
Supporting Information

A DFT Study of the Mechanisms of “In Water” Au(I)-Catalyzed Tandem [3,3] Rearrangement/Nazarov Reaction/[1,2]-Hydrogen Shift of Enynyl Acetates: A Proton-Transport Catalysis Strategy in the Water-Catalyzed [1,2]-Hydrogen Shift

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1. Full citation of Ref. 19

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. *Gaussian 03 (Revision C.02)*, Gaussian, Inc., Wallingford CT 2004.

2. Discussion of computational methods

The computed relative energies (activation energies and reaction energies) using MP2 method with larger 6-31+G(d,p)/SDD basis set on the geometries obtained by B3LYP/6-31G(d)/SDD are close to those obtained by B3LYP/6-31G(d)/SDD calculations, as compared by Figures 1 and S1. This demonstrates that DFT method and MP2 methods are both suitable to describe the Au(I)-catalyzed tandem reaction of enynyl acetates. The DFT method has been well applied in mechanistic studies of Au and other transition metal catalyzed reactions (see Ref. 17 of the text). Therefore, in the present study, we applied DFT to study the Au(I) catalyzed reactions.

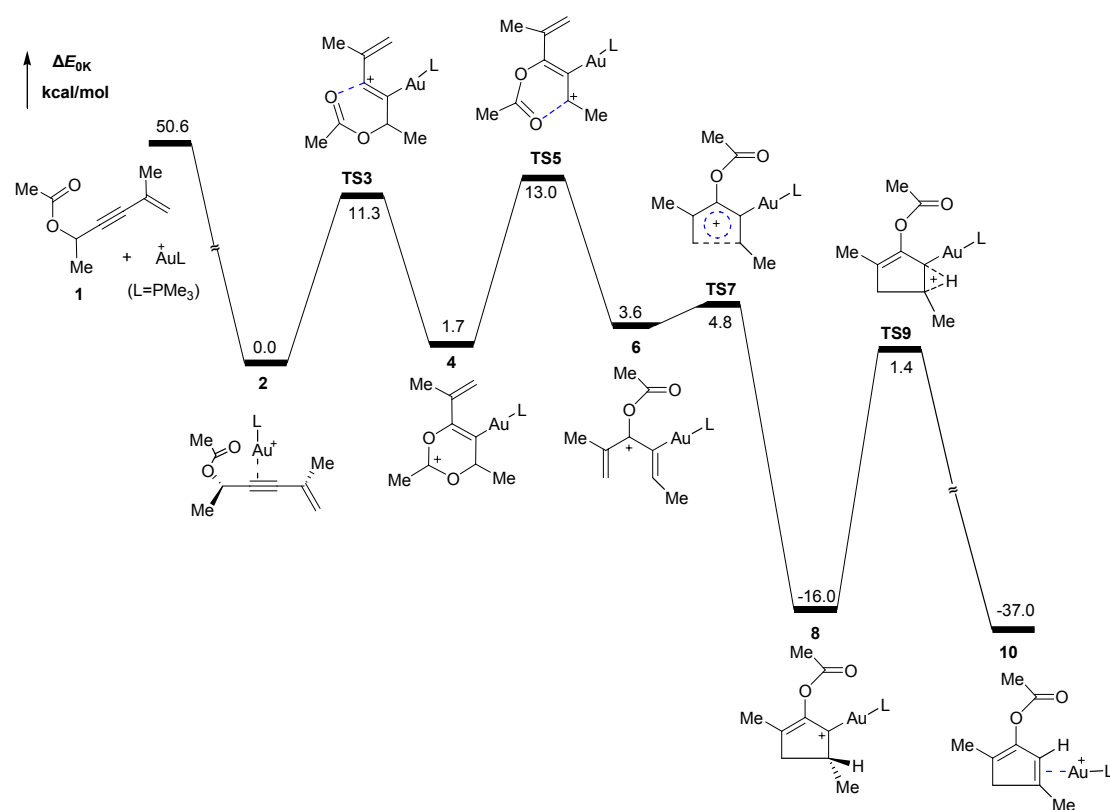


Figure S1. MP2/6-31+G(d,p)/SDD computed energy surface for the Au(I)-catalyzed tandem reaction of enynyl acetate based on the geometries obtained at the B3LYP/6-31G(d)/SDD level.

3. Ligand effects on the titled tandem reactions

We have computed the energy surface of $[\text{AuP}(\text{Ph})_3]^+$ catalyzed tandem reaction of enynyl acetate at the B3LYP/6-31G(d)/SDD level (Figure S2). Comparison of Figures 1 and S2 shows that using $\text{P}(\text{Me})_3$ as the ligand rather than $\text{P}(\text{Ph})_3$ will not change all the computed potential energy surfaces and conclusions in the text of the present paper. The present study present an example that the steric and electronic effects of the phenyls in triphenylphosphine have little effect on the potential energy surface of Au(I) catalyzed reactions.

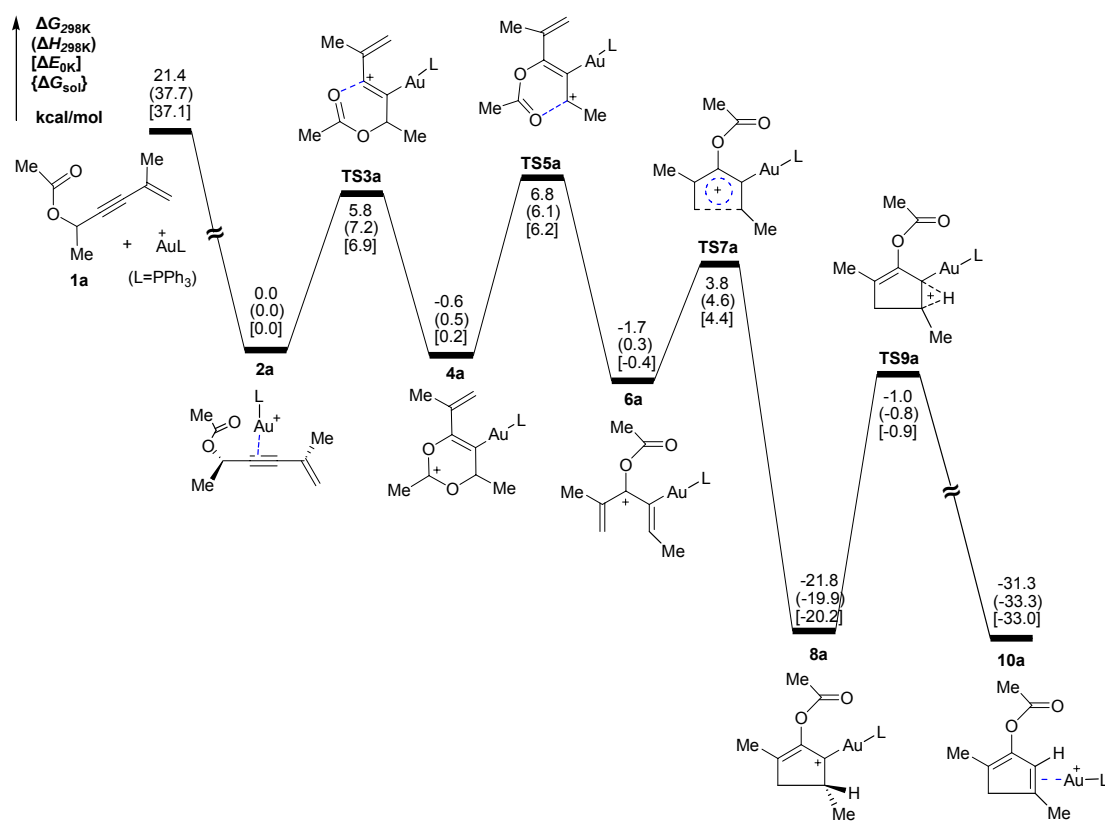


Figure S2. DFT computed energy surfaces for the tandem reaction of enynyl acetate.

4. The effects of water on the titled tandem reactions

We have computed how one water molecule affects the energy surface of the tandem reaction, which is given in Figure S3. Calculations indicate that the effect of water molecule on the [3,3] rearrangement and Nazarov reaction is negligible. It is found that the potential energy surface in the presence of one water molecule is very similar to that without water molecule. Calculations indicated that in wet CH_2Cl_2 , water molecule acts as a ligand coordinated to the Au(I) catalyst, and this coordination does not alter the reaction mechanisms of the tandem [3,3] rearrangement and Nazarov reaction.

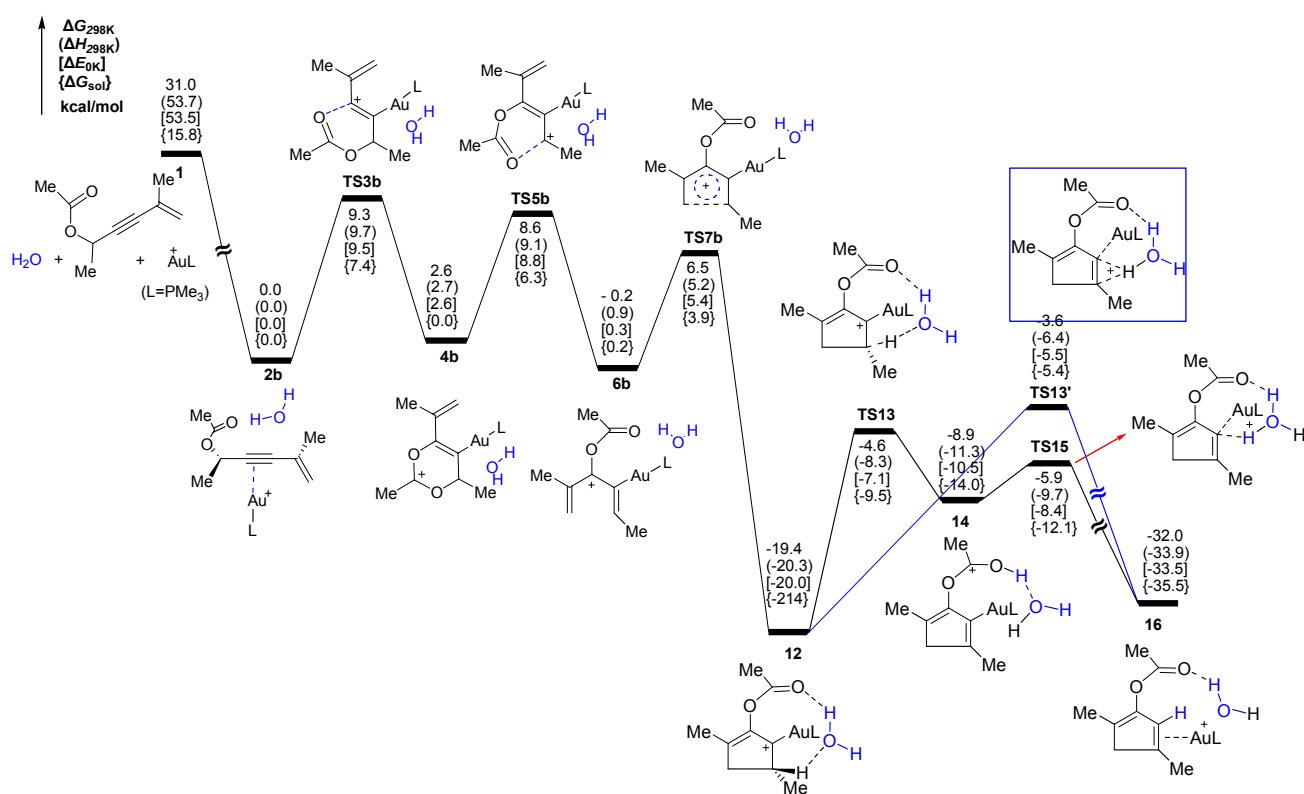


Figure S3. The DFT computed energy surfaces for the tandem reaction of enynyl acetate catalyzed by a single water molecule.

