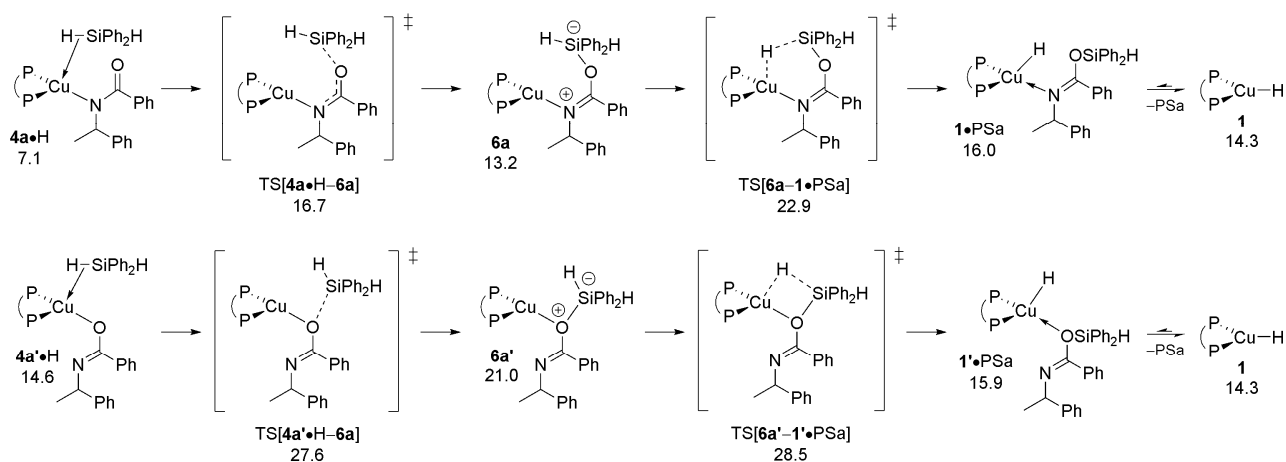


Fig. S14. Nucleophilic attack of the $\{\text{P}^\wedge\text{P}\}\text{Cu}^{\text{I}}$ amidate/imidate **4a/4a'** at Ph_2SiH_2 (H) with ensuing hydrogen-atom transfer at transient silicate **6a/6a'**.

Free energies are given in kcal mol^{-1} relative to $\{\text{4a} + \text{reactant}\}$.

Cartesian coordinates (in Å) of located key structures

A				S				dioxane			
O	2.165859	-1.049317	0.065240	C	1.321075	-1.335661	0.000164	O	-1.401457	-0.160703	0.087055
C	1.478932	0.127570	0.074469	C	0.257186	-2.230906	-0.001216	C	-0.783778	0.317923	-1.103226
N	2.235867	1.168934	0.148445	C	-1.041620	-1.745530	-0.001190	C	0.630773	-0.202265	-1.224478
O	3.555095	0.654495	0.193704	C	-1.271318	-0.379039	0.000084	O	1.406191	0.162996	-0.087444
C	3.508183	-0.706057	0.142664	C	-0.213986	0.536179	0.001096	C	0.788512	-0.315630	1.102837
C	0.033645	0.117365	0.005082	C	1.089839	0.027327	0.001337	C	-0.626038	0.204558	1.224090
O	4.423945	-1.462170	0.160163	H	2.337209	-1.705742	0.000485	H	-1.396872	-0.026583	-1.934347
C	-0.670029	1.325415	0.018211	H	0.442048	-3.295986	-0.002072	H	-0.775740	1.414848	-1.103595
C	-2.740672	0.112485	-0.126451	H	-1.877721	-2.431159	-0.002065	H	0.615645	-1.294052	-1.329942
C	-0.660672	-1.090851	-0.074317	H	-2.287732	-0.007221	0.000090	H	1.128608	0.225152	-2.093254
C	-2.044188	-1.087116	-0.139671	C	-0.515000	1.963584	0.001884	H	0.780474	-1.412555	1.103206
H	-2.578447	-2.024214	-0.201025	H	1.932038	0.704086	0.002953	H	1.401606	0.028876	1.933958
H	-0.117500	-2.023152	-0.084458	H	-1.574252	2.199000	0.006640	H	-0.610911	1.296345	1.329553
C	-2.050070	1.316638	-0.047444	C	0.346706	2.980702	-0.003034	H	-1.123873	-0.222859	2.092866
H	-0.128240	2.256977	0.079812	H	-0.001985	4.002707	-0.001823				
H	-3.820204	0.111393	-0.177404	H	1.418871	2.843207	-0.008652				
H	-2.591504	2.251604	-0.037019								

H				Pa (2,1-ins)				Pb (1,2-ins)			
Si	-1.577564	-0.000284	-0.578370	C	-3.211208	3.146058	0.056371	C	-1.139931	4.999442	1.235829
C	-0.559512	-1.538194	-0.260555	C	-3.550700	2.673619	1.332797	C	-0.058564	5.618292	0.587066
C	-0.597947	1.538726	-0.161840	C	-2.630584	1.883459	2.045982	C	0.976372	4.828677	0.056076
H	-2.816671	-0.099996	0.239199	C	-1.386651	1.570986	1.481073	C	0.927801	3.431019	0.173938
H	-1.990783	0.098236	-2.004413	C	-1.033293	2.040382	0.195969	C	-0.152543	2.796927	0.824818
C	0.179125	1.597791	0.998486	C	-1.961592	2.831093	-0.507594	C	-1.185291	3.599990	1.350156
C	0.847778	3.848913	0.485866	H	-3.924019	3.766526	-0.511468	H	-1.954105	5.610991	1.658893
C	-0.629064	2.661311	-0.991962	H	-4.530016	2.920627	1.774509	H	-0.020209	6.716400	0.497542
C	0.085312	3.807583	-0.672439	H	-2.885205	1.511431	3.052272	H	1.830979	5.306106	-0.451352
H	0.050058	4.666351	-1.329022	H	-0.668120	0.949052	2.040994	H	1.742292	2.812983	-0.241539
H	-1.214057	2.640804	-1.902652	C	0.331743	1.661367	-0.371518	C	-0.219017	1.288148	0.886831
C	0.894751	2.740717	1.321169	C	0.653328	2.226883	-1.761541	C	-0.740058	0.690572	-0.442512
H	0.234868	0.737598	1.653345	H	1.121565	2.020713	0.324672	H	-2.036152	3.119601	1.863493
H	1.407030	4.740182	0.735623	H	-1.714238	3.212586	-1.509938	H	-0.094855	1.045139	-1.272152
H	1.491189	2.767563	2.223063	H	-0.058940	1.855354	-2.531122	H	-1.776497	1.038052	-0.643400
C	-1.131628	-2.677167	0.310256	H	0.623402	3.338126	-1.760265	H	-0.877841	0.961591	1.722170
C	0.962368	-3.848864	0.176437	H	1.677287	1.911777	-2.050318	H	0.792063	0.865353	1.069738
C	0.794916	-1.581168	-0.602728	O	2.684432	0.221940	0.190693	O	1.501082	-0.848509	-1.012179
C	1.549673	-2.724413	-0.387904	C	1.656221	-0.414582	-0.056547	C	0.453549	-1.438364	-0.733239
H	2.596856	-2.738575	-0.658202	N	0.463116	0.203390	-0.346111	N	-0.718396	-0.762473	-0.471947
H	1.269251	-0.708272	-1.032668	C	1.631162	-1.922378	-0.057607	C	0.377149	-2.942278	-0.662382
C	-0.379972	-3.823677	0.526359	C	2.867234	-2.587058	-0.192419	C	-0.825276	-3.670026	-0.790436
H	-2.176003	-2.669467	0.595360	C	1.746620	-4.741041	-0.046387	C	0.392324	-5.761066	-0.533286
H	1.550459	-4.740386	0.346188	C	0.454950	-2.684358	0.105679	C	1.588874	-3.643223	-0.492986
H	-0.840437	-4.695310	0.971403	C	0.512916	-4.086875	0.111095	C	1.596444	-5.042953	-0.420252
				H	-0.410611	-4.672734	0.249095	H	2.548185	-5.580902	-0.278860
				H	-0.516778	-2.188170	0.266472	H	2.518479	-3.057138	-0.423634
				C	2.924626	-3.987361	-0.195263	C	-0.817384	-5.072382	-0.725728
				H	3.775126	-1.971903	-0.290871	H	-1.777144	-3.146483	-0.980274
				H	1.790769	-5.842656	-0.043939	H	0.397413	-6.862170	-0.480967
				H	3.895034	-4.497495	-0.310121	H	-1.760968	-5.631235	-0.837348
				H	-0.327577	-0.348754	-0.684643	H	-1.488775	-1.270078	-0.032077