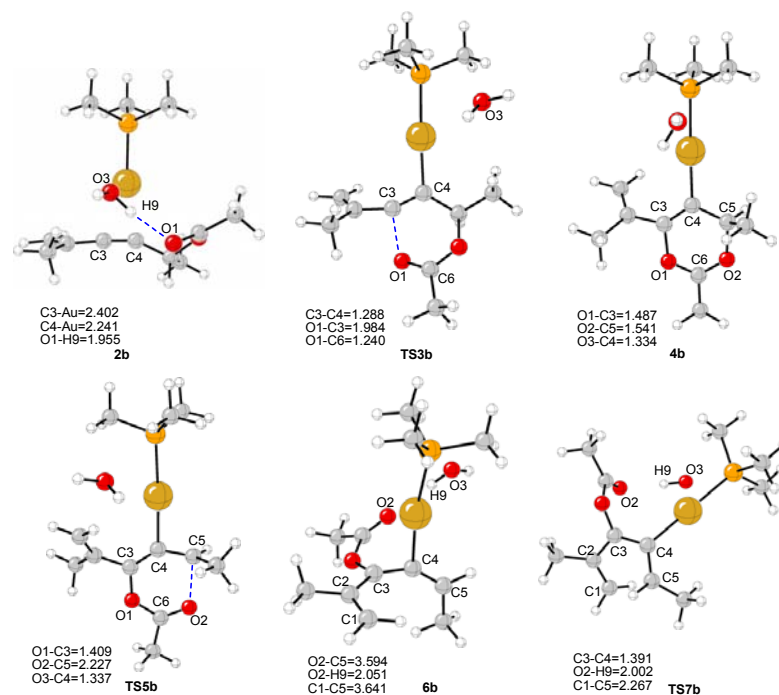


Figure S4. The DFT optimized key structures for the tandem reaction catalyzed by a single water molecule.

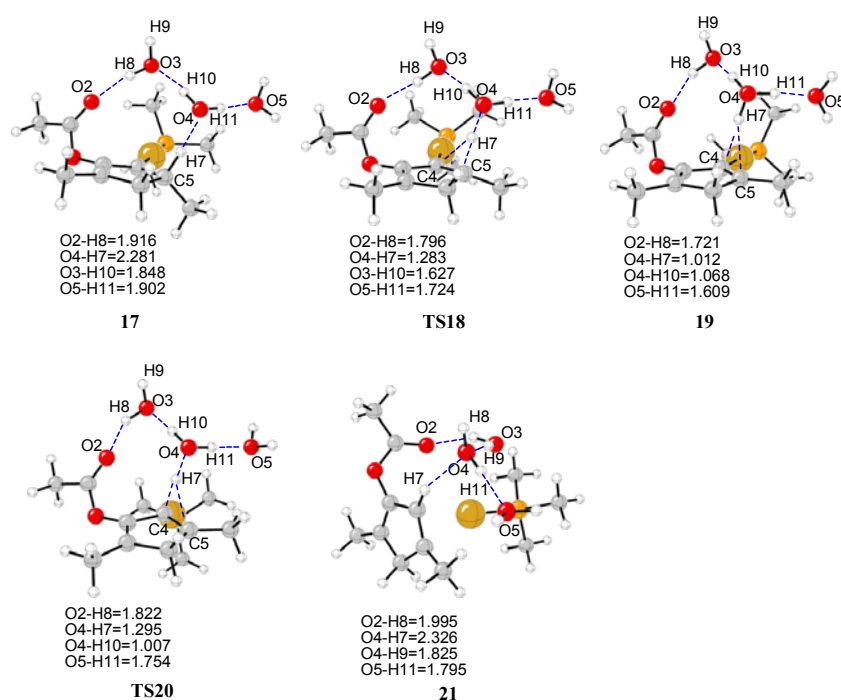


Figure S5. The DFT optimized key structures for the tandem reaction catalyzed by three-water cluster.

5. Discussion of substitute group (-CF₃) and possible autoionization process

The acetoxy group is replaced by a CF₃ group that can form hydrogen bond network with water. The [1,2]-hydride shift is turned to a two-step deprotonation/protonation process with high efficiency (see Figure S6).

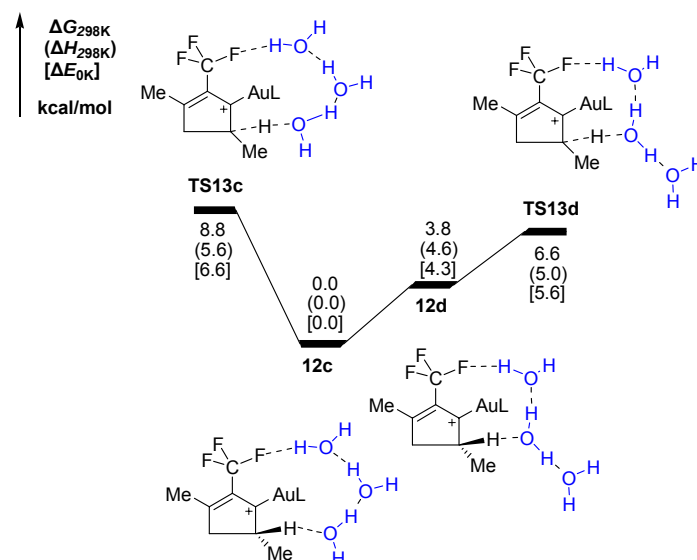
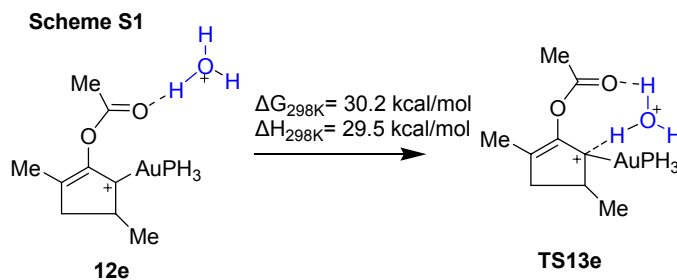


Figure S6. DFT computed energy surface for the three-water cluster catalyzed proton transfer (L=PMe₃).

We also calculated the reaction mechanism that the water molecules first carry out an autoionization process proposed in Scheme S1. Then one hydrogen atom in the hydronium shifts to the C4 atom (see **8** in Figure 2 for atom labeling). Finally, the H7 atom is abstracted by water. The free energy needed for H shift in room temperature is more than 30 kcal/mol, indicating this reaction path is not favorable.



6. The DFT optimized key structures for the four-water cluster catalyzed proton transfer and direct hydride shift of intermediate **22**

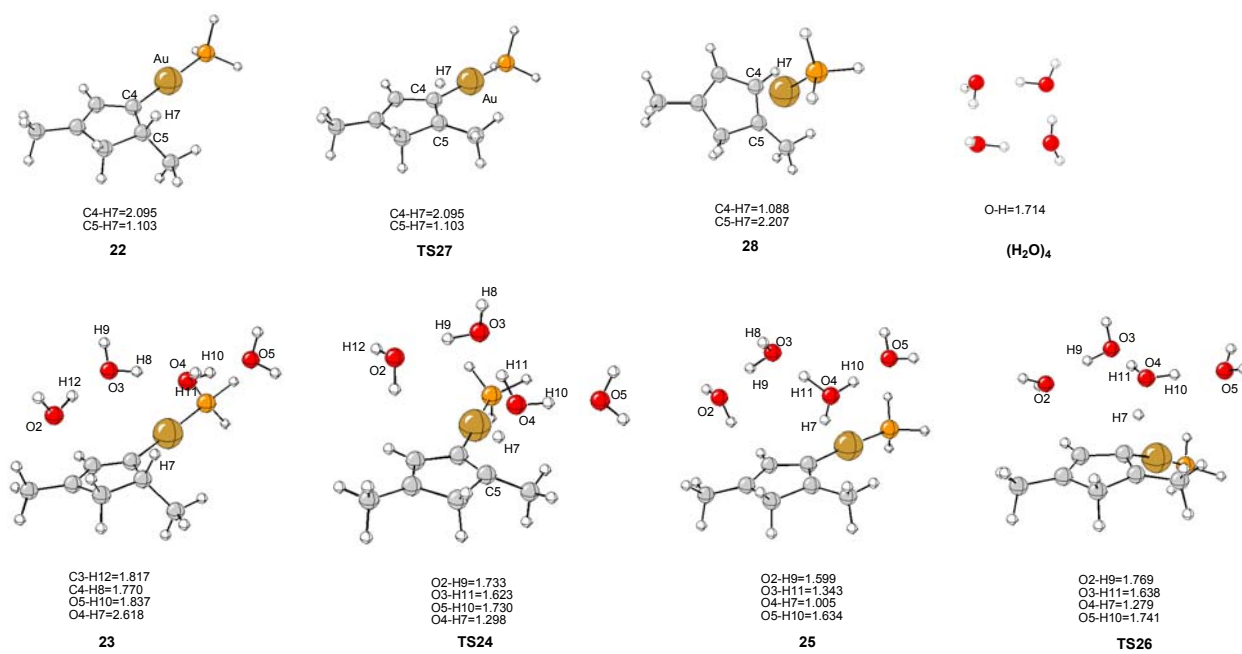
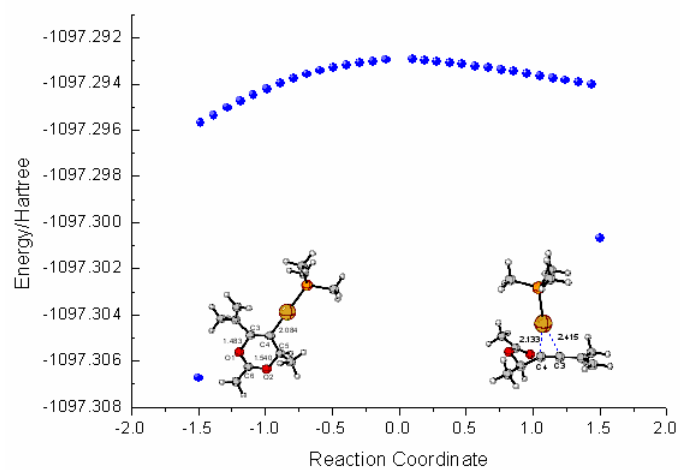


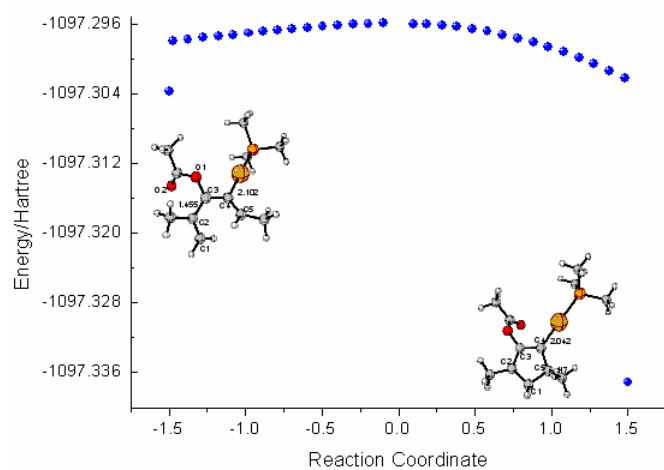
Figure S7. The DFT optimized key structures for the four-water cluster catalyzed proton transfer and direct hydride shift of intermediate **22** (L=PH₃).

7. IRC plots for selected transition states

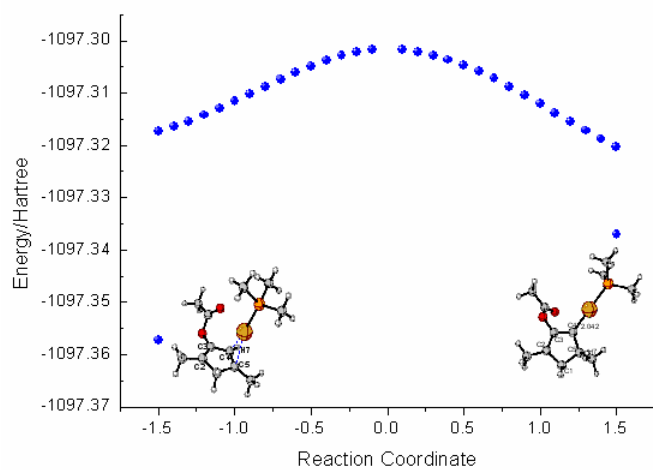
IRC for TS3



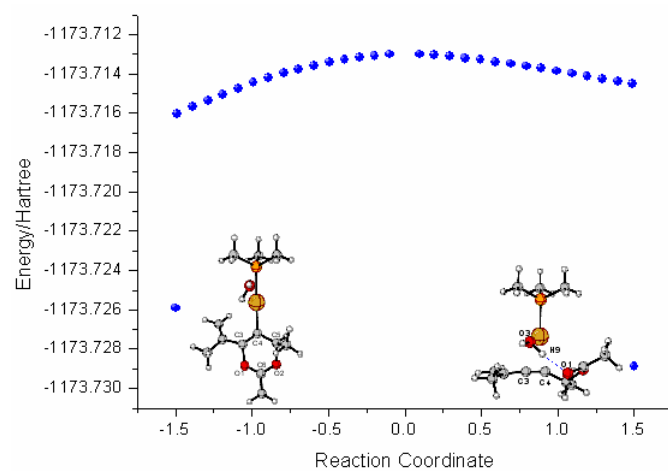
IRC for TS7



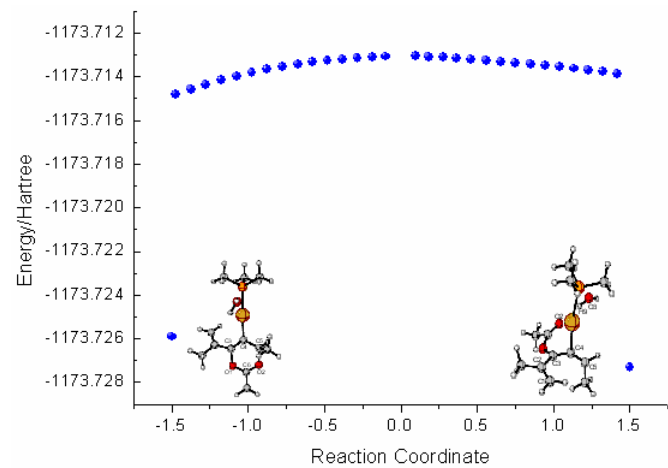
IRC for TS9



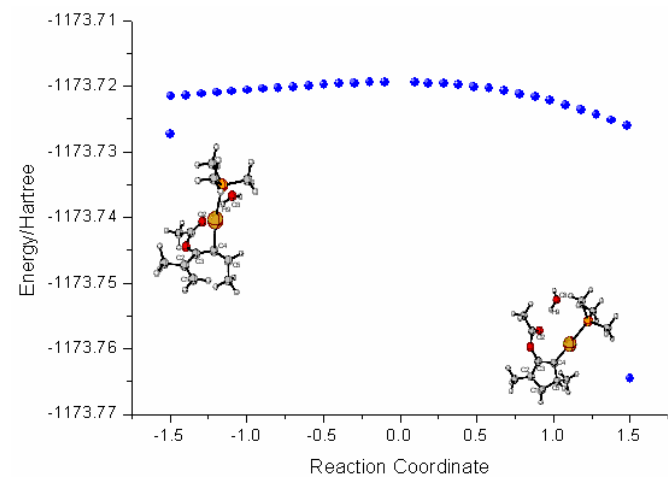
IRC for TS3b



IRC for TS5b



IRC for TS7b



8. Selected topological parameters at bond critical points in **12**

Three topological criteria are often applied to detect the existence of H-bond interactions.^{1,2} The first criterion states that there exists the bond critical point (BCP) between the proton donor and proton acceptor. The other two topological criteria require that the topological parameters at BCP be within the proper range of 0.002-0.035 au for the electron density (ρ) and 0.024-0.139 au for its Laplacian ($\nabla^2\rho$), respectively.¹ There exists weak interaction between oxygen atom and Au atom reflected by the topological properties at bond critical point (BCP3).

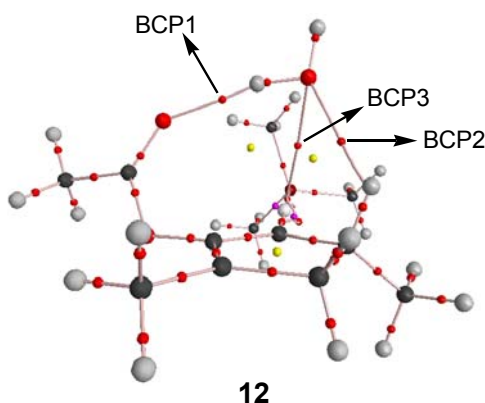


Figure S8. The bond critical points and molecular graphs in **12** (red circles correspond to the bond critical points).

Table S1. Selected topological properties (in au) at bond critical points

	ρ_b	$\nabla^2\rho$	λ_1	λ_2	λ_3
BCP1	0.0232	0.0815	-0.0316	-0.0312	0.1443
BCP2	0.0102	0.0366	-0.0097	-0.0086	0.0549
BCP3	0.0095	0.0270	-0.0060	-0.0034	0.0364

(1) Koch, U.; Popelier, P. L. A. *J. Phys. Chem.* **1995**, *99*, 9747.

(2) Popelier, P. L. A. *J. Phys. Chem. A* **1998**, *102*, 1873.

9. Energies of stationary points and imaginary frequencies

Table S2. Free energies and partial electronic energies (Hartree) computed at the MP2/6-31+G(d,p)/SDD level.

	ΔG_{298K}	ΔE_{0K}		ΔG_{298K}		ΔG_{298K}
2	-1097.052585	-1094.044506	2a	-1672.096620	2b	-1173.458309
TS3	-1097.041017	-1094.026472	TS3a	-1672.087300	TS3b	-1173.443511
4	-1097.053269	-1094.041759	4a	-1672.097604	4b	-1173.454086
TS5	-1097.039769	-1094.023769	TS5a	-1672.085838	TS5b	-1173.444649
6	-1097.053314	-1094.038713	6a	-1672.099323	6b	-1173.458597
TS7	-1097.044683	-1094.036839	TS7a	-1672.090593	TS7b	-1173.447959
8	-1097.083687	-1094.069977	8a	-1672.131364	12c	-1435.491912
TS9	-1097.052328	-1094.042208	TS9a	-1672.098186	12d	-1435.485842
10	-1097.103124	-1094.103501	10a	-1672.146453	TS13c	-1435.477912
12	-1173.489158	-1170.317745	17	-1326.301530	TS13d	-1435.481355
TS13	-1173.465614	-1170.298484	TS18	-1326.293848	23	-1056.968036
TS13'	-1173.464081	-1170.298042	19	-1326.301380	TS24	-1056.953013
14	-1173.472456	-1170.309141	TS20	-1326.295024	25	-1056.961257
TS15	-1173.467678	-1170.300506	21	-1326.323562	TS26	-1056.955362
16	-1173.509334	-1170.351642	22	-751.343930	TS27	-751.309809
					28	-751.350904

Table S3. Imaginary Frequencies (IF) of transition states discussed in the text.

	IF/cm ⁻¹		IF/cm ⁻¹		IF/cm ⁻¹
TS3	-200.5	TS3a	-215.0	TS3b	-220.7
TS5	-141.0	TS5a	-163.4	TS5b	-165.7
TS7	-301.1	TS7a	-309.6	TS7b	-306.0
TS9	-821.6	TS9a	-834.3	TS13c	-899.9
TS13	-967.6	TS13'	-578.3	TS13d	-864.1

TS18	-948. 2	TS20	-1028. 9	TS15	-700. 2
TS24	-926. 5	TS26	-956. 2	TS27	-797. 6

10. Cartesian coordinates

1

C	0.586627	0.478555	0.233658
C	0.586456	0.479952	1.446631
C	0.638203	0.479082	-1.229715
H	0.033972	1.306769	-1.613770
C	-1.274530	-0.749017	-1.994938
O	-1.989517	0.215416	-1.840285
O	0.061018	-0.755734	-1.749554
C	-1.726872	-2.107477	-2.478958
H	-2.769817	-2.05177	-2.792992
H	-1.098820	-2.449132	-3.307374
H	-1.626403	-2.838335	-1.668893
C	2.065598	0.550092	-1.772079
C	0.509792	0.519723	2.876231
C	-0.695202	1.223708	3.464425
H	-0.667968	1.200082	4.558014
H	-0.732257	2.269851	3.137871
H	-1.624889	0.750851	3.126418
C	1.465742	-0.043889	3.635063
H	2.321887	-0.544585	3.194495
H	1.407894	-0.015240	4.719566
H	2.648327	-0.309739	-1.429427
H	2.552531	1.464834	-1.420715
H	2.048642	0.554574	-2.866394

2

O	-1.102184	1.915695	-2.93995
C	-1.079569	1.792014	0.692078
C	-0.168321	1.830100	-0.150184
C	0.759609	2.480489	-1.124431
H	0.236545	3.372162	-1.487471
C	0.000876	1.465321	-3.140211
O	1.033519	1.627088	-2.248987
C	0.447702	0.686639	-4.348971
H	-0.410994	0.494951	-4.992893
H	1.199761	1.260319	-4.901382
H	0.914661	-0.257292	-4.050173
C	2.102054	2.849412	-0.499853

2'

O	-0.153631	0.706214	-5.39050
C	-0.206086	0.741213	-1.82780
C	0.694805	0.728864	-2.64442
C	1.805986	0.749271	-3.60167
H	1.762121	1.707643	-4.13359
C	0.655052	-0.190081	-5.45832
O	1.687278	-0.315161	-4.56712
C	0.698527	-1.287067	-6.48907
H	-0.207884	-1.251764	-7.09401
H	1.572781	-1.150221	-7.13514
H	0.798132	-2.264576	-6.00775
C	3.165949	0.576911	-2.91977

C	-2.232342	1.819162	1.546497	C	-1.356353	0.747259	-1.00404
C	-3.572217	1.558348	0.891484	C	-2.432848	-0.253951	-1.35131
H	-4.377466	1.635399	1.626485	H	-3.252399	-0.233322	-0.62907
H	-3.759073	2.278896	0.087919	H	-2.827473	4.96666	-2.34341
H	-3.602194	0.558543	0.44315	H	-2.025741	-1.267353	-1.42056
C	-2.071011	2.120519	2.850060	C	-1.531989	1.700741	-0.00119
H	-1.092224	2.310254	3.279262	H	-0.864383	2.559156	0.043505
H	-2.928963	2.198145	3.511541	H	-2.527047	1.834076	0.419961
H	2.626515	1.957263	-0.144559	H	3.219204	-0.38626	-2.404650
H	1.952735	3.532112	0.341718	H	3.331788	1.381538	-2.197630
H	2.723179	3.346284	-1.250079	H	3.952408	0.613406	-3.677990
Au	0.082694	-0.309564	0.438725	Au	-0.581018	0.284516	1.457482
P	0.704861	-2.534935	0.748971	P	0.328331	-0.900319	3.255375
C	2.220285	-2.970286	-0.191985	C	0.771495	-2.636626	2.849734
H	2.482391	-4.020075	-0.022052	H	1.519063	-2.654009	2.051488
H	2.05484	-2.811187	-1.261313	H	1.179501	-3.137825	3.734237
H	3.052524	-2.337254	0.129036	H	-0.115498	-3.178352	2.508904
C	1.075015	-2.951036	2.498917	C	1.864633	-0.141696	3.917043
H	0.189740	-2.780408	3.118241	H	2.237248	-0.724108	4.766565
H	1.373881	-4.001546	2.582107	H	2.631954	-0.113039	3.138022
H	1.885953	-2.317106	2.868886	H	1.664307	0.882208	4.245660
C	-0.575607	-3.737559	0.214136	C	-0.822915	-1.007302	4.682356
H	-0.222525	-4.762028	0.373872	H	-0.355489	-1.560614	5.504090
H	-1.494387	-3.582541	0.787109	H	-1.082195	-0.002784	5.029068
H	-0.800165	-3.596299	-0.846980	H	-1.741592	-1.519519	4.382288
TS3				4			
O	-0.153632	0.706215	-5.390496	O	-1.020340	-0.171441	-3.420046
C	-0.206086	0.741213	-1.827799	C	-1.016805	-0.187093	-1.937027
C	0.694805	0.728864	-2.644423	C	0.147618	-0.150864	-1.286814
C	1.805986	0.749271	-3.601671	C	1.433359	-0.22722	-2.046184
H	1.762122	1.707644	-4.133594	H	2.09076	0.613429	-1.817247
C	0.655052	-0.190081	-5.458319	C	0.067311	-0.03755	-4.085895
O	1.687278	-0.315161	-4.567123	O	1.228675	-0.01928	-3.557879
C	0.698527	-1.287067	-6.489068	C	-0.041486	0.136927	-5.561519
H	-0.207885	-1.251764	-7.094009	H	-0.923223	-0.386641	-5.936657
H	1.572781	-1.150222	-7.135137	H	-0.159331	1.206349	-5.779908
H	0.798132	-2.264576	-6.007747	H	0.865818	-0.218646	-6.052577
C	3.165949	0.576912	-2.919772	C	2.178846	-1.549033	-1.927267
C	-1.356353	0.747260	-1.004038	C	-2.419075	-0.212662	-1.480494
C	-2.432848	-0.253951	-1.351313	C	-3.386846	0.751114	-2.129544
H	-3.252399	-0.233323	-0.629069	H	-4.376536	0.666371	-1.673897
H	-2.827473	0.000050	-2.343407	H	-3.044997	1.788418	-2.021358
H	-2.025742	-1.267354	-1.420561	H	-3.492158	0.554607	-3.202482