PSa (2,1-ins)			PSb (1,2-ins)			1					
C	0.647711	4.455667	0.791550	C	-0.452058	4.813167	1.899605	Cu	2.495096	-0.212465	0.078163
C	-0.030904	4.473581	2.001339	C	-1.518781	5.700563	1.913919	C	-0.445637	-1.229803	-0.900400
C	-1.243570	3.805222	2.115936	C	-2.805865	5.226129	1.699681	C	-1.349583	-1.914888	-1.706844
C	-1.772321	3.127213	1.029532	C	-3.019813	3.874890	1.472164	C	-2.323080	-2.724495	-1.140643
C	-1.101053	3.107544	-0.191387	C	-1.956828	2.973731	1.455581	C	-2.403559	-2.854940	0.239897
C	0.113943	3.775348	-0.295272	C	-0.671062	3.462659	1.672545	C	-1.508810	-2.176815	1.054059
H	1.596638	4.965013	0.693647	H	0.555310	5.169574	2.066735	C	-0.528689	-1.360329	0.497874
H	0.383322	5.000696	2.849711	H	-1.350222	6.753576	2.093334	H	-1.276298	-1.830611	-2.781563
H	-1.775158	3.807539	3.057943	H	-3.644705	5.908854	1.714184	H	-3.015791	-3.257440	-1.777336
H	-2.706342	2.592983	1.126161	H	-4.026427	3.510727	1.308721	H	-3.157891	-3.490922	0.682147
C	-1.688783	2.388565	-1.384012	C	-2.186974	1.525322	1.149934	H	-1.561976	-2.291263	2.127053
C	-2.889767	3.134966	-1.948580	C	-2.216779	1.270071	-0.362030	P	0.886898	-0.138705	-1.549838
H	-0.913966	2.341387	-2.151840	H	0.165324	2.779594	1.661524	P	0.727240	-0.459946	1.487194
H	0.652474	3.754025	-1.233249	H	-2.992369	1.898083	-0.800010	C	0.074735	1.498782	-1.594996
H	-3.682274	3.200565	-1.206485	H	-1.261758	1.575508	-0.791467	C	-1.241576	1.673233	-0.771107
H	-2.608395	4.144014	-2.244214	H	-1.399824	0.916794	1.593853	C	-1.825035	2.929521	-1.980700
H	-3.283101	2.612058	-2.818265	H	-3.130200	1.184717	1.575955	C	-1.102878	4.018570	-1.510116
O	-0.006933	0.225652	-1.545988	O	-0.313508	-0.617282	-1.050173	C	0.205684	3.849778	-1.082207
C	-1.280311	0.093632	-1.047786	C	-1.649167	-0.944344	-0.927076	C	0.794531	2.595431	-1.126455
N	-2.108011	1.048868	-0.991057	N	-2.552112	-0.104777	-0.646593	H	-1.812689	0.824174	-2.364502
C	-1.651258	-1.260497	-0.595394	C	-1.966449	-2.359177	-1.196708	H	-2.847702	3.057613	-2.308588
C	-2.594978	-1.413919	0.419449	C	-3.201407	-2.882243	-0.805880	H	-1.563694	4.995849	-1.469193
C	-2.311008	-3.800404	0.344325	C	-2.588919	-5.034273	-1.688088	H	0.766044	4.691797	-0.701497
C	-1.049132	-2.393144	-1.140161	C	-1.051861	-3.192145	-1.840209	H	1.808814	2.454863	-0.777978
C	-1.383736	-3.656085	-0.677540	C	-1.363957	-4.520568	-2.086056	C	1.027549	-0.653966	-3.295478
H	-0.913784	-4.527272	-1.112637	H	-0.645622	-5.153408	-2.588456	C	1.546138	-1.926089	-3.547227
H	-0.318959	-2.284806	-1.925952	H	-0.099731	-2.796029	-2.153506	C	1.717875	-2.367974	-4.847688
C	-2.915494	-2.674373	0.890434	C	-3.506847	-4.209127	-1.047393	C	1.399417	-1.536634	-5.915072
H	-3.050303	-0.530635	0.839911	H	-3.905576	-2.229777	-0.312816	C	0.906495	-0.263478	-5.671246
H	-2.562946	-4.784860	0.714045	H	-2.830395	-6.071458	-1.875869	C	0.718069	0.177755	-4.368353
H	-3.634472	-2.781121	1.690942	H	-4.462828	-4.605076	-0.733508	H	1.816255	-2.568171	-2.719170
Si	1.417901	0.039391	-0.660026	Si	0.856984	-0.815181	0.134439	H	2.115208	-3.356893	-5.030002
C	2.406584	-1.320679	-1.465428	C	2.058213	-2.150265	-0.353517	H	1.544247	-1.877927	-6.930542
C	1.035194	-0.293261	1.127174	C	1.712657	0.827464	0.310207	H	0.664297	0.391379	-6.497089
H	2.118667	1.338721	-0.785510	H	0.173125	-1.211683	1.391155	H	0.331729	1.169716	-4.188264
C	2.205643	-1.654123	-2.807376	C	1.673600	1.780699	-0.709229	C	-0.057413	1.133158	1.900746
C	3.929171	-3.324934	-2.692354	C	3.017924	3.284691	0.596942	C	-1.354881	1.466871	1.524422
C	3.392564	-2.008325	-0.754097	C	2.424212	1.127917	1.474125	C	-1.858765	2.728388	1.804343
C	4.147373	-3.002299	-1.360361	C	3.070262	2.346631	1.619363	C	-1.078459	3.661070	2.471253
H	4.903312	-3.527779	-0.792802	H	3.608544	2.567581	2.530775	C	0.216644	3.332186	2.851566
H	3.569423	-1.772970	0.287355	H	2.467540	0.409089	2.283256	C	0.730106	2.079756	2.559241
C	2.957756	-2.647295	-3.416613	C	2.320752	2.999628	-0.568273	H	-1.965308	0.747064	1.000273
H	1.448000	-1.135492	-3.380295	H	1.119837	1.573441	-1.614645	H	-2.862888	2.983026	1.494924
H	4.515240	-4.100943	-3.165381	H	3.515338	4.238007	0.711005	H	-1.473906	4.643941	2.687160
H	2.786296	-2.894008	-4.455641	H	2.271100	3.731628	-1.362404	H	0.832575	4.057620	3.365009
C	0.856954	-1.588183	1.621922	C	3.186565	-1.856102	-1.123095	H	1.747607	1.832691	2.830867
C	0.246062	-0.715445	3.775192	C	3.795461	-4.179896	-1.181416	C	0.770749	-1.359586	3.074443
C	0.815407	0.785414	1.987739	C	1.824270	-3.481754	0.001126	C	-0.096909	-1.084253	4.129311
C	0.420523	0.576599	3.300682	C	2.683551	-4.489314	-0.409446	C	-0.020646	-1.820661	5.302270
H	0.245964	1.424473	3.948448	H	2.487529	-5.514845	-0.127671	C	0.918590	-2.835668	5.428452
H	0.937875	1.797558	1.629968	H	0.955304	-3.736740	0.593672	C	1.790770	-3.107249	4.382464
C	0.466288	-1.798613	2.934085	C	4.047499	-2.861833	-1.537038	C	1.724549	-2.366667	3.212530
H	1.002172	-2.438869	0.971668	H	3.398107	-0.830247	-1.395638	H	-0.824448	-0.290819	4.033887
H	-0.064748	-0.879675	4.798184	H	4.466894	-4.964682	-1.502071	H	-0.693921	-1.600640	6.119508
H	0.323252	-2.806687	3.298358	H	4.916143	-2.618510	-2.133519	H	0.977684	-3.406856	6.344566
								H	2.533906	-3.885936	4.484064
								H	2.424560	-2.547597	2.407531
								H	4.038368	-0.194548	0.224876

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1•D				1•H				1•H (cont)			
Cu	1.516068	-0.211367	-0.126434	Cu	1.597069	-1.007230	-0.677979	H	2.264694	3.435098	2.531194
C	-1.236214	-1.443912	-1.023626	C	-1.275256	-2.154792	-1.327228	C	3.249175	-0.156937	3.523623
C	-2.040365	-2.259559	-1.815365	C	-2.199407	-2.915039	-2.039985	H	3.280094	-0.579032	1.426402
C	-2.903630	-3.175811	-1.234524	C	-3.056396	-3.782683	-1.381179	H	3.125066	0.538041	5.549801
C	-2.967433	-3.286969	0.147803	C	-2.993386	-3.903206	0.000740	H	3.497326	-1.171982	3.800289
C	-2.159636	-2.490686	0.945349	C	-2.069512	-3.160171	0.718870				
C	-1.288356	-1.568184	0.374779	C	-1.205071	-2.284180	0.069536				
H	-1.975387	-2.186284	-2.891565	H	-2.235992	-2.835500	-3.116832				
H	-3.520238	-3.806360	-1.860249	H	-3.767280	-4.369398	-1.946492				
H	-3.635032	-4.003832	0.605650	H	-3.655375	-4.583865	0.518028				
H	-2.190049	-2.604783	2.018575	H	-2.006277	-3.274366	1.790950				
P	-0.077174	-0.202794	-1.730057	P	-0.108599	-0.994260	-2.150114				
P	-0.133525	-0.543186	1.384976	P	0.065070	-1.306307	0.983099				
C	-1.156515	1.249061	-2.030485	C	-1.100980	0.515389	-2.434880				
C	-2.533262	1.162161	-2.230095	C	-2.487491	0.566970	-2.313289				
C	-3.292702	2.311187	-2.394526	C	-3.163759	1.761707	-2.517111				
C	-2.684821	3.559018	-2.367037	C	-2.463891	2.911178	-2.854525				
C	-1.312699	3.652776	-2.177897	C	-1.083158	2.863788	-2.989932				
C	-0.552801	2.505990	-2.004850	C	-0.405603	1.676895	-2.771787				
H	-3.015660	0.195605	-2.243087	H	-3.040055	-0.325865	-2.059632				
H	-4.361237	2.231582	-2.542744	H	-4.240164	1.792132	-2.414163				
H	-3.278371	4.454239	-2.491271	H	-2.990525	3.843266	-3.005303				
H	-0.834759	4.622491	-2.151421	H	-0.528740	3.759661	-3.227595				
H	0.510938	2.577665	-1.828923	H	0.672187	1.651255	-2.849872				
C	0.256328	-0.861856	-3.402925	C	0.076022	-1.708876	-3.822713				
C	1.249316	-1.837837	-3.499790	C	1.069914	-2.672871	-3.990089				
C	1.551974	-2.401720	-4.728250	C	1.250165	-3.277172	-5.223973				
C	0.886315	-1.981398	-5.873567	C	0.456373	-2.910589	-6.303663				
C	-0.086454	-0.996000	-5.784087	C	-0.520773	-1.937682	-6.145087				
C	-0.404726	-0.438550	-4.552914	C	-0.714119	-1.338651	-4.908168				
H	1.787329	-2.131854	-2.607740	H	1.705909	-2.926005	-3.151737				
H	2.320083	-3.159989	-4.795051	H	2.021957	-4.024362	-5.347294				
H	1.131859	-2.414721	-6.833375	H	0.605948	-3.375174	-7.268554				
H	-0.600268	-0.658901	-6.674197	H	-1.133745	-1.642665	-6.985930				
H	-1.163137	0.328041	-4.489145	H	-1.473198	-0.579105	-4.788760				
C	-1.195948	0.792183	2.042980	C	-0.928059	-0.007735	1.800173				
C	-2.288389	1.261859	1.314616	C	-2.141694	0.421195	1.263671				
C	-2.965961	2.403099	1.714288	C	-2.818036	1.494768	1.822419				
C	-2.574065	3.087408	2.856458	C	-2.297219	2.151395	2.928895				
C	-1.496078	2.619191	3.597477	C	-1.087948	1.730629	3.467069				
C	-0.808380	1.486525	3.192590	C	-0.403099	0.665902	2.905460				
H	-2.606365	0.740254	0.426462	H	-2.558882	-0.081788	0.406056				
H	-3.804050	2.754808	1.128614	H	-3.755573	1.816491	1.389779				
H	-3.103893	3.976462	3.168710	H	-2.824741	2.988768	3.364062				
H	-1.187842	3.139314	4.494392	H	-0.663806	2.240540	4.320609				
H	0.030541	1.135536	3.776298	H	0.541188	0.360790	3.326448				
C	0.210871	-1.592858	2.845306	C	0.555780	-2.418059	2.353817				
C	-0.638261	-1.694569	3.946603	C	-0.111312	-2.487822	3.574907				
C	-0.314160	-2.534071	5.001614	C	0.333730	-3.351932	4.564523				
C	0.855818	-3.281802	4.963194	C	1.440966	-4.159004	4.339970				
C	1.704801	-3.181827	3.869475	C	2.104494	-4.096972	3.121762				
C	1.389459	-2.336486	2.816069	C	1.670015	-3.226427	2.134315				
H	-1.546380	-1.110116	3.984646	H	-0.968054	-1.856816	3.760464				
H	-0.975911	-2.605735	5.854189	H	-0.185651	-3.394853	5.512296				
H	1.106874	-3.935383	5.787341	H	1.787350	-4.830569	5.113594				
H	2.620611	-3.756014	3.839392	H	2.970845	-4.719085	2.943162				
H	2.050367	-2.233516	1.964194	H	2.199592	-3.145013	1.193165				
H	2.814751	-1.093191	-0.153717	H	2.941406	-1.803613	-0.716225				
O	2.231015	1.985487	-0.133609	Si	2.564463	1.928410	-0.000197				
C	3.662236	2.064819	-0.234215	H	2.016318	0.753840	-0.768621				
C	4.307311	1.686589	1.075065	H	3.861639	2.265530	-0.641877				
O	3.833232	2.514536	2.137352	C	2.767635	1.475007	1.802003				
C	2.419517	2.405658	2.238360	C	1.404173	3.374645	-0.218212				
C	1.753322	2.801261	0.944356	C	1.777462	4.501544	-0.954253				
H	3.937597	3.084570	-0.521552	C	-0.371704	5.509082	-0.573702				
H	3.945744	1.370186	-1.019792	C	0.119650	3.337862	0.330550				
H	5.385608	1.826035	1.025235	C	-0.759136	4.394033	0.157173				
H	4.089904	0.635551	1.285990	H	-1.749369	4.339034	0.587014				
H	2.103770	3.060974	3.047926	H	-0.201352	2.476369	0.894977				
H	2.141956	1.375454	2.488569	C	0.897742	5.560959	-1.132288				
H	1.965019	3.851068	0.716946	H	2.766829	4.556519	-1.390306				
H	0.678222	2.654781	0.990387	H	-1.057749	6.334123	-0.710987				
				H	1.205033	6.428101	-1.701516				
				C	3.127505	0.179305	2.183448				
				C	3.033383	0.801795	4.504832				
				C	2.558231	2.429137	2.800286				
				C	2.694576	2.098161	4.140876				
				H	2.525162	2.848339	4.901744				

1dim				1dim (cont)				1•A			
Cu	-1.148842	0.099741	-0.392290	H	7.332286	-1.569245	-2.549150	Cu	1.408229	-0.015141	0.734289
C	-3.992026	-1.236859	-0.868692	H	6.294776	-3.791850	-2.856830	C	-1.703172	-0.654310	-0.211911
C	-4.887137	-2.056485	-1.546117	H	3.848123	-4.052080	-2.617840	C	-2.738741	-1.114547	-1.019893
C	-5.599444	-3.034026	-0.864016	H	2.445728	-2.090048	-2.061584	C	-3.823879	-1.776440	-0.464764
C	-5.426596	-3.193295	0.504093	C	3.021649	1.839958	-2.922782	C	-3.886922	-1.973272	0.908226
C	-4.537082	-2.378425	1.191105	C	2.177643	2.947119	-2.811717	C	-2.866211	-1.508492	1.724426
C	-3.813571	-1.401221	0.516649	C	2.131283	3.892215	-3.822477	C	-1.766722	-0.854625	1.175693
H	-5.008290	-1.946840	-2.614629	C	2.906536	3.732816	-4.965034	H	-2.682824	-0.982311	-2.090681
H	-6.284205	-3.674607	-1.402832	C	3.728545	2.622454	-5.089778	H	-4.616186	-2.141277	-1.103693
H	-5.976655	-3.957748	1.035650	C	3.789654	1.679156	-4.072692	H	-4.729517	-2.492115	1.344125
H	-4.389946	-2.513399	2.253272	H	1.547844	3.047415	-1.937358	H	-2.915704	-1.663748	2.792277
P	-2.978546	0.070707	-1.681106	H	1.476486	4.747581	-3.726911	P	-0.212065	0.207332	-0.862524
P	-2.547749	-0.336019	1.310269	H	2.861128	4.466209	-5.758329	P	-0.359884	-0.222710	2.178925
C	-4.083183	1.526666	-1.541353	H	4.325918	2.487541	-5.981341	C	-0.784027	1.918602	-1.153195
C	-5.463530	1.455587	-1.718731	H	4.429965	0.816033	-4.178054	C	-1.904583	2.220014	-1.925210
C	-6.251768	2.579813	-1.529217	C	3.491274	-1.820867	1.289906	C	-2.326767	3.533326	-2.052669
C	-5.668896	3.782177	-1.150798	C	4.880658	-1.874494	1.235748	C	-1.637401	4.552087	-1.404928
C	-4.296264	3.857010	-0.964797	C	5.529920	-3.095530	1.119461	C	-0.520693	4.254898	-0.638389
C	-3.505522	2.734645	-1.158751	C	4.800305	-4.273689	1.073059	C	-0.089278	2.942116	-0.514391
H	-5.925083	0.516113	-1.986989	C	3.412521	-4.227064	1.126237	H	-2.448656	1.431153	-2.424109
H	-7.323082	2.515122	-1.664253	C	2.761955	-3.008532	1.217935	H	-3.197258	3.763404	-2.651924
H	-6.286378	4.654999	-0.988057	H	5.454799	-0.960520	1.265997	H	-1.974915	5.575348	-1.498291
H	-3.840984	4.785819	-0.650594	H	6.609247	-3.123390	1.058837	H	0.013305	5.042767	-0.126045
H	-2.439083	2.772982	-0.980541	H	5.308501	-5.223732	0.981113	H	0.772459	2.690889	0.089854
C	-3.007748	-0.411262	-3.441334	H	2.836308	-5.140958	1.073926	C	0.034804	-0.535654	-2.500566
C	-2.163177	-1.460444	-3.810663	H	1.681897	-2.968201	1.198451	C	0.009900	-1.927322	-2.625784
C	-2.111732	-1.882855	-5.128205	C	2.048664	-0.097841	3.087852	C	0.378674	-2.532800	-3.815839
C	-2.882375	-1.249651	-6.096205	C	2.694439	-0.747447	4.136872	C	0.797802	-1.760841	-4.890599
C	-3.704894	-0.191749	-5.737782	C	2.222312	-0.609161	5.434038	C	0.838934	-0.378382	-4.768827
C	-3.771113	0.226346	-4.415352	C	1.104605	0.173663	5.689994	C	0.465021	0.231986	-3.582908
H	-1.536927	-1.925441	-3.060465	C	0.456489	0.820243	4.646286	H	-0.313496	-2.535796	-1.792562
H	-1.456540	-2.697602	-5.404705	C	0.923122	0.681704	3.350035	H	0.347990	-3.610490	-3.899192
H	-2.832983	-1.573626	-7.126664	H	3.554172	-1.370993	3.936032	H	1.095549	-2.233752	-5.815855
H	-4.298680	0.311867	-6.488602	H	2.723111	-1.120003	6.245489	H	1.172144	0.228426	-5.599156
H	-4.411786	1.052280	-4.144332	H	0.728505	0.265539	6.699569	H	0.509240	1.307594	-3.492497
C	-3.498307	1.098043	1.929911	H	-0.430506	1.407455	4.838604	C	-0.884290	1.493728	2.545364
C	-4.887504	1.170970	1.898095	H	0.406921	1.142287	2.518366	C	-2.167189	1.967528	2.286095
C	-5.537416	2.325150	2.312188	H	-0.001913	-1.141355	-0.743222	C	-2.482603	3.297568	2.523697
C	-4.808715	3.409410	2.776867					C	-1.524584	4.160301	3.034899
C	-3.421121	3.343232	2.810784					C	-0.244536	3.690947	3.300939
C	-2.769804	2.201824	2.375537					C	0.080411	2.368721	3.045397
H	-5.460912	0.332305	1.532383					H	-2.917187	1.304340	1.881990
H	-6.616507	2.377258	2.264801					H	-3.477037	3.659823	2.301981
H	-5.317410	4.308065	3.097719					H	-1.771066	5.197504	3.216585
H	-2.845549	4.191253	3.156526					H	0.509983	4.361741	3.688501
H	-1.689637	2.172683	2.345176					H	1.090473	2.015641	3.193017
C	-2.061579	-1.229510	2.824823					C	-0.567517	-1.101788	3.768755
C	-2.712318	-1.090030	4.048155					C	-0.080558	-2.407041	3.850645
C	-2.245461	-1.769949	5.163690					C	-0.217315	-3.131476	5.023563
C	-1.128097	-2.588105	5.065121					C	-0.819900	-2.553371	6.133941
C	-0.475043	-2.727122	3.847894					C	-1.291147	-1.250185	6.062735
C	-0.936410	-2.047370	2.733316					C	-1.169935	-0.526266	4.884748
H	-3.571790	-0.439667	4.129542					H	0.406253	-2.851715	2.993777
H	-2.750107	-1.654506	6.113542					H	0.159539	-4.143549	5.075509
H	-0.756115	-3.103050	5.940104					H	-0.916073	-3.115334	7.052575
H	0.411693	-3.341020	3.774447					H	-1.757649	-0.794478	6.925514
H	-0.416325	-2.108750	1.786734					H	-1.542841	0.485910	4.832115
H	0.003938	1.349515	-0.184028					H	2.392699	1.184297	1.048398
Cu	1.150556	0.076438	-0.392499					O	2.850521	-3.431182	-1.260047
C	3.994448	1.485761	-0.240040					C	2.816494	-2.078874	-1.062640
C	4.891603	2.515461	-0.498389					N	2.213477	-1.751602	0.042451
C	5.600154	3.106977	0.539056					O	1.814113	-3.003738	0.630366
C	5.421469	2.666338	1.843232					C	2.201687	-4.012451	-0.191358
C	4.529866	1.636834	2.112305					C	3.421627	-1.214356	-2.042681
C	3.810080	1.042366	1.081868					O	2.019482	-5.177272	-0.030565
H	5.017301	2.872951	-1.510723					C	3.524213	0.163718	-1.819104
H	6.286551	3.915762	0.328607					C	4.557328	0.429356	-3.976665
H	5.968598	3.129714	2.652824					C	3.902095	-1.761199	-3.238157
H	4.378188	1.304980	3.129621					C	4.463891	-0.938094	-4.196665
P	2.985577	0.651870	-1.537611					H	4.825605	-1.366050	-5.120802
P	2.541963	-0.258666	1.338752					H	3.825033	-2.822490	-3.413808
C	4.090982	-0.725146	-2.029012					C	4.092600	0.971471	-2.784836
C	5.471988	-0.586357	-2.153246					H	3.156833	0.589975	-0.892320
C	6.260480	-1.684448	-2.459181					H	4.992419	1.069733	-4.731484
C	5.677162	-2.932644	-2.633442					H	4.169500	2.034294	-2.603843
C	4.303839	-3.078519	-2.502986								
C	3.512862	-1.980211	-2.201870								
H	5.933775	0.377201	-1.992270								