C	-1.531990	1.700742	-0.001195	C	-2.784716	-1.072291	-0.517252
H	-0.864383	2.559156	0.043505	H	-2.088205	-1.789581	-0.094685
H	-2.527047	1.834077	0.419962	H	-3.800723	-1.081359	-0.132725
H	3.219204	-0.386260	-2.404652	H	1.528152	-2.390679	-2.184699
H	3.331788	1.381539	-2.197629	H	2.508762	-1.676346	-0.89199
H	3.952409	0.613407	-3.677989	H	3.059115	-1.555127	-2.576792
Au	-0.581019	0.284517	1.457482	Au	0.271839	0.043725	0.784754
P	0.328331	-0.900320	3.255376	P	0.433488	0.349162	3.112038
C	0.771495	-2.636626	2.849734	C	2.131183	0.129167	3.786950
H	1.519063	-2.654010	2.051488	H	2.140250	0.293969	4.869645
H	1.179501	-3.137826	3.734237	H	2.485218	-0.884543	3.577303
H	-0.115498	-3.178353	2.508904	H	2.814783	0.838935	3.311869
C	1.864634	-0.141697	3.917043	C	-0.073859	2.027830	3.670462
H	2.237248	-0.724108	4.766565	H	0.014684	2.117317	4.758485
H	2.631954	-0.113040	3.138022	H	0.559332	2.783491	3.196246
H	1.664307	0.882205	4.245661	H	-1.111372	2.216611	3.379103
C	-0.822915	-1.007302	4.682357	C	-0.609055	-0.800078	4.101778
H	-0.355490	-1.560615	5.504091	H	-0.494495	-0.600598	5.172608
H	-1.082195	-0.002784	5.029069	H	-1.660538	-0.676529	3.826148
H	-1.741593	-1.519520	4.382289	H	-0.318505	-1.834887	3.897706
TS5				6			
O	3.474942	-1.619472	0.825625	O	-2.047328	0.851705	-0.923938
C	1.614208	-1.782345	-0.471461	C	-2.139670	0.679305	0.411088
C	1.247478	-0.444808	-0.355401	C	-0.927225	0.720449	1.134319
O	3.422113	0.527770	0.032376	C	-0.924127	1.266247	2.394671
C	2.085352	0.628986	-0.343525	C	-3.549890	-0.070186	2.231170
H	1.135707	-2.508802	0.184497	C	-2.747780	0.024654	-1.845771
C	3.968610	-0.512959	0.745649	O	-3.263577	-0.99552	-1.496744
C	5.255815	-0.092229	1.389823	C	-2.660219	0.619316	-3.217857
H	5.901280	0.389279	0.648165	H	-3.151751	1.598127	-3.232461
H	5.052178	0.644545	2.174996	H	-1.612846	0.777696	-3.493979
H	5.753366	-0.961634	1.819734	H	-3.141607	-0.050235	-3.930840
C	2.355296	-2.358496	-1.628608	C	0.186381	1.209732	3.382966
C	1.741562	2.049454	-0.583561	C	-3.451952	0.543078	1.024756
C	2.387260	3.098854	0.290511	C	-4.673043	1.111112	0.329909
H	2.005608	4.091708	0.039983	H	-5.098816	0.384567	-0.369085
H	2.185763	2.910732	1.352660	H	-5.441738	1.350083	1.069584
H	3.474936	3.109206	0.164229	H	-4.437598	2.024461	-0.22528
C	0.922752	2.353556	-1.603759	H	-4.501585	-0.112145	2.753841
H	0.506337	1.590768	-2.255229	H	-2.722481	-0.608481	2.677439
H	0.664573	3.384921	-1.825952	H	0.636067	2.207266	3.496779
H	2.935298	-1.605736	-2.167930	H	0.968590	0.503348	3.094539
H	1.621204	-2.789366	-2.326132	H	-0.206085	0.945381	4.374101

H	2.996186	-3.181770	-1.296840	H	-1.778784	1.875220	2.699907
Au	-0.839338	-0.219945	-0.070768	Au	0.812793	-0.017652	0.213686
P	-3.137006	0.026845	0.329032	P	2.768351	-0.882387	-0.77486
C	-4.194893	-1.118204	-0.646533	C	2.844204	-2.720413	-0.782572
H	-3.936862	-2.154763	-0.410679	H	1.989510	-3.125030	-1.332679
H	-5.252618	-0.951079	-0.416022	H	3.770641	-3.066517	-1.253373
H	-4.031522	-0.955637	-1.715873	H	2.801849	-3.096911	0.243736
C	-3.607474	-0.271335	2.081371	C	4.320385	-0.353389	0.059143
H	-4.686930	-0.144128	2.21662	H	4.309339	-0.677077	1.104109
H	-3.327569	-1.288011	2.372274	H	5.192928	-0.788024	-0.440211
H	-3.079129	0.431504	2.732175	H	4.401422	0.737349	0.036003
C	-3.778642	1.706562	-0.056209	C	2.998374	-0.39795	-2.535254
H	-3.60642	1.936877	-1.111672	H	3.923304	-0.827122	-2.935210
H	-4.852488	1.763812	0.151620	H	2.153423	-0.75483	-3.131610
H	-3.256481	2.451959	0.550755	H	3.044873	0.69196	-2.617537
6' (optimization in CH ₂ Cl ₂)				TS7			
O	-2.029196	0.922704	-0.870770	O	2.116568	1.228929	-0.587930
C	-2.029244	0.923114	0.482073	C	2.262191	-0.085450	-0.243870
C	-0.767043	0.921661	1.108329	C	1.162559	-0.944150	-0.260990
C	-0.611893	1.597073	2.295545	C	1.499905	-2.310810	-0.364630
C	-3.357062	0.556273	2.471927	C	3.463220	-1.911580	0.681383
C	-2.858160	0.063580	-1.626900	C	2.676429	2.212933	0.242157
O	-3.432940	-0.857859	-1.119940	O	3.234567	1.934458	1.267675
C	-2.827336	0.475344	-3.066060	C	2.444053	3.573054	-0.346710
H	-3.235185	1.487045	-3.170410	H	2.890147	3.631857	-1.345050
H	-1.794405	0.502488	-3.427850	H	1.370091	3.754320	-0.459500
H	-3.414910	-0.227899	-3.656820	H	2.883656	4.328120	0.305045
C	0.558131	1.51946	3.208987	C	0.665164	-3.437770	0.160663
C	-3.294578	1.003724	1.192533	C	3.528684	-0.668140	0.057414
C	-4.501917	1.612528	0.509547	C	4.832266	-0.073000	-0.396460
H	-5.042243	0.861974	-0.076320	H	5.262216	0.535330	0.407500
H	-5.190444	2.006176	1.262204	H	5.549769	-0.866080	-0.629960
H	-4.218991	2.431027	-0.159940	H	4.707745	0.565709	-1.275500
H	-4.262186	0.689066	3.058644	H	4.312200	-2.591530	0.631791
H	-2.555687	-0.012038	2.929176	H	2.779971	-2.093590	1.502436
H	1.118188	2.466075	3.173712	H	-0.043298	-3.751730	-0.619430
H	1.234830	0.699183	2.957391	H	0.092719	-3.154200	1.047568
H	0.213395	1.414633	4.246743	H	1.286670	-4.310500	0.386765
H	-1.369005	2.332372	2.580062	H	2.204369	-2.594970	-1.146450
Au	0.818611	-0.074000	0.157252	Au	-0.801955	-0.281830	-0.09086
P	2.604161	-1.213449	-0.866810	P	-3.038357	0.448275	0.096582
C	2.547667	-3.037715	-0.643390	C	-3.482031	1.070718	1.770012
H	1.619766	-3.433129	-1.067390	H	-2.843544	1.919415	2.032358

H	3.401305	-3.511968	-1.139790	H	-4.529825	1.388453	1.797000
H	2.571724	-3.278952	0.423549	H	-3.328203	0.281888	2.512264
C	4.258561	-0.717147	-0.236340	C	-4.276872	-0.865450	-0.256940
H	4.316812	-0.909549	0.839162	H	-4.145916	-1.697250	0.441530
H	5.047442	-1.281004	-0.745890	H	-5.294357	-0.472430	-0.157500
H	4.413049	0.352463	-0.406990	H	-4.137627	-1.242910	-1.274290
C	2.706597	-0.969286	-2.686770	C	-3.477311	1.822096	-1.045830
H	3.559047	-1.519436	-3.099810	H	-4.527071	2.107049	-0.917990
H	1.787205	-1.326514	-3.160400	H	-2.844278	2.690936	-0.843100
H	2.822369	0.095335	-2.910920	H	-3.314241	1.510653	-2.08179
8				TS9			
O	-2.411523	0.262609	-1.410878	O	2.22169	1.572179	0.559274
C	-2.416445	0.245565	-0.032507	C	2.458561	0.240871	0.288887
C	-1.283823	0.236554	0.804492	C	1.37945	-0.71979	-0.067893
C	-1.767214	0.300236	2.225665	C	2.030385	-1.96568	-0.238941
C	-1.849634	-0.823499	-2.073233	C	1.710451	2.340938	-0.470811
O	-1.380079	-1.763294	-1.484988	O	1.458319	1.87748	-1.556197
C	-1.93448	-0.623453	-3.559689	C	1.540051	3.767507	-0.02931
H	-2.976677	-0.483544	-3.864114	H	0.886273	3.817857	0.847749
H	-1.388612	0.281728	-3.847012	H	2.508247	4.185668	0.265419
H	-1.51341	-1.491934	-4.066442	H	1.119591	4.352645	-0.847429
C	-1.228042	-0.845513	3.110443	C	1.389506	-3.28545	-0.528393
C	-3.602812	0.335394	0.677976	C	3.669582	-0.3444	0.387878
C	-4.965018	0.414326	0.098936	C	4.978989	0.287996	0.726716
H	-5.614584	-0.348343	0.547628	H	5.426805	-0.18166	1.611527
H	-5.417719	1.384401	0.349568	H	5.696572	0.170283	-0.095177
H	-4.958298	0.300564	-0.986201	H	4.857901	1.354457	0.929573
C	-3.310899	0.361491	2.138207	C	3.504727	-1.80216	0.044891
H	-0.134851	-0.834386	3.136041	H	0.360078	-3.16467	-0.876184
H	-1.553176	-1.819742	2.730630	H	1.359747	-3.86373	0.404676
H	-1.599016	-0.729841	4.133353	H	1.961921	-3.86926	-1.256273
H	-1.378129	1.242813	2.642925	H	1.569216	-1.07623	-1.249693
Au	0.677589	0.175179	0.236551	Au	-0.67333	-0.32434	0.003027
P	2.963873	0.078847	-0.387079	P	-2.97682	0.133516	0.142954
H	-3.796788	-0.491084	2.634137	H	3.770355	-2.47228	0.877822
H	-3.734024	1.258701	2.611945	H	4.133723	-2.11961	-0.798958
C	3.397815	-1.442536	-1.325782	C	-4.04339	-1.35004	-0.066206
H	2.8037	-1.495637	-2.242759	H	-5.10126	-1.07463	0.001103
H	4.461746	-1.444486	-1.585571	H	-3.85566	-1.8084	-1.041677
H	3.174404	-2.326848	-0.721746	H	-3.81525	-2.08462	0.711708
C	3.508301	1.47095	-1.459958	C	-3.49153	0.86027	1.752113
H	4.568146	1.367493	-1.715861	H	-4.56909	1.05599	1.757377
H	2.918281	1.48379	-2.381039	H	-3.24883	0.170871	2.566138