S13

1•Sa				1•Sb				2a			
Cu	1.888343	-0.629160	0.289998	Cu	1.593185	-0.017689	-0.542432	Cu	1.482935	-0.567382	-0.245607
C	-0.843612	-1.915232	-0.638686	C	-1.184257	-1.226326	-1.450618	C	-1.417213	-1.567137	-1.128735
C	-1.539563	-2.809834	-1.442059	C	-1.946090	-2.043893	-2.277782	C	-2.319402	-2.268402	-1.922293
C	-2.282768	-3.834040	-0.871024	C	-2.763777	-3.023995	-1.733082	C	-3.253414	-3.115064	-1.343400
C	-2.338735	-3.966444	0.509322	C	-2.828584	-3.189343	-0.356332	C	-3.293586	-3.267615	0.036581
C	-1.638996	-3.083756	1.320733	C	-2.069657	-2.379459	0.476446	C	-2.397216	-2.576249	0.837998
C	-0.884014	-2.061689	0.757449	C	-1.243574	-1.397964	-0.059181	C	-1.456103	-1.723538	0.268960
H	-1.483936	-2.717363	-2.517397	H	-1.880735	-1.930566	-3.350449	H	-2.276805	-2.165818	-2.997158
H	-2.815231	-4.529690	-1.505033	H	-3.345590	-3.661352	-2.384754	H	-3.947075	-3.658702	-1.969849
H	-2.916374	-4.764066	0.955721	H	-3.462278	-3.955015	0.069546	H	-4.019358	-3.929422	0.488551
H	-1.662527	-3.202425	2.394413	H	-2.106055	-2.518722	1.547268	H	-2.418098	-2.706366	1.910454
P	0.147291	-0.507055	-1.277585	P	-0.069570	0.094013	-2.077114	P	-0.151465	-0.411768	-1.795310
P	0.166614	-0.926368	1.744740	P	-0.160983	-0.333092	0.972013	P	-0.205174	-0.806044	1.245602
C	-1.150198	0.788128	-1.393471	C	-1.213618	1.528139	-2.157484	C	-1.026680	1.192178	-1.815827
C	-2.420958	0.529140	-1.907121	C	-2.517735	1.425565	-2.639910	C	-2.348429	1.131900	-2.241467
C	-3.383848	1.525387	-1.927348	C	-3.362273	2.523873	-2.613725	C	-2.982988	2.544846	-2.197480
C	-3.088524	2.790129	-1.432759	C	-2.915621	3.734544	-2.099386	C	-2.306270	3.660084	-1.719755
C	-1.828496	3.051093	-0.917386	C	-1.621281	3.842962	-1.614111	C	-0.993867	3.541151	-1.287409
C	-0.865397	2.054100	-0.894526	C	-0.775581	2.744313	-1.642310	C	-0.354761	2.311814	-1.332946
H	-2.661433	-0.453607	-2.285286	H	-2.877652	0.482323	-3.024348	H	-2.883368	0.445868	-2.599271
H	-4.367204	1.314251	-2.325545	H	-4.373680	2.433290	-2.986224	H	-4.009490	2.632709	-2.526532
H	-3.842951	3.565065	-1.444051	H	-3.579811	4.587240	-2.068154	H	-2.807029	4.617386	-1.674491
H	-1.590417	4.027353	-0.519816	H	-1.273927	4.777777	-1.197017	H	-0.467624	4.399514	-0.894783
H	0.102887	2.254863	-0.470302	H	0.221115	2.812427	-1.234152	H	0.657166	2.216846	-0.965999
C	0.506332	-0.948316	-3.009135	C	0.224010	-0.378803	-3.814547	C	-0.003855	-0.907301	-3.545701
C	1.310214	-2.067372	-3.239688	C	0.990152	-1.525126	-4.038961	C	0.552944	-2.159993	-3.812336
C	1.682124	-2.403418	-4.530502	C	1.279870	-1.925267	-5.332300	C	0.733175	-2.582580	-5.118032
C	1.280314	-1.615825	-5.603311	C	0.830629	-1.177436	-6.414600	C	0.385371	-1.749836	-5.217267
C	0.502901	-0.489695	-5.375815	C	0.088139	-0.026851	-6.194900	C	-0.146236	-0.495420	-5.916271
C	0.113435	-0.156349	-4.085503	C	-0.218535	0.371701	-4.900469	C	-0.343890	-0.074133	-4.608012
H	1.650011	-2.657215	-2.399070	H	1.363103	-2.085598	-3.192272	H	0.844934	-2.801568	-2.991185
H	2.297232	-3.276629	-4.699829	H	1.868559	-2.817295	-5.497017	H	1.159174	-3.557107	-5.312746
H	1.579369	-1.875156	-6.609467	H	1.065705	-1.487277	-7.423464	H	0.536411	-2.075866	-7.194822
H	0.192204	0.131313	-6.205107	H	-0.258138	0.563646	-7.032198	H	-0.412036	0.160045	-6.734261
H	-0.494692	0.719401	-3.915415	H	-0.799748	1.267102	-4.738030	H	-0.760954	0.902829	-4.415054
H	-0.940178	0.471215	2.148653	C	-1.274958	1.027787	1.474399	H	-0.993313	0.787320	1.647539
C	-2.304341	0.466913	1.870631	C	-2.559153	1.182401	0.956762	C	-2.345324	1.045514	1.436840
C	-3.071391	1.595902	2.116801	C	-3.309997	2.307939	1.262010	C	-2.860204	2.305030	1.704369
C	-2.488358	2.733326	2.654819	C	-2.798062	3.286593	2.100214	C	-2.035804	3.307938	2.194958
C	-1.128678	2.743145	2.939845	C	-1.523185	3.135381	2.631933	C	-0.686855	3.053437	2.404663
C	-0.357505	1.623687	2.676120	C	-0.764512	2.021852	3.125232	C	-0.162715	1.803899	2.119426
H	-2.761986	-0.411591	1.441441	H	-2.969058	0.429213	0.302250	H	-2.989649	0.270405	1.048905
H	-4.125544	1.588418	1.877238	H	-4.298865	2.418277	0.839097	H	-3.907328	2.504185	1.522679
H	-3.087728	3.613609	2.841598	H	-3.385700	4.162531	2.337656	H	-2.441211	4.289476	2.398891
H	-0.666730	3.630050	3.351617	H	-1.116109	3.891306	3.289805	H	-0.030804	3.833845	2.763761
H	0.706911	1.642251	2.868260	H	0.228770	1.913416	2.724499	H	0.897014	1.626828	2.236927
C	0.380091	-1.809185	3.328817	C	0.087434	-1.311506	2.492584	C	-0.141584	-1.708630	2.830026
C	-0.384091	-1.542296	4.461906	C	-0.652217	-1.129435	3.658428	C	-0.835129	-1.301089	3.966663
C	-0.166502	-2.257353	5.631590	C	-0.389546	-1.908060	4.776772	C	-0.735850	-2.033244	5.141481
C	0.806625	-3.245848	5.674568	C	0.602900	-2.877422	4.734544	C	0.049116	-3.176810	5.187965
C	1.570124	-3.514621	4.544946	C	1.339385	-3.061509	3.571656	C	0.744078	-3.585815	4.056416
C	1.365988	-2.795321	3.378631	C	1.090868	-2.279186	2.456712	C	0.657499	-2.850824	2.885537
H	-1.145553	-0.776644	4.429844	H	-1.428479	-0.379116	3.693618	H	-1.446220	-0.411003	3.932739
H	-0.761354	-2.043610	6.509174	H	-0.965759	-1.760163	5.680219	H	-1.273701	-1.709206	6.021915
H	0.973266	-3.802463	6.586489	H	0.806073	-3.482852	5.607336	H	0.126144	-3.744053	6.105094
H	2.332902	-4.280494	4.576272	H	2.124748	-3.803661	3.538615	H	1.366127	-4.469413	4.091683
H	1.965147	-2.985585	2.497737	H	1.680090	-2.393658	1.557162	H	1.217566	-3.152152	2.010148
H	2.288103	-2.127299	0.034257	H	2.019425	-1.517331	-0.756918	H	3.505790	-1.696733	1.805253
C	2.145776	3.050817	-2.621752	C	3.197245	0.345936	3.898615	C	3.371547	2.510477	2.260173
C	1.749029	4.276853	-2.097498	C	3.985747	-0.781219	4.077347	C	3.188592	3.548770	1.355475
C	1.802878	4.474184	-0.725568	C	4.585698	-1.373374	2.973139	C	3.153218	3.246100	-0.003806
C	2.237732	3.457154	0.109890	C	4.383807	-0.853737	1.707531	C	3.277061	1.940802	-0.439755
C	2.635002	2.215475	-0.400488	C	3.586730	0.278023	1.508452	C	3.432758	0.859524	0.459481
C	2.585787	2.038638	-1.790627	C	3.007917	0.872698	2.632562	C	3.485688	1.198098	1.828884
H	2.100049	2.878277	-3.688419	H	2.727430	0.817899	4.750759	H	3.424899	2.724419	3.320649
H	1.398626	5.063252	-2.750947	H	4.127533	-1.196252	5.065253	H	3.104373	4.571374	1.696153
H	1.499847	5.422058	-0.301176	H	5.204012	-2.252007	3.099088	H	3.039722	4.040948	-0.730771
H	2.266721	3.618281	1.179755	H	4.822915	-1.338981	0.846355	H	3.258312	1.725964	-1.501540
C	3.077628	1.171780	0.514633	C	3.392511	0.792359	0.151962	C	3.468923	-0.519096	-0.028273
C	3.814058	0.054175	0.168937	C	2.558433	1.830628	-0.211850	C	4.066570	-1.571554	0.878799
H	3.010080	1.423356	1.565766	H	4.106573	0.434958	-0.577664	H	3.904623	-0.561650	-1.025966
H	2.857264	1.085474	-2.219747	H	2.417102	1.768867	2.515993	H	3.624676	0.415688	2.560850
H	4.158595	-0.104444	-0.841787	H	1.990077	2.389401	0.516068	H	4.068691	-2.542376	0.385092
H	4.342312	-0.501056	0.927632	H	2.686459	2.304157	-1.173448	H	5.102981	-1.348249	1.164530