H	3.357098	2.421617	-0.940135	H	-2.95694	1.798998	1.924391
C	4.126731	0.101919	1.037684	C	-3.56825	1.324423	-1.12756
H	5.163464	0.047645	0.688917	H	-4.64327	1.502142	-1.016519
H	3.990887	1.02198	1.613781	H	-3.03475	2.273817	-1.023828
H	3.925871	-0.749939	1.694087	H	-3.3714	0.928079	-2.128004
10				11			
O	-0.947310	-2.011430	-2.361300	O	-0.180480	0.167873	-1.459740
C	-1.025220	-1.998020	-0.981500	C	-0.194800	0.210998	-0.070240
C	0.153489	-2.000540	-0.097000	C	0.988267	0.196955	0.799935
C	-0.279230	-2.049080	1.222039	C	0.582867	0.356007	2.076855
C	-0.324450	-0.968280	-3.000270	C	0.661096	-0.687220	-2.114760
O	0.146879	-0.020650	-2.409780	O	1.411794	-1.458250	-1.567310
C	-0.321550	-1.185220	-4.486910	C	0.503951	-0.513420	-3.607080
H	0.207541	-2.113330	-4.727470	H	-0.534180	-0.699600	-3.901610
H	-1.348110	-1.293900	-4.851770	H	0.744281	0.515808	-3.894160
H	0.162839	-0.342110	-4.979430	H	1.167322	-1.207440	-4.124230
C	-2.172480	-2.060200	-0.271620	C	-1.332720	0.381998	0.635601
C	-3.576130	-2.06121	-0.781780	C	-2.736760	0.471452	0.129443
H	-4.116550	-2.95686	-0.450540	H	-3.375240	-0.310340	0.564408
H	-4.135510	-1.19514	-0.404610	H	-3.201150	1.434732	0.383929
H	-3.597950	-2.03507	-1.874020	H	-2.765670	0.363024	-0.95882
C	-1.799870	-2.10969	1.192223	C	-0.927850	0.485437	2.088268
Au	0.402806	0.21205	0.601604	H	-1.395500	-0.303960	2.696766
P	0.882042	2.491132	0.619772	H	-1.246140	1.439886	2.535766
H	-2.121570	-3.05413	1.657512	H	2.003974	0.062155	0.452755
H	-2.280100	-1.31294	1.776913	C	1.424435	0.397916	3.314280
H	1.165773	-2.20164	-0.437480	H	1.155579	-0.404900	4.015128
C	0.523146	-2.42985	2.435279	H	2.487005	0.288547	3.073759
H	0.231025	-1.84883	3.316030	H	1.298245	1.344284	3.858859
H	0.344341	-3.48751	2.672681				
H	1.596470	-2.30014	2.271664				
C	1.758196	3.089418	2.118577				
H	1.968175	4.161021	2.032303				
H	1.142394	2.915156	3.005603				
H	2.701059	2.548066	2.238469				
C	1.952930	2.939073	-0.802410				
H	2.111650	4.022391	-0.834160				
H	2.920349	2.437046	-0.708950				
H	1.480417	2.607842	-1.731450				
C	-0.610830	3.549956	0.465688				
H	-1.274940	3.388317	1.319661				
H	-0.323150	4.606303	0.430951				
H	-1.151010	3.295007	-0.450590				

12				TS13			
O	-2.228820	1.518869	-0.785036	O	-2.035242	1.568691	-0.801319
C	-2.361066	0.193609	-0.402303	C	-2.256321	0.197447	-0.626899
C	-1.299817	-0.701181	-0.157347	C	-1.189844	-0.727402	-0.235204
C	-1.904185	-2.018478	0.220536	C	-1.821858	-1.940979	0.028006
C	-1.703762	2.418681	0.112464	C	-1.951472	2.320916	0.316845
O	-1.375207	2.114556	1.236583	O	-2.056537	1.868423	1.449908
C	-1.612095	3.785857	-0.502319	C	-1.724905	3.770804	0.003901
H	-0.917234	3.764136	-1.349154	H	-0.808617	3.886997	-0.584018
H	-2.587245	4.093875	-0.892178	H	-2.550317	4.150793	-0.60729
H	-1.265057	4.499034	0.245394	H	-1.65463	4.341383	0.929746
C	-1.277702	-3.250266	-0.455575	C	-1.158973	-3.276321	0.261428
C	-3.602261	-0.411259	-0.326262	C	-3.462608	-0.396739	-0.780895
C	-4.916832	0.245647	-0.526298	C	-4.767963	0.226081	-1.149481
H	-5.511119	-0.302626	-1.268371	H	-5.215118	-0.286632	-2.009906
H	-5.490606	0.208657	0.410720	H	-5.488051	0.144402	-0.324727
H	-4.815955	1.285876	-0.840477	H	-4.652389	1.282609	-1.404348
C	-3.426674	-1.854754	-0.002912	C	-3.278318	-1.847883	-0.428185
H	-0.210107	-3.315994	-0.227399	H	-0.144916	-3.150736	0.654354
H	-1.394551	-3.208634	-1.544128	H	-1.081054	-3.838726	-0.677948
H	-1.761992	-4.162759	-0.093713	H	-1.730522	-3.896710	0.961302
H	-1.705965	-2.081476	1.304401	H	-1.917480	-1.210247	1.342568
Au	0.699739	-0.293612	-0.149323	Au	0.816865	-0.268941	-0.104765
P	3.028461	0.136051	-0.103326	P	3.139479	0.198901	-0.063444
H	-3.779348	-2.472165	-0.842658	H	-3.428326	-2.498706	-1.302380
H	-4.039252	-2.148086	0.86046	H	-4.007221	-2.180814	0.324009
H	-1.026418	0.581582	2.410569	H	-2.262267	0.354616	2.068627
O	-0.867673	-0.303779	2.785418	O	-2.320835	-0.615457	2.355615
H	-0.614181	-0.150041	3.708043	H	-1.695549	-0.747740	3.091763
C	4.055262	-1.37848	0.083969	C	4.077665	-0.703977	-1.363931
H	5.119662	-1.122211	0.112675	H	5.144284	-0.460880	-1.311851
H	3.786207	-1.895606	1.009733	H	3.949519	-1.782546	-1.232424
H	3.873112	-2.056087	-0.755432	H	3.695833	-0.431217	-2.352243
C	3.678182	0.956856	-1.616534	C	3.571804	1.968566	-0.326214
H	4.757944	1.120512	-1.533843	H	3.125138	2.580910	0.462809
H	3.476869	0.33239	-2.491944	H	4.658234	2.106352	-0.312603
H	3.180843	1.920709	-1.759309	H	3.181641	2.307055	-1.290677
C	3.546663	1.226897	1.284975	C	3.981497	-0.249270	1.511191
H	4.629827	1.387686	1.266736	H	3.854154	-1.317655	1.709592
H	3.038986	2.192957	1.208416	H	5.051428	-0.021632	1.455931
H	3.268557	0.766943	2.237817	H	3.540388	0.311269	2.340794

TS13'

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O	-2.421986	-0.107388	-1.279647	O	-2.392176	-0.251519	-1.303936
C	-2.417049	-0.105048	0.108775	C	-2.382003	-0.223158	0.126189
C	-1.160906	-0.102687	0.90826	C	-1.12763	-0.193051	0.903073
C	-1.573052	-0.144701	2.243151	C	-1.538405	-0.256863	2.208665
C	-2.01271	1.015408	-1.93765	C	-2.151024	0.793409	-2.03079
O	-1.648708	2.027629	-1.373469	O	-1.907811	1.956994	-1.597471
C	-2.085129	0.823433	-3.426169	C	-2.15799	0.567628	-3.505751
H	-1.445117	-0.012889	-3.726786	H	-1.122764	0.41816	-3.837767
H	-3.108105	0.568553	-3.721615	H	-2.736085	-0.322171	-3.757768
H	-1.769228	1.737642	-3.92863	H	-2.549576	1.450906	-4.014526
C	-0.704815	-0.204708	3.459909	C	-0.693928	-0.30452	3.447049
C	-3.528362	-0.181233	0.86579	C	-3.514151	-0.329099	0.84469
C	-4.956775	-0.213832	0.430015	C	-4.937496	-0.412158	0.397946
H	-5.458971	-1.117935	0.796509	H	-5.417012	-1.319151	0.786405
H	-5.512677	0.643267	0.830995	H	-5.521827	0.438987	0.770721
H	-5.037998	-0.197827	-0.659532	H	-5.022086	-0.430851	-0.692584
C	-3.084301	-0.202492	2.306981	C	-3.052989	-0.360204	2.281585
H	0.335921	0.025555	3.217375	H	0.365148	-0.164512	3.209691
H	-0.738269	-1.222329	3.870468	H	-0.797898	-1.272111	3.956522
H	-1.055264	0.47397	4.245017	H	-0.991044	0.462778	4.174308
H	-1.135895	1.061451	1.503217	H	-1.303468	1.888728	1.243349
Au	0.76689	-0.290194	0.132973	Au	0.800669	-0.225827	0.166083
P	2.935685	-0.556786	-0.743816	P	3.037914	-0.397212	-0.594801
H	-3.384601	-1.124655	2.827872	H	-3.358592	-1.296077	2.773344
H	-3.509568	0.622137	2.897013	H	-3.502094	0.449799	2.875288
H	-1.491783	3.40213	1.643184	H	-1.819657	2.195015	-0.539882
O	-0.931267	2.712101	1.253053	O	-1.629911	2.68232	0.750912
H	-1.156224	2.683841	0.29753	H	-0.931371	3.357534	0.80279
C	3.912303	-1.881655	0.077681	C	3.964397	-1.762823	0.221732
H	4.909292	-1.958775	-0.369206	H	4.989585	-1.82094	-0.159458
H	4.015132	-1.659831	1.144043	H	3.993765	-1.59585	1.302644
H	3.397599	-2.841388	-0.026599	H	3.45793	-2.714776	0.036559
C	2.97417	-0.990424	-2.531534	C	4.083839	1.09235	-0.312252
H	2.488628	-0.202038	-3.114272	H	4.104145	1.332326	0.75506
H	4.006238	-1.106902	-2.878987	H	5.108712	0.919864	-0.657815
H	2.433985	-1.92722	-2.697636	H	3.66577	1.948696	-0.849905
C	3.978828	0.951651	-0.602835	C	3.217704	-0.742945	-2.395285
H	4.075419	1.237619	0.448679	H	2.777901	0.073502	-2.976019
H	4.976058	0.772295	-1.018618	H	4.273097	-0.845677	-2.66927
H	3.508291	1.779486	-1.141425	H	2.693104	-1.669466	-2.647394
17				TS18			
O	-2.361711	-1.015132	-1.756371	O	1.756903	-2.374482	-0.190136
C	-2.472747	-0.899661	-0.377662	C	2.153561	-1.077052	-0.519574