2b				2a•A				2a•A (cont)			
Cu	1.545579	-0.494612	-0.584926	Cu	0.588518	-0.261149	-0.290115	O	1.756841	2.250501	-1.254768
C	-1.456358	-1.427595	-1.522022	C	-2.278906	-1.390328	-1.176952	C	2.918234	2.957969	-1.208654
C	-2.400460	-2.062612	-2.323853	C	-3.143392	-2.132012	-1.975993	C	3.027941	1.339684	1.965703
C	-3.378419	-2.864911	-1.755360	C	-4.004031	-3.060074	-1.408542	O	3.332981	3.695573	-2.043729
C	-3.424703	-3.037082	-0.377290	C	-4.010435	-3.250740	-0.033180	C	2.181047	0.458817	2.647041
C	-2.491392	-2.407424	0.431985	C	-3.160405	-2.510258	0.775171	C	3.713879	0.398545	4.494945
C	-1.504545	-1.600661	-0.127126	C	-2.289473	-1.580495	0.215398	C	4.216009	1.761031	2.575271
H	-2.356408	-1.944504	-3.396956	H	-3.133993	-1.986907	-3.046389	C	4.550658	1.288264	3.830232
H	-4.103330	-3.358273	-2.388140	H	-4.667576	-3.634454	-2.039897	H	5.472984	1.611409	4.291956
H	-4.185090	-3.665206	0.065853	H	-4.678389	-3.975367	0.411644	H	4.876302	2.434451	2.051717
H	-2.520321	-2.547496	1.503044	H	-3.163550	-2.665079	1.844288	C	2.528516	-0.012693	3.897570
P	-0.111603	-0.349545	-2.163859	P	-1.104106	-0.154276	-1.858455	H	1.274106	0.121368	2.174035
P	-0.207913	-0.755517	0.855278	P	-1.144784	-0.531605	1.191535	H	3.985213	0.028780	5.473814
C	-0.872913	1.311875	-2.141282	C	-2.099585	1.373155	-1.981848	H	1.868335	-0.701359	4.404563
C	-2.175580	1.544965	-2.576977	C	-3.448347	1.428150	-1.639681				
C	-2.724150	2.814123	-2.486925	C	-4.126233	2.637572	-1.663272				
C	-1.980687	3.856980	-1.949443	C	-3.472554	3.799843	-2.044563				
C	-0.685732	3.629519	-1.507876	C	-2.129147	3.750775	-2.393719				
C	-0.131795	2.362667	-1.606033	C	-1.442156	2.548917	-2.349333				
H	-2.762941	0.731334	-2.978202	H	-3.966209	0.530375	-1.338915				
H	-3.736594	2.988070	-2.825134	H	-5.168873	2.669771	-1.378991				
H	-2.415041	4.843636	-1.866292	H	-4.004246	4.741104	-2.062460				
H	-0.110184	4.433813	-1.072513	H	-1.609608	4.652620	-2.686937				
H	0.870208	2.175834	-1.243975	H	-0.390224	2.522795	-2.592539				
C	-0.011313	-0.805140	-3.927968	C	-0.891733	-0.699967	-3.589717				
C	0.386241	-2.107736	-4.239066	C	-0.233581	-1.911974	-3.809113				
C	0.544708	-2.496837	-5.557908	C	-0.009762	-2.364870	-5.098154				
C	0.334408	-1.584517	-6.585209	C	-0.425986	-1.607847	-6.186224				
C	-0.037574	-0.283259	-6.282116	C	-1.076381	-0.401103	-5.974752				
C	-0.211876	0.106918	-4.961337	C	-1.313261	0.051176	-4.684023				
H	0.569043	-2.817480	-3.442902	H	0.095776	-2.503703	-2.967361				
H	0.845759	-3.510104	-5.785688	H	0.500100	-3.305430	-5.253931				
H	0.468136	-1.886009	-7.614670	H	-0.242068	-1.957101	-7.192595				
H	-0.196800	0.433738	-7.075881	H	-1.407316	0.191400	-6.816640				
H	-0.504802	1.121333	-4.735455	H	-1.828933	0.986845	-4.529746				
C	-0.949317	0.840769	1.327198	C	-2.170148	0.953172	1.520911				
C	-2.255008	1.198995	1.002389	C	-3.492913	0.856989	1.949210				
C	-2.730029	2.461293	1.324737	C	-4.248244	2.002025	2.142266				
C	-1.913091	3.369097	1.983553	C	-3.690376	3.252098	1.904477				
C	-0.611521	3.013242	2.312451	C	-2.375053	3.353001	1.477796				
C	-0.124865	1.761034	1.976607	C	-1.617030	2.207671	1.284629				
H	-2.894337	0.499203	0.485670	H	-3.933426	-0.113633	2.126385				
H	-3.740457	2.736150	1.055401	H	-5.275575	1.920153	2.470330				
H	-2.287396	4.352371	2.233603	H	-4.284574	4.144601	2.043740				
H	0.036390	3.713436	2.821234	H	-1.941731	4.322400	1.276749				
H	0.892911	1.499314	2.217831	H	-0.602526	2.279094	0.921968				
C	-0.150365	-1.712053	2.408265	C	-1.033175	-1.343172	2.824339				
C	-0.790269	-1.308994	3.576685	C	-1.234293	-0.635346	4.008570				
C	-0.665518	-2.063269	4.734685	C	-0.997433	-1.239274	5.235442				
C	0.093827	-3.224891	4.733942	C	-0.559203	-2.554111	5.296387				
C	0.732361	-3.632461	3.568882	C	-0.351278	-3.263628	4.119636				
C	0.617039	-2.876499	2.414127	C	-0.576726	-2.661213	2.893556				
H	-1.372682	-0.399588	3.583637	H	-1.573311	0.388919	3.972411				
H	-1.160156	-1.740066	5.640403	H	-1.157724	-0.678022	6.145710				
H	0.194669	-3.807661	5.638953	H	-0.375406	-3.022658	6.253073				
H	1.332463	-4.531866	3.565576	H	-0.003535	-4.286679	4.156771				
H	1.138871	-3.175261	1.514191	H	-0.394340	-3.214076	1.984270				
H	3.887659	1.644687	-0.230721	C	5.459528	-0.055937	-0.319376				
C	2.643746	-0.026833	3.762719	C	5.614884	0.555176	-1.552600				
C	2.650326	1.230681	4.349073	C	4.598126	0.421265	-2.497946				
C	3.114732	2.317557	3.619285	C	3.459256	-0.301396	-2.206255				
C	3.561307	2.141314	2.317258	C	3.273800	-0.930975	-0.957699				
C	3.561193	0.884321	1.711222	C	4.310094	-0.775786	-0.021631				
C	3.092146	-0.193701	2.459737	H	6.235167	0.034640	0.430592				
H	2.272018	-0.880260	4.312488	H	6.504603	1.124948	-1.780522				
H	2.292389	1.364302	5.360855	H	4.698418	0.892088	-3.466991				
H	3.121467	3.305091	4.062210	H	2.677162	-0.391998	-2.950274				
H	3.915529	2.995997	1.753706	C	2.046076	-1.663730	-0.675451				
C	4.073982	0.711770	0.306932	C	2.116623	-2.748362	0.380334				
C	3.509746	-0.462652	-0.488989	H	1.665396	-2.079590	-1.606962				
H	5.170782	0.648947	0.379187	H	4.219838	-1.236261	0.951257				
H	3.063536	-1.173222	2.009604	H	1.196175	-3.330309	0.382172				
H	3.936591	-0.424487	-1.494480	H	2.941726	-3.450012	0.202698				
H	3.873773	-1.404090	-0.063882	H	2.243050	-2.361136	1.389439				
				O	3.499249	2.688264	0.009993				
				C	2.687764	1.799324	0.649401				
				N	1.618893	1.509380	-0.042502				

3a'				3a' (cont)				3a			
Cu	1.047945	0.365043	-0.692818	C	3.309991	1.049923	2.053720	Cu	0.962863	0.095177	-0.530661
C	-2.052247	-0.582734	-1.406001	C	2.932447	-0.286522	2.132177	C	-1.952266	-1.186452	-1.263180
C	-3.024104	-1.200702	-2.186120	C	4.347459	-0.604279	4.046728	C	-2.811300	-1.948975	-2.047655
C	-3.921191	-2.090597	-1.612578	C	4.218724	1.550815	2.985400	C	-3.532664	-2.992027	-1.483187
C	-3.856025	-2.363138	-0.252913	C	4.739844	0.727138	3.969881	C	-3.399308	-3.278541	-0.131306
C	-2.899226	-1.741129	0.536218	H	5.448622	1.123993	4.684427	C	-2.568857	-2.503450	0.666099
C	-1.992122	-0.849187	-0.025260	H	4.493720	2.593635	2.925724	C	-1.853188	-1.447707	0.115147
H	-3.066825	-0.998020	-3.246350	C	3.438545	-1.107699	3.126793	H	-2.896925	-1.745331	-3.104730
H	-4.666662	-2.573498	-2.228830	H	2.224037	-0.678982	1.421635	H	-4.188289	-3.587477	-2.103014
H	-4.550542	-3.060395	0.194777	H	4.745730	-1.243614	4.823322	H	-3.945138	-4.104109	0.304011
H	-2.842620	-1.962464	1.592094	H	3.111159	-2.135996	3.185740	H	-2.462877	-2.724205	1.718540
P	-0.768530	0.520196	-2.101785					P	-0.844240	0.108397	-1.935730
P	-0.679426	0.006315	0.924513					P	-0.758531	-0.330767	1.067170
C	-1.383990	2.215117	-1.832976					C	-1.738519	1.685550	-1.807084
C	-2.730586	2.489916	-1.613448					C	-3.127031	1.745345	-1.730016
C	-3.142723	3.794030	-1.387680					C	-3.759733	2.972748	-1.619153
C	-2.216590	4.827391	-1.391297					C	-3.012073	4.142425	-1.597995
C	-0.873306	4.555328	-1.610057					C	-1.628033	4.083232	-1.673464
C	-0.452678	3.252440	-1.818835					C	-0.985757	2.858341	-1.764389
H	-3.450856	1.684999	-1.597534					H	-3.708721	0.835101	-1.734040
H	-4.186349	4.000485	-1.195889					H	-4.837120	3.015678	-1.541441
H	-2.539583	5.842121	-1.204612					H	-3.508969	5.098459	-1.507496
H	-0.143686	5.351990	-1.584336					H	-1.041482	4.990198	-1.632992
H	0.601160	3.036403	-1.920397					H	0.092344	2.807985	-1.755156
C	-0.871580	0.284806	-3.911548					C	-0.743241	-0.231134	-3.724948
C	-0.324060	-0.865940	-4.481674					C	-0.376808	-1.502737	-4.173437
C	-0.371661	-1.061753	-5.852318					C	-0.206442	-1.747363	-5.526385
C	-0.950200	-0.103715	-6.673999					C	-0.386889	-0.726010	-6.448982
C	-1.483725	1.048984	-6.116030					C	-0.744106	0.540742	-6.010046
C	-1.446461	1.244626	-4.743142					C	-0.922185	0.789567	-4.657434
H	0.139959	-1.615306	-3.858552					H	-0.242803	-2.311177	-3.470782
H	0.055046	-1.958491	-6.279349					H	0.072179	-2.737636	-5.858444
H	-0.979302	-0.253080	-7.744140					H	-0.248478	-0.916834	-7.503818
H	-1.932670	1.801031	-6.749874					H	-0.890912	1.340449	-6.722560
H	-1.862716	2.144806	-4.317404					H	-1.205599	1.777050	-4.326250
C	-1.489846	1.539269	1.498852					C	-1.901197	1.016771	1.532160
C	-2.823367	1.550216	1.904572					C	-3.263164	0.807946	1.742341
C	-3.398574	2.721529	2.368626					C	-4.082716	1.866201	2.102693
C	-2.645352	3.887394	2.433838					C	-3.549145	3.139345	2.249226
C	-1.318576	3.877591	2.031796					C	-2.195787	3.351364	2.028258
C	-0.737242	2.709264	1.560041					C	-1.369444	2.298104	1.667505
H	-3.412541	0.646116	1.853464					H	-3.687697	-0.176762	1.609858
H	-4.434797	2.725663	2.678631					H	-5.139213	1.697706	2.262008
H	-3.095521	4.801602	2.796035					H	-4.190134	3.965965	2.523754
H	-0.725584	4.779866	2.073861					H	-1.779881	4.344976	2.120777
H	0.290747	2.719863	1.232254					H	-0.324809	2.468541	1.444559
C	-0.455867	-0.970143	2.444213					C	-0.381211	-1.205865	2.615363
C	-0.458391	-0.368536	3.700721					C	-1.223874	-1.177542	3.726080
C	-0.145549	-1.114119	4.827688					C	-0.890211	-1.891923	4.866577
C	0.163958	-2.461405	4.713583					C	0.285600	-2.630585	4.906462
C	0.171992	-3.061923	3.460839					C	1.132522	-2.644813	3.807314
C	-0.123509	-2.320088	2.330647					C	0.809912	-1.927791	2.665859
H	-0.693536	0.680370	3.797925					H	-2.130313	-0.590659	3.705120
H	-0.142730	-0.636938	5.797732					H	-1.544734	-1.865370	5.727040
H	0.410339	-3.037852	5.594403					H	0.545439	-3.183802	5.798665
H	0.426283	-4.107720	3.357100					H	2.056599	-3.204347	3.836091
H	-0.084177	-2.787635	1.359637					H	1.489448	-1.902248	1.830115
C	2.416914	-4.176939	0.516477					C	3.316317	-3.780179	0.823413
C	1.224715	-4.770223	0.121866					C	2.236482	-4.652447	0.822179
C	0.403602	-4.099102	-0.779220					C	1.138719	-4.373971	0.013970
C	0.776233	-2.865106	-1.273943					C	1.134180	-3.247884	-0.784664
C	1.990432	-2.250880	-0.908149					C	2.219557	-2.353240	-0.805367
C	2.795238	-2.943938	0.014651					C	3.310552	-2.644589	0.029199
H	3.065728	-4.684419	1.217755					H	4.172261	-3.983012	1.453465
H	0.936559	-5.736839	0.510584					H	2.242803	-5.532923	1.449552
H	-0.535188	-4.536697	-1.090742					H	0.284188	-5.037133	0.010827
H	0.111978	-2.354425	-1.953133					H	0.265076	-3.033734	-1.391024
C	2.400584	-0.985900	-1.500432					C	2.177104	-1.170185	-1.647328
C	3.844509	-0.582571	-1.434300					C	3.442979	-0.466697	-2.027868
H	1.991573	-0.857247	-2.499305					H	1.525774	-1.311068	-2.501452
H	3.734812	-2.516431	0.325406					H	4.149762	-1.969407	0.054826
H	3.991296	0.385553	-1.901374					H	3.230919	0.388376	-2.665900
H	4.470848	-1.315049	-1.956160					H	4.104636	-1.139474	-2.584799
H	4.213734	-0.499812	-0.416570					H	3.983161	-0.104043	-1.158787
O	2.754212	3.240486	1.262829					O	1.457997	2.171230	0.069986
C	2.738715	1.988667	1.044923					C	2.350877	1.544916	0.798070
N	2.203199	1.614202	-0.083024					N	2.443946	0.255433	0.708367