C	-1.395061	-0.724856	0.517392	C	1.244024	0.034612	-0.711981
C	-1.970442	-0.673565	1.896703	C	2.037468	1.148446	-1.053807
H	-1.818394	0.380888	2.190995	H	2.063095	1.671031	0.221806
O	-0.225959	1.979946	1.856444	O	2.205796	2.29938	1.330754
C	-1.942160	0.076859	-2.46884	C	1.239035	-2.644916	1.032044
O	-1.732190	1.151287	-1.951292	O	1.110494	-1.818278	1.914174
C	-1.795108	-0.25878	-3.925496	C	0.852804	-4.094424	1.143489
H	-1.610446	0.652582	-4.494591	H	0.037773	-4.311773	0.444058
H	-0.955124	-0.950966	-4.05519	H	1.695314	-4.735191	0.866307
H	-2.691877	-0.763338	-4.296677	H	0.53296	-4.312122	2.162597
C	-1.237392	-1.540936	2.93662	C	1.525483	2.349548	-1.835721
C	-3.686766	-1.052251	0.260392	C	3.443361	-0.774249	-0.830474
C	-5.007059	-1.252771	-0.387548	C	4.642256	-1.656257	-0.735553
H	-5.498587	-2.147655	0.015224	H	5.165066	-1.708779	-1.698761
H	-5.668144	-0.407793	-0.149235	H	5.362095	-1.255587	-0.009563
H	-4.925206	-1.345025	-1.472003	H	4.373213	-2.671093	-0.433086
C	-3.477344	-0.982447	1.735149	C	3.473316	0.658279	-1.270394
H	-0.18788	-1.242836	3.008292	H	0.523456	2.637751	-1.501713
H	-1.277835	-2.603219	2.67099	H	1.468286	2.127242	-2.908566
H	-1.700422	-1.415255	3.920624	H	2.192246	3.211686	-1.715693
Au	0.571783	-0.393273	0.088993	Au	-0.790167	0.006578	-0.419541
P	2.838978	0.041975	-0.428918	P	-3.132066	0.003993	-0.073700
H	-3.74954	-1.941792	2.199774	H	3.738535	0.729363	-2.336326
H	-4.136242	-0.232384	2.194108	H	4.234922	1.238834	-0.730786
H	-0.163648	2.453009	0.998194	H	1.728560	1.727700	2.015459
H	0.590022	2.226026	2.336349	H	1.691301	3.149917	1.259980
H	-0.589435	2.503284	-1.217094	H	1.116335	5.295386	0.602914
O	-0.00575	3.108958	-0.722198	O	0.720095	4.566435	1.106463
H	-0.381854	3.991960	-0.862305	H	0.442088	4.961518	1.948225
C	3.881326	0.450816	1.029090	H	0.904154	-0.151573	2.551781
H	4.901743	0.693243	0.712633	O	0.861879	0.735881	2.971070
H	3.454289	1.298185	1.574506	H	1.209620	0.60886	3.868205
H	3.914815	-0.411429	1.702717	C	-3.757107	1.528685	0.747711
C	3.728766	-1.343793	-1.252832	H	-3.523924	2.401788	0.130975
H	3.218262	-1.613076	-2.182146	H	-4.840779	1.475048	0.897653
H	4.761421	-1.058443	-1.480995	H	-3.265358	1.650932	1.717418
H	3.736581	-2.220803	-0.598812	C	-4.127260	-0.130618	-1.616285
C	3.028421	1.466126	-1.578691	H	-5.198799	-0.118107	-1.389966
H	4.082485	1.744527	-1.684112	H	-3.891822	0.70411	-2.283207
H	2.634226	1.18944	-2.561726	H	-3.881065	-1.062278	-2.134331
H	2.448056	2.316876	-1.210106	C	-3.746489	-1.368739	0.988557
H	2.302765	2.424026	4.064013	H	-4.831395	-1.300163	1.122481
O	2.236494	2.729634	3.145488	H	-3.505247	-2.330985	0.526909
H	2.340783	3.692961	3.197639	H	-3.260497	-1.324474	1.967792

19				TS20			
O	-2.483177	-0.678943	-1.381595	O	2.289371	-1.746611	-0.156885
C	-2.45977	-0.597401	0.02098	C	2.426425	-0.393929	-0.48684
C	-1.207195	-0.477606	0.803245	C	1.842551	1.760232	-0.948459
C	-1.593269	-0.548352	2.115227	C	1.36275	0.636956	-0.304377
H	-1.002516	1.460641	1.327156	H	1.045638	1.093969	0.959544
O	-0.798177	2.436849	1.500699	O	0.918922	1.667143	2.113654
C	-2.149196	0.399821	-2.104239	C	1.970801	-2.122028	1.097441
O	-1.883069	1.480428	-1.599891	O	1.811376	-1.329207	2.007723
C	-2.150064	0.107493	-3.580013	C	1.858291	-3.619326	1.206759
H	-1.320174	-0.567357	-3.818895	H	1.11727	-3.996129	0.494443
H	-3.074288	-0.402262	-3.866795	H	2.816882	-4.082669	0.950625
H	-2.040098	1.034796	-4.143146	H	1.576734	-3.897182	2.222825
C	-0.723925	-0.544397	3.339437	C	1.193179	3.101601	-1.042935
C	-3.564249	-0.747597	0.77557	C	3.495577	0.054424	-1.169189
C	-4.984875	-0.924141	0.345285	C	4.728631	-0.685195	-1.578708
H	-5.40353	-1.863016	0.7305	H	4.849415	-0.685432	-2.669959
H	-5.622815	-0.114546	0.723815	H	5.630638	-0.220449	-1.159742
H	-5.069726	-0.941421	-0.74485	H	4.695385	-1.724845	-1.242583
C	-3.097429	-0.727736	2.209995	C	3.216814	1.495669	-1.512728
H	-0.973017	0.281691	4.023303	H	0.225738	3.121328	-0.532176
H	0.335419	-0.48153	3.062615	H	1.024221	3.374141	-2.09346
H	-0.852791	-1.467177	3.920289	H	1.839483	3.883407	-0.621423
Au	0.702573	-0.469596	0.011803	Au	-0.693136	0.072903	-0.389082
P	2.890141	-0.563305	-0.888651	P	-2.907579	-0.630302	-0.653747
H	-3.345145	-1.667726	2.726622	H	3.236269	1.677018	-2.599057
H	-3.581129	0.069947	2.794098	H	3.958622	2.187947	-1.085734
H	-0.626277	2.920484	0.563936	H	0.686772	0.98327	2.815309
H	0.034356	2.468849	2.082001	H	0.162061	2.308439	2.070989
H	1.281866	1.699333	3.680932	H	-0.843612	4.399208	1.959642
O	1.321708	2.434948	3.047655	O	-1.144268	3.476954	1.99924
H	1.503612	3.230447	3.574985	H	-1.741699	3.439664	2.76337
H	-0.898303	2.862246	-1.311261	H	0.773266	-0.892192	3.440429
O	-0.411804	3.502557	-0.734099	O	0.242979	-0.200876	3.891525
H	-0.849167	4.362675	-0.850882	H	0.645494	-0.096843	4.768579
C	3.999357	-1.751728	-0.022594	C	-3.431879	-0.738365	-2.413747
H	4.994017	-1.764537	-0.480905	H	-4.472062	-1.072928	-2.489128
H	4.094914	-1.470266	1.03044	H	-3.335324	0.242363	-2.888811
H	3.570199	-2.757086	-0.069857	H	-2.788363	-1.443234	-2.948445
C	2.964331	-1.089177	-2.652706	C	-4.15326	0.470645	0.135123
H	2.412574	-0.378048	-3.274875	H	-4.066743	1.480794	-0.275772
H	4.001282	-1.137969	-3.001979	H	-5.167261	0.096241	-0.042178
H	2.503112	-2.075051	-2.764232	H	-3.972398	0.518488	1.212994

C	3.817731	1.028326	-0.856757	C	-3.259303	-2.297692	0.040832
H	3.913808	1.378141	0.175532	H	-4.310757	-2.565604	-0.109029
H	4.817029	0.909137	-1.289255	H	-2.628238	-3.044152	-0.450638
H	3.268856	1.785511	-1.424683	H	-3.036527	-2.306620	1.111972
21				22			
O	3.340769	0.068782	0.746985	C	0.898094	-0.43413	-2.01656
C	2.550657	0.142649	-0.390356	C	0.875763	-0.18063	-0.6347
C	1.409300	1.065589	-0.549168	C	2.289194	-0.11327	-0.12273
O	-1.080701	0.688162	2.346986	C	2.601547	1.142314	0.717537
C	0.933005	0.939349	-1.850472	C	2.201019	-0.51758	-2.49108
C	2.765621	-0.207411	1.951118	C	2.607924	-0.80193	-3.88828
O	1.580596	-0.436814	2.079515	H	3.296845	-0.02817	-4.25234
C	3.78939	-0.188272	3.051638	H	3.172216	-1.74519	-3.92325
H	4.581496	-0.913266	2.837877	H	1.755576	-0.87642	-4.56689
H	4.26035	0.798775	3.107250	C	3.170804	-0.28494	-1.38074
H	3.311604	-0.428275	4.001556	H	1.947336	1.198659	1.592339
C	0.07136	1.916025	-2.604333	H	2.466367	2.054973	0.127276
C	2.805218	-0.540675	-1.52578	H	3.637832	1.108967	1.066963
C	3.857109	-1.572955	-1.769456	Au	-0.79834	0.029013	0.504001
H	3.409567	-2.537278	-2.043687	P	-2.7546	0.276457	1.831569
H	4.514734	-1.281443	-2.598262	H	3.768539	0.614325	-1.59132
H	4.475651	-1.723424	-0.881091	H	3.895342	-1.10774	-1.30721
C	1.805785	-0.084448	-2.562692	H	0.019458	-0.55244	-2.6416
H	-0.502124	2.562014	-1.933855	H	-3.36992	-0.90439	2.287266
H	-0.62414	1.404748	-3.278229	H	-3.85027	0.935429	1.243768
H	0.712064	2.555547	-3.228049	H	-2.63069	0.99189	3.036942
Au	-0.528917	-0.208934	-0.320771	H	2.413398	-0.9878	0.537691
P	-2.36437	-1.541087	0.237789	C	0.898094	-0.43413	-2.01656
H	1.232883	-0.915721	-2.994365				
H	2.309447	0.407244	-3.409381				
H	-0.221706	0.27734	2.550542				
H	-0.8439	1.614611	2.112925				
H	0.036874	3.833364	2.21621				
O	-0.160936	3.19718	1.512019				
H	-0.765506	3.664072	0.890937				
C	-2.051188	-2.573684	1.723239				
H	-1.8016	-1.91493	2.558746				
H	-2.941748	-3.160329	1.973901				
H	-1.212359	-3.251788	1.54205				
C	-3.843672	-0.542877	0.668229				
H	-4.669934	-1.193742	0.974489				
H	-3.57537	0.124225	1.491658				
H	-4.158273	0.0548	-0.19236				
C	-2.922947	-2.717861	-1.060786				

H	-3.782483	-3.298903	-0.709028
H	-3.207155	-2.169555	-1.963757
H	-2.108321	-3.4028	-1.313896
H	1.172263	1.877869	0.135684
H	-2.761657	4.452059	-0.204558
O	-1.811125	4.376438	-0.382561
H	-1.557354	5.224344	-0.779887