3a (cont)				4a				4a (cont)			
C	3.213241	2.320831	1.724881	Cu	1.020331	-0.019945	-0.202682	C	2.969820	-2.124089	-1.287749
C	4.126878	1.683617	2.564664	C	-1.792960	-1.119667	-1.154674	C	1.869437	-2.676876	-0.633683
C	4.810442	3.808270	3.462383	C	-2.617691	-1.872849	-1.983643	C	1.689953	-4.404328	-2.292470
C	3.107749	3.709092	1.766616	C	-3.504586	-2.793139	-1.444627	C	3.435783	-2.749736	-2.441856
C	3.902815	4.448526	2.629976	C	-3.579975	-2.962975	-0.068121	C	2.798919	-3.874551	-2.943284
H	3.815535	5.526826	2.653128	C	-2.760996	-2.219757	0.768972	H	3.168417	-4.343869	-3.845343
H	2.397752	4.190498	1.110140	C	-1.859532	-1.299904	0.240772	H	4.310673	-2.341019	-2.925141
C	4.919051	2.422453	3.426955	H	-2.548911	-1.751582	-3.054985	C	1.228433	-3.803927	-1.129153
H	4.199710	0.606189	2.530073	H	-4.135278	-3.378155	-2.099495	H	1.542487	-2.240185	0.300301
H	5.430572	4.384403	4.135960	H	-4.271608	-3.678604	0.354050	H	1.195361	-5.282341	-2.684790
H	5.624074	1.919602	4.075541	H	-2.809341	-2.362913	1.838686	H	0.374458	-4.213839	-0.606235
				P	-0.585518	0.110271	-1.784615				
				P	-0.675591	-0.355947	1.270910				
				C	-1.534978	1.670696	-1.752721				
				C	-2.872293	1.729482	-2.139401				
				C	-3.558592	2.932132	-2.094121				
				C	-2.918245	4.082332	-1.651590				
				C	-1.589536	4.027552	-1.257758				
				C	-0.899325	2.826435	-1.309312				
				H	-3.377639	0.833090	-2.468908				
				H	-4.596717	2.970685	-2.394392				
				H	-3.457790	5.018107	-1.606295				
				H	-1.091851	4.916374	-0.897236				
				H	0.129986	2.776828	-0.983806				
				C	-0.405321	-0.291947	-3.553871				
				C	0.276421	-1.466580	-3.873922				
				C	0.482238	-1.813694	-5.197739				
				C	0.030511	-0.984224	-6.216806				
				C	-0.630366	0.194521	-5.902599				
				C	-0.849976	0.542615	-4.576862				
				H	0.649143	-2.106588	-3.090161				
				H	1.012579	-2.726596	-5.428820				
				H	0.201501	-1.250967	-7.250421				
				H	-0.976626	0.849239	-6.690464				
				H	-1.362332	1.463313	-4.342656				
				C	-1.501216	1.221660	1.654070				
				C	-2.851736	1.451987	1.411784				
				C	-3.404288	2.691919	1.694994				
				C	-2.618448	3.700313	2.235264				
				C	-1.271693	3.470444	2.482657				
				C	-0.708918	2.241621	2.180421				
				H	-3.464968	0.670458	0.988445				
				H	-4.450296	2.871140	1.488869				
				H	-3.053862	4.665112	2.456000				
				H	-0.650043	4.251293	2.898149				
				H	0.342029	2.073954	2.355722				
				C	-0.648265	-1.246830	2.863983				
				C	-1.177517	-0.705065	4.032449				
				C	-1.058142	-1.386861	5.235091				
				C	-0.414365	-2.614756	5.283564				
				C	0.110992	-3.163013	4.119770				
				C	0.000935	-2.481362	2.919549				
				H	-1.672532	0.253551	4.005224				
				H	-1.469478	-0.954334	6.136702				
				H	-0.317600	-3.141231	6.222604				
				H	0.618284	-4.117133	4.149303				
				H	0.425359	-2.910613	2.023234				
				C	2.518859	2.947394	3.645833				
				C	2.125378	1.892648	4.455717				
				C	2.212822	0.594783	3.968303				
				C	2.685648	0.362338	2.687226				
				C	3.082759	1.411841	1.855683				
				C	2.987210	2.708479	2.359068				
				H	2.456590	3.963909	4.011616				
				H	1.752025	2.078483	5.453394				
				H	1.902217	-0.238404	4.582903				
				H	2.748808	-0.646787	2.309721				
				C	3.636490	1.104289	0.480261				
				C	3.617263	2.280048	-0.486899				
				H	4.684428	0.816380	0.608581				
				H	3.279997	3.548274	1.747002				
				H	2.602700	2.654924	-0.627114				
				H	4.246037	3.103831	-0.152467				
				H	3.993481	1.944732	-1.448793				
				O	4.933002	-0.845696	-0.944232				
				C	3.705407	-0.921272	-0.756673				
				N	2.941766	-0.035327	-0.098263				