23				TS24			
C	-1.96107	-1.24587	-0.58239	C	2.202722	-0.76512	0.005509
C	-0.97065	-0.70644	0.244342	C	1.095012	0.142059	-0.23789
C	-1.61391	-0.03358	1.425893	C	1.458196	1.422947	0.231394
O	0.149256	3.044582	0.586882	H	0.780181	1.340869	1.415432
C	-1.12253	-0.57606	2.784559	O	0.218014	1.521557	2.571766
C	-3.23042	-0.95423	-0.09062	C	0.880315	2.725711	-0.30629
C	-4.51465	-1.2404	-0.76445	C	3.283745	-0.09819	0.512776
H	-5.29891	-1.5185	-0.0522	C	4.603013	-0.6682	0.916619
H	-4.82001	-0.28644	-1.22483	H	5.422431	-0.16153	0.391352
H	-4.42486	-1.99927	-1.54562	H	4.782106	-0.51516	1.98926
C	-3.13042	-0.19032	1.183153	H	4.668794	-1.73927	0.705074
H	-0.04025	-0.45049	2.887492	C	2.934204	1.356522	0.634347
H	-1.35508	-1.64117	2.892975	H	-0.20111	2.645927	-0.45658
H	-1.6105	-0.03444	3.600956	H	1.334654	2.988359	-1.26952
Au	1.027097	-0.70778	-0.13819	H	1.071743	3.555039	0.384219
P	3.351215	-0.66483	-0.59711	Au	-0.70534	-0.40367	-1.0372
H	-3.65761	-0.70759	1.996688	P	-2.77379	-1.03158	-2.0144
H	-3.63439	0.775747	1.032898	H	3.546813	1.94975	-0.062
H	-0.12264	3.889599	0.975405	H	3.149544	1.75535	1.635797
H	1.131007	3.026224	0.630064	H	-0.27117	0.669392	2.820462
H	3.253835	2.996815	1.687562	H	-0.48073	2.219791	2.446851
O	2.961583	2.95314	0.762697	H	-1.48905	4.30216	2.168694
H	3.434927	3.674685	0.317573	O	-1.73651	3.364975	2.121351
H	-0.86782	2.632934	-2.44599	H	-2.53671	3.285909	2.664562
O	-1.14825	2.135791	-1.66321	H	-0.44027	-1.43671	2.922112
H	-0.65548	2.52428	-0.90127	O	-1.07717	-0.70576	3.127733
H	-1.77913	-1.77822	-1.50959	H	-1.29848	-0.81561	4.066268
H	3.767355	-0.8084	-1.93491	H	2.188644	-1.82396	-0.24004
H	4.164628	-1.63515	0.019511	H	-3.25612	-2.33419	-1.7805
H	4.033346	0.513376	-0.23872	H	-2.85813	-0.98754	-3.41963
H	-2.92888	2.07151	-1.30648	H	-3.91755	-0.28233	-1.67605
O	-3.84578	1.939531	-0.97436	H	1.472397	-2.05577	1.907721
H	-4.34601	2.710558	-1.27795	O	0.875426	-2.49677	2.53607
H	-1.32513	1.027772	1.371004	H	0.679354	-3.3632	2.146836

25				TS26			
C	-1.78775	-1.11991	-0.7405	C	-2.18305	0.164378	-0.566000
C	-0.77417	-0.72151	0.273817	C	-1.59235	-1.602990	0.804590
C	-1.37914	-0.7876	1.501111	C	-1.08332	-0.447360	0.237615
H	-0.7134	1.299161	0.785386	H	-0.64713	0.36535	1.273523
O	-0.74082	2.291825	0.941522	O	-0.44441	1.194854	2.225042
C	-0.78628	-0.55817	2.859687	O	-1.57282	3.739546	-1.20719
C	-2.97567	-1.42856	-0.16102	C	-0.90526	-2.56037	1.720819
C	-4.22766	-1.94733	-0.80341	C	-3.31182	-0.56912	-0.48495
H	-4.49792	-2.93026	-0.39673	C	-4.64063	-0.31731	-1.12747
H	-5.08568	-1.28638	-0.62327	H	-4.93371	-1.14707	-1.7844
H	-4.1062	-2.06092	-1.88592	H	-5.43825	-0.21243	-0.37981
C	-2.81881	-1.23221	1.32955	H	-4.62234	0.595295	-1.73161
H	0.270229	-0.27817	2.790898	C	-3.03601	-1.76218	0.40175
H	-0.84769	-1.46862	3.470559	H	0.116626	-2.23951	1.946256
H	-1.31922	0.225268	3.415707	H	-0.85051	-3.5607	1.270312
Au	1.219409	-0.50261	-0.16795	H	-1.4604	-2.67639	2.661482
P	3.525207	-0.42451	-0.70882	Au	0.901529	-0.37523	-0.47046
H	-3.00102	-2.17411	1.86949	P	3.038808	-0.3657	-1.41928
H	-3.54136	-0.51365	1.745919	H	-3.18811	-2.71949	-0.12236
H	-1.43432	2.776286	0.224733	H	-3.69638	-1.80618	1.281787
H	0.192414	2.667169	0.842956	H	-0.29237	2.093646	1.78924
H	2.040027	3.672036	1.566798	H	0.410223	0.938743	2.665915
O	1.671624	3.351451	0.727015	H	1.82096	-0.12868	4.174127
H	1.772087	4.084041	0.097217	O	1.911211	0.440671	3.393081
H	-2.76478	2.638317	-1.15778	H	2.505856	1.15668	3.668184
O	-2.24439	3.360594	-0.67357	H	-0.52588	3.612053	0.212571
H	-2.9028	3.941798	-0.25687	O	0.045866	3.493564	1.008865
H	-1.56627	-1.22234	-1.80055	H	-0.07604	4.295289	1.540551
H	3.969795	0.476645	-1.69805	H	3.128306	-0.61603	-2.80234
H	4.113687	-1.60981	-1.19331	H	3.968668	-1.30815	-0.9384
H	4.440105	-0.1128	0.317346	H	3.81232	0.808952	-1.33237
H	-3.18631	0.529444	-1.34951	H	-2.07056	1.090226	-1.12228
O	-3.55595	1.36425	-1.71299	H	-2.5066	3.981211	-1.10526
H	-3.5897	1.247812	-2.67566	H	-1.26184	4.226643	-1.98616
TS27				28			
C	0.849152	-0.2166	-2.14741	C	-0.67411	1.748253	-1.69905
C	0.883632	-0.25543	-0.66200	C	-0.65378	1.724473	-0.23765
C	2.254404	-0.24123	-0.28471	C	0.665257	1.633386	0.230934
C	2.81625	-0.19515	1.097993	C	0.598102	1.714711	-2.1734
C	2.094947	-0.16117	-2.66683	C	1.047541	1.707093	-3.59753
C	2.500061	-0.11091	-4.10425	H	1.739507	2.534964	-3.79687
H	3.099156	0.784271	-4.31392	H	1.589806	0.781835	-3.83422

H	3.120877	-0.97645	-4.36863	H	0.202232	1.792433	-4.28539
H	1.627841	-0.10167	-4.7628	C	1.555591	1.655013	-1.00562
C	3.094291	-0.18807	-1.53441	Au	-0.24649	-0.50978	0.446768
H	2.059549	-0.43377	1.850509	P	-0.62573	-2.77603	0.873134
H	3.163568	0.829049	1.290739	H	2.187385	2.555857	-0.96818
H	3.679875	-0.85757	1.214685	H	2.257716	0.81177	-1.07149
H	1.327671	-1.35364	-0.30324	H	-1.51088	1.962714	0.388687
Au	-0.78516	0.034552	0.544362	C	1.167257	2.039919	1.594506
P	-2.71525	0.432864	1.831483	H	2.033372	1.448193	1.906751
H	-3.51038	-0.68168	2.1561	H	1.487689	3.090243	1.562071
H	-2.5375	1.012653	3.101101	H	0.390486	1.95394	2.359828
H	-3.67854	1.295509	1.277029	H	-1.10416	-3.09765	2.155476
H	3.710456	0.72484	-1.49791	H	-1.55921	-3.42674	0.04677
H	3.812268	-1.01817	-1.59808	H	0.489922	-3.6248	0.763577
H	-0.0747	-0.23467	-2.71275	H	-1.58032	1.793205	-2.29188
2a				TS3a			
O	2.906956	-1.836906	-1.735306	O	-5.268226	-0.420887	0.373046
C	3.068530	1.548110	0.035526	C	-3.316400	-0.841426	0.309447
C	3.156849	0.330928	0.266623	C	-2.713605	0.293451	0.363540
C	3.934813	-0.914415	0.555527	C	-3.424348	1.606550	0.627497
H	4.702668	-0.98463	-0.222956	H	-3.702681	1.628525	1.688764
C	2.721704	-2.505594	-0.742957	C	-5.532929	0.686693	-0.115466
O	3.133363	-2.107444	0.498985	O	-4.687596	1.702767	-0.115588
C	2.020534	-3.837084	-0.679285	C	-6.857506	1.003372	-0.744135
H	1.823435	-4.190087	-1.691674	H	-7.367315	0.080979	-1.024429
H	2.631669	-4.564499	-0.136672	H	-7.475396	1.542554	-0.016075
H	1.073106	-3.735000	-0.138605	H	-6.722281	1.654415	-1.611732
C	4.566316	-0.872841	1.945828	C	-2.651160	2.860347	0.256818
C	3.036293	2.937890	-0.317312	C	-3.412297	-2.269676	0.184856
C	2.874142	3.279556	-1.783231	C	-4.041865	-2.846864	-1.061859
H	2.916785	4.361809	-1.929946	H	-3.979932	-3.938119	-1.053771
H	3.663400	2.813077	-2.383101	H	-5.096782	-2.561293	-1.123628
H	1.913943	2.914299	-2.165818	H	-3.542431	-2.473376	-1.963365
C	3.199694	3.854264	0.657263	C	-2.909578	-3.015865	1.188274
H	3.315759	3.570852	1.698532	H	-2.490036	-2.564878	2.081677
H	3.234362	4.914185	0.422352	H	-2.896547	-4.1006	1.123372
H	3.797646	-0.80294	2.720813	H	-2.377175	2.848086	-0.802368
H	5.235238	-0.011739	2.030317	H	-1.736294	2.914771	0.854215
H	5.145648	-1.786607	2.105119	H	-3.255898	3.749124	0.457766
Au	0.934784	0.394159	0.149999	Au	-0.616126	0.124127	0.160516
P	-1.366726	-0.00317	0.049179	P	1.724833	0.014102	-0.046786
C	-1.735541	-1.354504	-1.125011	C	2.463614	1.676642	-0.25901
C	-0.957815	-1.483439	-2.288906	C	3.620478	2.065044	0.43208