4a'				4a' (cont)				5a			
Cu	0.694577	-0.378973	-0.320109	C	3.599890	2.239539	1.082289	Cu	0.500969	-0.071709	-0.470062
C	-2.361958	-1.157403	-1.092166	C	4.823619	2.190416	1.749740	C	-2.460523	-1.218577	-1.180300
C	-3.420930	-1.664045	-1.840954	C	4.416035	4.355025	2.721488	C	-3.401129	-1.904326	-1.942534
C	-4.481524	-2.305390	-1.220402	C	2.795065	3.365665	1.245590	C	-4.257499	-2.813914	-1.338667
C	-4.500062	-2.431865	0.162357	C	3.201989	4.418440	2.052070	C	-4.188873	-3.036229	0.030494
C	-3.451727	-1.931507	0.918630	H	2.572001	5.292641	2.157029	C	-3.267908	-2.342186	0.801478
C	-2.367907	-1.306433	0.306193	H	1.852358	3.404210	0.722683	C	-2.403340	-1.432078	0.204184
H	-3.407605	-1.566387	-2.916759	C	5.224334	3.234755	2.566727	H	-3.451899	-1.745813	-3.009556
H	-5.294452	-2.699407	-1.814378	H	5.447462	1.320875	1.608786	H	-4.976275	-3.352824	-1.939939
H	-5.330382	-2.920593	0.652856	H	4.732785	5.172077	3.355797	H	-4.853326	-3.749307	0.497802
H	-3.468549	-2.035007	1.993219	H	6.173205	3.178865	3.083726	H	-3.211181	-2.508626	1.867449
P	-0.963067	-0.232862	-1.836557					P	-1.290941	0.023837	-1.855603
P	-0.934822	-0.647797	1.247455					P	-1.186762	-0.439081	1.141924
C	-1.593422	1.482936	-1.905707					C	-2.243770	1.580442	-1.829767
C	-2.891433	1.778827	-2.317426					C	-3.534120	1.629545	-2.357946
C	-3.339315	3.089678	-2.315893					C	-4.259539	2.807039	-2.301690
C	-2.495726	4.112304	-1.899501					C	-3.702956	3.939310	-1.717182
C	-1.203266	3.820481	-1.491168					C	-2.420639	3.890131	-1.194370
C	-0.747455	2.509876	-1.492395					C	-1.684140	2.714341	-1.247194
H	-3.555618	0.985830	-2.628901					H	-3.973641	0.750396	-2.806813
H	-4.348959	3.313648	-2.632215					H	-5.260379	2.841796	-2.709730
H	-2.850100	5.133902	-1.889216					H	-4.274775	4.855724	-1.666546
H	-0.546854	4.611268	-1.156481					H	-1.986999	4.762211	-0.726527
H	0.251951	2.280644	-1.150894					H	-0.696706	2.673372	-0.809597
C	-0.913867	-0.793694	-3.567691					C	-1.115533	-0.376367	-3.621796
C	-0.814287	-2.160991	-3.836230					C	-0.905332	-1.693972	-4.029735
C	-0.659074	-2.610929	-5.136526					C	-0.647892	-1.981194	-5.360175
C	-0.581913	-1.702796	-6.185262					C	-0.580249	-0.956901	-6.295087
C	-0.666434	-0.342879	-5.923469					C	-0.772902	0.356932	-5.892824
C	-0.831275	0.112525	-4.623426					C	-1.037893	0.649059	-4.563461
H	-0.873375	-2.872679	-3.025042					H	-0.952281	-2.497200	-3.309112
H	-0.591806	-3.672273	-5.332091					H	-0.494087	-3.006495	-5.666116
H	-0.453567	-2.054195	-7.199301					H	-0.372912	-1.182052	-7.331620
H	-0.606547	0.369648	-6.734486					H	-0.717616	1.159384	-6.614881
H	-0.899357	1.172502	-4.428353					H	-1.190205	1.673403	-4.256728
C	-1.415336	1.076695	1.621321					C	-2.127210	1.015719	1.692622
C	-2.710378	1.555110	1.443221					C	-3.450808	1.232593	1.315073
C	-3.001745	2.885834	1.700324					C	-4.087162	2.413390	1.663385
C	-2.009434	3.741912	2.156726					C	-3.410910	3.383414	2.389065
C	-0.717539	3.268172	2.338696					C	-2.093819	3.167940	2.772206
C	-0.414795	1.946268	2.054840					C	-1.450947	1.992002	2.425146
H	-3.486171	0.895600	1.084556					H	-3.980299	0.491626	0.736200
H	-4.005520	3.254185	1.540292					H	-5.109907	2.578426	1.354626
H	-2.239935	4.779028	2.358197					H	-3.905917	4.309007	2.648455
H	0.066011	3.930076	2.678796					H	-1.550778	3.922081	3.322971
H	0.604299	1.599131	2.136924					H	-0.422474	1.845479	2.716272
C	-1.039951	-1.499294	2.862108					C	-0.825906	-1.414032	2.628892
C	-1.035810	-0.800256	4.067118					C	-1.342764	-1.085867	3.879899
C	-1.018501	-1.485760	5.273595					C	-1.017380	-1.856344	4.986515
C	-1.012843	-2.872730	5.292937					C	-0.176928	-2.952082	4.851383
C	-1.021356	-3.575174	4.094245					C	0.335559	-3.282908	3.604026
C	-1.025979	-2.894874	2.888688					C	0.017413	-2.518053	2.494653
H	-1.050770	0.279018	4.065269					H	-1.990194	-0.229235	3.989926
H	-1.016713	-0.930503	6.201421					H	-1.416183	-1.593599	5.956447
H	-1.000611	-3.403802	6.234397					H	0.086499	-3.541988	5.718142
H	-1.018515	-4.656707	4.099124					H	1.006268	-4.123525	3.498400
H	-1.022866	-3.445766	1.960797					H	0.451756	-2.744529	1.533488
C	1.063029	-3.618340	-0.704742					C	5.212615	0.891144	-0.702304
C	1.252960	-4.003592	0.611220					C	5.139584	2.237917	-1.037731
C	2.118676	-3.278668	1.423861					C	4.035291	2.715002	-1.734690
C	2.819546	-2.201072	0.911245					C	3.010909	1.855849	-2.076052
C	2.679593	-1.824114	-0.430508					C	3.058335	0.495124	-1.735593
C	1.767982	-2.533815	-1.225095					C	4.190513	0.028291	-1.049774
H	0.382739	-4.170934	-1.338770					H	6.066268	0.515314	-0.155300
H	0.725739	-4.860421	1.007110					H	5.934521	2.912862	-0.752553
H	2.245721	-3.558434	2.460350					H	3.966266	3.763529	-1.988491
H	3.502299	-1.637840	1.530268					H	2.133422	2.236405	-2.580689
C	3.604810	-0.790129	-1.050448					C	1.942203	-0.362671	-2.059743
C	4.837254	-1.498322	-1.610074					C	2.131111	-1.841351	-2.125456
H	3.061365	-0.342314	-1.893169					H	1.335419	0.040391	-2.861589
H	1.670639	-2.279914	-2.272377					H	4.250822	-1.009150	-0.762716
H	5.488512	-0.770088	-2.088114					H	1.222411	-2.343521	-2.445116
H	4.562643	-2.260908	-2.338126					H	2.918487	-2.095551	-2.841988
H	5.394155	-1.971423	-0.803460					H	2.417817	-2.244969	-1.156810
O	1.893503	1.148577	-0.138526					O	2.055713	1.123031	1.981257
C	3.148286	1.113527	0.210364					C	2.306482	-0.163978	1.586674
N	4.036375	0.233591	-0.128236					N	1.814342	-0.848916	0.646449

5a (cont)				4a•H				4a•H (cont)			
O	0.951351	1.910082	0.085533	Cu	0.906830	-0.704929	0.143078	N	2.711396	-1.460377	0.302036
C	1.499737	2.221919	1.168657	C	-1.960851	-1.757905	-0.771561	C	2.249693	-3.506942	-0.954819
C	3.313099	-0.786243	2.498677	C	-2.840175	-2.474150	-1.577435	C	0.910124	-3.648706	-0.611953
O	1.638878	3.294301	1.721511	C	-3.752354	-3.357487	-1.023665	C	0.584020	-5.287671	-2.333650
C	3.665294	-2.125761	2.329354	C	-3.794355	-3.538949	0.351968	C	2.751719	-4.299863	-1.987413
C	5.196040	-1.990546	4.178077	C	-2.922019	-2.835611	1.166273	C	1.924952	-5.168601	-2.680112
C	3.920214	-0.056687	3.520088	C	-2.002910	-1.939232	0.621895	H	2.326966	-5.761332	-3.491149
C	4.854386	-0.657588	4.351905	H	-2.793736	-2.362235	-2.649252	H	3.801945	-4.218668	-2.224713
H	5.317864	-0.078206	5.139089	H	-4.420447	-3.912869	-1.667160	C	0.080799	-4.532494	-1.285757
H	3.656256	0.980057	3.651519	H	-4.498667	-4.232558	0.789782	H	0.511137	-3.062209	0.199085
C	4.597067	-2.722868	3.159650	H	-2.938589	-2.994361	2.234371	H	-0.059043	-5.971930	-2.870274
H	3.196074	-2.683153	1.532692	P	-0.733159	-0.572894	-1.478248	H	-0.954756	-4.625409	-0.992318
H	5.925671	-2.455685	4.827141	P	-0.781744	-1.048697	1.672480	Si	1.571491	2.707030	-0.191771
H	4.860882	-3.761957	3.012762	C	-1.808660	0.889874	-1.774250	H	1.226852	1.316441	0.271349
				C	-2.939764	1.121475	-0.993814	H	2.921086	3.051254	0.306298
				C	-3.750358	2.220628	-1.231684	C	0.412869	3.985561	0.517689
				C	-3.450582	3.100169	-2.262064	C	1.576038	2.683961	-2.058937
				C	-2.322774	2.879353	-3.040846	C	1.970711	1.534483	-2.747949
				C	-1.502504	1.789449	-2.796518	C	1.608285	2.629656	-4.856155
				H	-3.200283	0.437893	-0.204396	C	1.210712	3.809776	-2.799697
				H	-4.620529	2.382345	-0.610643	C	1.227051	3.785103	-4.186326
				H	-4.086109	3.953477	-2.453715	H	0.935646	4.664116	-4.745535
				H	-2.068304	3.561225	-3.839658	H	0.889601	4.707922	-2.289129
				H	-0.636488	1.631755	-3.416256	C	1.983177	1.504574	-4.134660
				C	-0.427607	-1.162662	-3.185874	H	2.249544	0.645462	-2.199196
				C	0.796353	-1.768456	-3.449204	H	1.611773	2.605070	-5.937263
				C	1.089175	-2.241057	-4.718658	H	2.266474	0.598233	-4.649650
				C	0.166873	-2.096615	-5.744212	C	0.871929	4.892578	-4.176350
				C	-1.051345	-1.476986	-5.494547	C	-1.296416	5.923307	1.594736
				C	-1.349446	-1.013340	-4.222987	C	-0.919869	4.070014	0.112704
				H	1.520176	-1.872298	-2.658083	C	-1.767205	5.028456	0.643634
				H	2.039592	-2.722255	-4.898765	H	-2.797395	5.070027	0.317982
				H	0.396291	-2.459233	-6.736695	H	-1.302737	3.379174	-0.619919
				H	-1.771325	-1.353875	-6.292017	C	0.025430	5.852855	2.013035
				H	-2.290251	-0.514157	-4.045139	H	1.901611	4.850296	1.806746
				C	-1.659573	0.429956	2.281940	H	-1.956497	6.672954	2.009918
				C	-3.046193	0.497164	2.404660	H	0.398151	6.548769	2.752594
				C	-3.646033	1.639202	2.912456				
				C	-2.864859	2.715054	3.314149				
				C	-1.483937	2.645106	3.209458				
				C	-0.881663	1.512316	2.686841				
				H	-3.656137	-0.343265	2.105469				
				H	-4.723197	1.687311	2.997866				
				H	-3.331997	3.608632	3.704037				
				H	-0.872620	3.484768	3.503439				
				H	0.193122	1.465470	2.602620				
				C	-0.710451	-2.119459	3.158985				
				C	-1.307993	-1.763931	4.365773				
				C	-1.198665	-2.592808	5.473621				
				C	-0.492333	-3.783575	5.389886				
				C	0.106453	-4.143509	4.189209				
				C	0.002721	-3.316790	3.083097				
				H	-1.848836	-0.833865	4.446831				
				H	-1.664324	-2.302288	6.405386				
				H	-0.403029	-4.425444	6.255055				
				H	0.666785	-5.064920	4.115132				
				H	0.491280	-3.602004	2.163731				
				C	2.813686	1.813181	3.778009				
				C	2.111187	1.004057	4.657580				
				C	1.940988	-0.340767	4.352110				
				C	2.451903	-0.854694	3.172950				
				C	3.153367	-0.053874	2.271313				
				C	3.338758	1.284494	2.604411				
				H	2.964242	2.860173	4.006728				
				H	1.704110	1.413221	5.572142				
				H	1.405012	-0.989102	5.029802				
				H	2.314747	-1.898629	2.937289				
				C	3.734533	-0.698996	1.036203				
				C	4.493931	0.229318	0.104224				
				H	4.466351	-1.430160	1.389593				
				H	3.900331	1.928170	1.947535				
				H	3.849724	0.989456	-0.329619				
				H	5.315807	0.731583	0.613122				
				H	4.914553	-0.362496	-0.702830				
				O	4.396965	-2.953431	-0.188898				
				C	3.204061	-2.592327	-0.239619				

6a				6a (cont)				1•PSa			
Cu	0.262309	0.094637	-0.360447	N	1.717254	-1.248851	0.002930	Cu	0.452776	-0.204539	-0.296936
C	-2.715461	-0.747982	-1.193561	C	2.915339	-2.113080	1.982843	C	-2.714740	-1.087570	-0.901483
C	-3.722275	-1.279549	-1.994229	C	4.005165	-1.751496	2.774462	C	-3.797649	-1.656179	-1.565186
C	-4.780295	-1.974101	-1.428155	C	4.178050	-4.008885	3.582870	C	-4.745240	-2.393241	-0.870358
C	-4.855029	-2.121001	-0.049421	C	2.450782	-3.427108	2.016490	C	-4.625037	-2.558348	0.502672
C	-3.859130	-1.590800	0.756728	C	3.077605	-4.367837	2.816501	C	-3.565912	-1.971114	1.180028
C	-2.772320	-0.923255	0.199422	H	2.699428	-5.380260	2.849541	C	-2.606742	-1.233821	0.492325
H	-3.673087	-1.152157	-3.065665	H	1.576523	-3.700028	1.445642	H	-3.888958	-1.537398	-2.634473
H	-5.551291	-2.389800	-2.062002	C	4.640648	-2.698885	3.559311	H	-5.573082	-2.841847	-1.402235
H	-5.687522	-2.646333	0.397905	H	4.335731	-0.723121	2.767090	H	-5.356647	-3.139309	1.047684
H	-3.923701	-1.704616	1.828809	H	4.668195	-4.745009	4.205288	H	-3.474783	-2.099508	2.248832
P	-1.324212	0.233787	-1.896676	H	5.492412	-2.414815	4.161754	P	-1.359935	-0.178614	-1.754627
P	-1.385218	-0.240529	1.201147	Si	2.414993	1.698682	1.003214	P	-1.179571	-0.394387	1.303449
C	-2.002588	1.936935	-1.907576	H	1.008820	1.478242	0.123339	C	-1.975906	1.548934	-1.785024
C	-3.351557	2.216722	-1.709027	H	3.681762	1.707265	1.852896	C	-3.306935	1.880388	-1.552346
C	-3.790981	3.530917	-1.639536	C	3.305147	2.132663	-0.625061	C	-3.711519	3.206622	-1.578651
C	-2.890572	4.576811	-1.776618	C	1.537174	3.134921	1.859068	C	-2.795526	4.210339	-1.858789
C	-1.544390	4.304507	-1.983600	C	4.578142	2.704212	-0.558731	C	-1.466848	3.884468	-2.095638
C	-1.101120	2.993599	-2.040079	C	4.662693	2.935205	-2.950943	C	-1.053701	2.562589	-2.043068
H	-4.058223	1.410076	-1.586449	C	2.742049	1.962549	-1.887780	H	-4.025116	1.105195	-1.331442
H	-4.838341	3.735938	-1.466240	C	3.406921	2.350128	-3.042029	H	-4.744096	3.455547	-1.375513
H	-3.233770	5.600157	-1.713705	H	2.950388	2.191941	-4.010811	H	-3.113357	5.243949	-1.879540
H	-0.833797	5.113383	-2.081413	H	1.768917	1.492757	-1.962842	H	-0.744521	4.663469	-2.299082
H	-0.047332	2.789169	-2.157370	C	5.246684	3.114875	-1.703431	H	-0.009901	2.308433	-2.159019
C	-1.308607	-0.255951	-3.657698	H	5.048121	2.829035	0.408992	C	-1.550823	-0.677640	-3.513183
C	-0.797612	-1.515461	-3.975863	H	5.186261	3.243350	-3.846313	C	-1.490376	-2.033082	-3.844906
C	-0.742748	-1.933354	-5.294595	H	6.227643	3.565555	-1.625946	C	-1.528294	-2.437703	-5.168344
C	-1.176403	-1.093075	-6.312926	C	1.335138	3.146213	3.238544	C	-1.611745	-1.497670	-6.187469
C	-1.673967	0.164568	-6.002687	C	0.285474	5.305684	3.118509	C	-1.663341	-0.148706	-5.867359
C	-1.745359	0.582595	-4.680732	C	1.092529	4.234761	1.123446	C	-1.636345	0.260581	-4.541556
H	-0.451194	-2.169601	-3.191160	C	0.492387	5.319479	1.744849	H	-1.422325	-2.774643	-3.067241
H	-0.350980	-2.914335	-5.524972	H	0.176011	6.173203	1.158643	H	-1.486754	-3.493327	-5.399161
H	-1.124301	-1.416392	-7.343340	H	1.229837	4.246118	0.049193	H	-1.634614	-1.813743	-7.221317
H	-2.013179	0.823046	-6.790645	C	0.698202	4.210431	3.863265	H	-1.734110	0.592766	-6.651753
H	-2.140595	1.559529	-4.445154	H	1.689659	2.314830	3.836031	H	-1.689882	1.312988	-4.308693
C	-2.158603	1.183410	2.044498	H	-0.196988	6.143125	3.604820	C	-1.943167	1.220286	1.735423
C	-3.015950	1.023603	3.132761	H	0.535491	4.192511	4.933078	C	-3.148313	1.308212	2.429295
C	-3.631132	2.127590	3.699494					C	-3.714794	2.545569	2.689948
C	-3.404236	3.395654	3.177341					C	-3.086883	3.704697	2.249716
C	-2.546572	3.557197	2.100544					C	-1.891911	3.619856	1.551880
C	-1.915623	2.457139	1.541131					C	-1.318328	2.382678	1.298204
H	-3.185934	0.040695	3.548317					H	-3.647210	0.410111	2.763812
H	-4.290007	1.999354	4.547649					H	-4.650384	2.606383	3.229480
H	-3.886297	4.256313	3.620586					H	-3.536325	4.669474	2.442610
H	-2.343434	4.539948	1.704447					H	-1.407981	4.516292	1.190241
H	-1.223575	2.587856	0.725419					H	-0.395753	2.298434	0.740339
C	-1.073492	-1.430905	2.547077					C	-1.015557	-1.256680	2.905283
C	-0.296584	-0.971478	3.615268					C	-0.922169	-0.557087	4.106412
C	0.144426	-1.846739	4.591510					C	-0.636226	-1.224153	5.288598
C	-0.171484	-3.197095	4.517149					C	-0.439056	-2.596527	5.290930
C	-0.937416	-3.662702	3.459649					C	-0.530227	-3.302543	4.097042
C	-1.381743	-2.788676	2.477914					C	-0.806217	-2.638290	2.914620
H	-0.023222	0.071957	3.667944					H	-1.057001	0.512536	4.119389
H	0.754058	-1.476018	5.403436					H	-0.558367	-0.660838	6.207607
H	0.188515	-3.881722	5.271957					H	-0.215094	-3.114082	6.213509
H	-1.185861	-4.712913	3.388575					H	-0.381728	-4.374194	4.086653
H	-1.968035	-3.172858	1.658736					H	-0.861460	-3.200494	1.994170
C	-1.207283	-4.040915	-1.144996					C	-1.456543	-4.512282	-1.045711
C	-0.979790	-4.967201	-2.149950					C	-1.423256	-5.423569	-2.089746
C	0.284973	-5.054869	-2.718801					C	-0.314259	-5.460730	-2.926653
C	1.299960	-4.206603	-2.303932					C	0.739863	-4.583160	-2.728546
C	1.076314	-3.252630	-1.309901					C	0.708580	-3.651613	-1.691957
C	-0.182535	-3.204429	-0.726707					C	-0.394023	-3.641877	-0.848780
H	-2.186654	-3.954541	-0.695316					H	-2.315409	-4.459787	-0.391416
H	-1.775789	-5.616849	-2.486393					H	-2.250340	-6.100992	-2.251061
H	0.480750	-5.783800	-3.493564					H	-0.272296	-6.174158	-3.738618
H	2.274323	-4.290140	-2.763829					H	1.596151	-4.624694	-3.388430
C	2.176041	-2.300249	-0.895150					C	1.874285	-2.703887	-1.504346
C	2.805208	-1.610859	-2.105545					C	2.097384	-1.792442	-2.703882
H	2.955909	-2.888110	-0.405444					H	2.758770	-3.332908	-1.396732
H	-0.357658	-2.484615	0.051795					H	-0.432295	-2.917184	-0.055247
H	2.051257	-1.047644	-2.649520					H	1.242305	-1.142513	-2.856244
H	3.257386	-2.328618	-2.785204					H	2.253771	-2.374916	-3.608166
H	3.572964	-0.916239	-1.778348					H	2.971076	-1.167325	-2.535119
O	2.112082	0.078164	1.800499					O	2.088424	-1.428823	1.850024
C	2.222196	-1.078541	1.187196					C	2.376018	-2.136338	0.741073
								N	1.696282	-1.882470	-0.309973

1•PSa (cont)

C	3.433378	-3.158464	0.903336
C	4.623887	-3.091705	0.181417
C	5.422320	-5.062906	1.302493
C	3.253550	-4.176969	1.838035
C	4.240916	-5.129738	2.028889
H	4.091103	-5.921899	2.749170
H	2.337866	-4.212482	2.411259
C	5.613518	-4.039020	0.384719
H	4.784193	-2.274062	-0.505445
H	6.195896	-5.801916	1.458307
H	6.540253	-3.970176	-0.167318
Si	3.251440	-0.739113	2.875196
H	1.305296	1.147938	-0.336869
H	3.772901	-1.742687	3.836640
C	4.632753	-0.155652	1.776060
C	2.352913	0.579811	3.814184
C	5.965889	-0.425929	2.087907
C	6.684525	0.585747	0.031047
C	4.340689	0.497227	0.573953
C	5.361763	0.860547	-0.291574
H	5.120417	1.359840	-1.220481
H	3.312174	0.703603	0.292323
C	6.986685	-0.056840	1.224361
H	6.211084	-0.950637	3.002940
H	7.478825	0.869474	-0.646485
H	8.015460	-0.275858	1.477070
C	1.632680	1.575559	3.148995
C	1.042150	2.580540	5.254093
C	2.406415	0.606170	5.208562
C	1.756367	1.599186	5.926666
H	1.801992	1.604479	7.007553
H	2.948240	-0.164513	5.742409
C	0.981960	2.567008	3.866655
H	1.558349	1.558174	2.068644
H	0.530390	3.354955	5.809619
H	0.411199	3.320118	3.343992