C	-2.797644	-2.244241	-0.897291	C	1.856247	2.575169	-1.153196
C	-1.248751	-2.48349	-3.216561	C	4.161651	3.336593	0.22839
H	-0.124535	-0.809704	-2.470947	H	4.096815	1.382629	1.12867
C	-3.079129	-3.245483	-1.828248	C	2.404983	3.840134	-1.356869
H	-3.39949	-2.161995	0.002363	H	0.957992	2.283651	-1.692273
C	-2.308236	-3.365025	-2.986583	C	3.557181	4.222982	-0.664083
H	-0.643014	-2.577029	-4.113004	H	5.056065	3.631756	0.769149
H	-3.900238	-3.932354	-1.645559	H	1.931832	4.528085	-2.051513
H	-2.52987	-4.146778	-3.707219	H	3.980299	5.211218	-0.818795
C	-2.059318	-0.472215	1.673301	C	2.511287	-0.731219	1.429743
C	-3.361249	-0.098473	2.042497	C	3.626589	-1.575828	1.321763
C	-1.283283	-1.246458	2.55189	C	1.993123	-0.428059	2.700325
C	-3.878529	-0.502437	3.274628	C	4.215623	-2.104797	2.471953
H	-3.967262	0.509269	1.37762	H	4.033062	-1.824868	0.346542
C	-1.807607	-1.649007	3.779252	C	2.589535	-0.954603	3.845262
H	-0.269261	-1.529715	2.280009	H	1.124573	0.219425	2.793556
C	-3.104877	-1.276718	4.141479	C	3.700352	-1.794894	3.731800
H	-4.884947	-0.207816	3.55678	H	5.076813	-2.760211	2.380812
H	-1.201819	-2.24498	4.455462	H	2.184094	-0.714516	4.823832
H	-3.509509	-1.584891	5.101035	H	4.160325	-2.210031	4.623812
C	-2.272008	1.482999	-0.5146	C	2.254179	-0.98105	-1.489769
C	-3.216564	1.417565	-1.548878	C	3.379891	-0.629096	-2.250064
C	-2.013531	2.712727	0.116155	C	1.527734	-2.136498	-1.822151
C	-3.896519	2.572061	-1.944401	C	3.773375	-1.427796	-3.325558
H	-3.421838	0.474667	-2.045098	H	3.944990	0.265861	-2.008816
C	-2.699973	3.858557	-0.280217	C	1.928344	-2.932399	-2.894447
H	-1.281973	2.773722	0.918417	H	0.649760	-2.412107	-1.243045
C	-3.640678	3.789519	-1.312614	C	3.050538	-2.577914	-3.647861
H	-4.625788	2.516006	-2.747070	H	4.643890	-1.148197	-3.911674
H	-2.499070	4.805219	0.212717	H	1.362054	-3.824439	-3.145947
H	-4.170407	4.684949	-1.624184	H	3.358006	-3.194966	-4.487085
4a				TS5a			
O	-4.99386	0.506598	0.014657	O	5.098328	-1.733816	0.449362
C	-3.529752	0.699408	0.176224	C	2.887178	-1.758857	0.11641
C	-2.7181	-0.353785	0.069373	C	2.750486	-0.386647	-0.058009
C	-3.287299	-1.727429	-0.078646	O	4.995652	0.503245	0.008879
H	-2.898728	-2.235158	-0.963187	C	3.599601	0.643042	-0.121028
C	-5.482062	-0.633319	-0.308641	H	2.808617	-2.158319	1.127586
O	-4.793002	-1.702629	-0.409354	C	5.642594	-0.653393	0.280804
C	-6.939111	-0.703074	-0.61406	C	7.127851	-0.439729	0.341853
H	-7.465921	0.118806	-0.126497	H	7.492281	-0.10144	-0.634359
H	-7.074172	-0.610528	-1.699507	H	7.36435	0.34323	1.06947
H	-7.343321	-1.668663	-0.303221	H	7.62039	-1.372131	0.618326

C	-3.16996	-2.612947	1.15386	C	2.842446	-2.76799	-0.985327
C	-3.285791	2.135061	0.408348	C	3.258408	2.069562	-0.333448
C	-3.992779	3.123374	-0.491692	C	3.95644	3.082981	0.543421
H	-3.689216	4.145496	-0.25201	H	3.588266	4.090946	0.335933
H	-3.760432	2.933499	-1.547401	H	3.796013	2.866374	1.60724
H	-5.081481	3.060737	-0.382873	H	5.038421	3.072975	0.373076
C	-2.451958	2.513266	1.388885	C	2.376713	2.413641	-1.285049
H	-1.987295	1.791835	2.053426	H	1.94054	1.680949	-1.957423
H	-2.216681	3.561454	1.550042	H	2.086274	3.449873	-1.43268
H	-3.588477	-2.115796	2.034623	H	2.918514	-2.305397	-1.971351
H	-2.111495	-2.811576	1.345687	H	1.916423	-3.353541	-0.925698
H	-3.681748	-3.566595	0.994073	H	3.670906	-3.469934	-0.834713
Au	-0.639602	-0.190053	0.060677	Au	0.625855	-0.235079	-0.039248
P	1.714656	-0.023002	-0.045196	P	-1.722758	-0.00895	0.046495
C	2.500679	0.109293	1.60551	C	-2.267471	1.697104	-0.329822
C	1.856283	0.857418	2.604844	C	-3.417782	1.948526	-1.093117
C	3.734349	-0.49752	1.886301	C	-1.527763	2.77509	0.185073
C	2.441983	1.003132	3.861769	C	-3.82224	3.263347	-1.333043
H	0.896985	1.32549	2.398821	H	-3.994764	1.125464	-1.502992
C	4.314135	-0.352211	3.148215	C	-1.940607	4.085157	-0.053456
H	4.239514	-1.085741	1.126583	H	-0.630668	2.591439	0.771301
C	3.670952	0.397065	4.135009	C	-3.087111	4.330448	-0.814011
H	1.937178	1.583487	4.628672	H	-4.711755	3.451113	-1.927126
H	5.267937	-0.827142	3.358829	H	-1.365605	4.913641	0.349797
H	4.123717	0.505447	5.116307	H	-3.404144	5.351662	-1.004124
C	2.479353	-1.478869	-0.856866	C	-2.544467	-1.108386	-1.165507
C	3.53806	-1.349897	-1.767665	C	-3.698529	-1.835198	-0.83774
C	1.99792	-2.759159	-0.534896	C	-2.008182	-1.206434	-2.461134
C	4.107023	-2.487661	-2.344569	C	-4.30797	-2.646623	-1.797489
H	3.916888	-0.367107	-2.029693	H	-4.120573	-1.773152	0.160214
C	2.573879	-3.891628	-1.108381	C	-2.624814	-2.0132	-3.415909
H	1.174479	-2.868516	0.166775	H	-1.11166	-0.649771	-2.723944
C	3.628292	-3.756719	-2.015804	C	-3.774452	-2.735906	-3.084029
H	4.92471	-2.379176	-3.051156	H	-5.199883	-3.208519	-1.536319
H	2.197528	-4.877761	-0.851932	H	-2.206348	-2.08182	-4.415793
H	4.072683	-4.639041	-2.467113	H	-4.250549	-3.369195	-3.826844
C	2.254257	1.446109	-0.999423	C	-2.394531	-0.428455	1.696296
C	3.395676	2.181543	-0.645798	C	-3.490609	0.262018	2.236269
C	1.509005	1.827543	-2.12783	C	-1.814107	-1.48206	2.42211
C	3.786535	3.27903	-1.41557	C	-3.998352	-0.102536	3.484681
H	3.975882	1.904147	0.228813	H	-3.943946	1.082966	1.6897
C	1.90741	2.920832	-2.896077	C	-2.328822	-1.844469	3.66599
H	0.617459	1.269838	-2.403973	H	-0.960353	-2.017785	2.014617
C	3.045885	3.648335	-2.539956	C	-3.420293	-1.153708	4.198902

H	4.669594	3.845146	-1.13382	H	-4.844488	0.438052	3.898446
H	1.326542	3.2081	-3.76778	H	-1.874629	-2.659674	4.22155
H	3.352295	4.50362	-3.135215	H	-3.816306	-1.431862	5.171161
6a				TS7a			
O	-4.99386	0.506598	0.014657	O	5.098328	-1.733816	0.449362
C	-3.529752	0.699408	0.176224	C	2.887178	-1.758857	0.11641
C	-2.7181	-0.353785	0.069373	C	2.750486	-0.386647	-0.058009
C	-3.287299	-1.727429	-0.078646	O	4.995652	0.503245	0.008879
H	-2.898728	-2.235158	-0.963187	C	3.599601	0.643042	-0.121028
C	-5.482062	-0.633319	-0.308641	H	2.808617	-2.158319	1.127586
O	-4.793002	-1.702629	-0.409354	C	5.642594	-0.653393	0.280804
C	-6.939111	-0.703074	-0.61406	C	7.127851	-0.439729	0.341853
H	-7.465921	0.118806	-0.126497	H	7.492281	-0.10144	-0.634359
H	-7.074172	-0.610528	-1.699507	H	7.36435	0.34323	1.06947
H	-7.343321	-1.668663	-0.303221	H	7.62039	-1.372131	0.618326
C	-3.16996	-2.612947	1.15386	C	2.842446	-2.76799	-0.985327
C	-3.285791	2.135061	0.408348	C	3.258408	2.069562	-0.333448
C	-3.992779	3.123374	-0.491692	C	3.95644	3.082981	0.543421
H	-3.689216	4.145496	-0.25201	H	3.588266	4.090946	0.335933
H	-3.760432	2.933499	-1.547401	H	3.796013	2.866374	1.60724
H	-5.081481	3.060737	-0.382873	H	5.038421	3.072975	0.373076
C	-2.451958	2.513266	1.388885	C	2.376713	2.413641	-1.285049
H	-1.987295	1.791835	2.053426	H	1.94054	1.680949	-1.957423
H	-2.216681	3.561454	1.550042	H	2.086274	3.449873	-1.43268
H	-3.588477	-2.115796	2.034623	H	2.918514	-2.305397	-1.971351
H	-2.111495	-2.811576	1.345687	H	1.916423	-3.353541	-0.925698
H	-3.681748	-3.566595	0.994073	H	3.670906	-3.469934	-0.834713
Au	-0.639602	-0.190053	0.060677	Au	0.625855	-0.235079	-0.039248
P	1.714656	-0.023002	-0.045196	P	-1.722758	-0.00895	0.046495
C	2.500679	0.109293	1.60551	C	-2.267471	1.697104	-0.329822
C	1.856283	0.857418	2.604844	C	-3.417782	1.948526	-1.093117
C	3.734349	-0.49752	1.886301	C	-1.527763	2.77509	0.185073
C	2.441983	1.003132	3.861769	C	-3.82224	3.263347	-1.333043
H	0.896985	1.32549	2.398821	H	-3.994764	1.125464	-1.502992
C	4.314135	-0.352211	3.148215	C	-1.940607	4.085157	-0.053456
H	4.239514	-1.085741	1.126583	H	-0.630668	2.591439	0.771301
C	3.670952	0.397065	4.135009	C	-3.087111	4.330448	-0.814011
H	1.937178	1.583487	4.628672	H	-4.711755	3.451113	-1.927126
H	5.267937	-0.827142	3.358829	H	-1.365605	4.913641	0.349797
H	4.123717	0.505447	5.116307	H	-3.404144	5.351662	-1.004124
C	2.479353	-1.478869	-0.856866	C	-2.544467	-1.108386	-1.165507
C	3.53806	-1.349897	-1.767665	C	-3.698529	-1.835198	-0.83774
C	1.99792	-2.759159	-0.534896	C	-2.008182	-1.206434	-2.461134

C	4.107023	-2.487661	-2.344569	C	-4.30797	-2.646623	-1.797489
H	3.916888	-0.367107	-2.029693	H	-4.120573	-1.773152	0.160214
C	2.573879	-3.891628	-1.108381	C	-2.624814	-2.0132	-3.415909
H	1.174479	-2.868516	0.166775	H	-1.11166	-0.649771	-2.723944
C	3.628292	-3.756719	-2.015804	C	-3.774452	-2.735906	-3.084029
H	4.92471	-2.379176	-3.051156	H	-5.199883	-3.208519	-1.536319
H	2.197528	-4.877761	-0.851932	H	-2.206348	-2.08182	-4.415793
H	4.072683	-4.639041	-2.467113	H	-4.250549	-3.369195	-3.826844
C	2.254257	1.446109	-0.999423	C	-2.394531	-0.428455	1.696296
C	3.395676	2.181543	-0.645798	C	-3.490609	0.262018	2.236269
C	1.509005	1.827543	-2.12783	C	-1.814107	-1.48206	2.42211
C	3.786535	3.27903	-1.41557	C	-3.998352	-0.102536	3.484681
H	3.975882	1.904147	0.228813	H	-3.943946	1.082966	1.6897
C	1.90741	2.920832	-2.896077	C	-2.328822	-1.844469	3.66599
H	0.617459	1.269838	-2.403973	H	-0.960353	-2.017785	2.014617
C	3.045885	3.648335	-2.539956	C	-3.420293	-1.153708	4.198902
H	4.669594	3.845146	-1.13382	H	-4.844488	0.438052	3.898446
H	1.326542	3.2081	-3.76778	H	-1.874629	-2.659674	4.22155
H	3.352295	4.50362	-3.135215	H	-3.816306	-1.431862	5.171161
8a				TS9a			
O	-3.596691	1.475972	0.559333	O	-3.467656	1.475229	-0.553601
C	-3.767878	0.122388	0.358065	C	-3.792065	0.160996	-0.290295
C	-2.735356	-0.82156	0.188345	C	-2.773594	-0.851682	0.09681
C	-3.373292	-2.176505	0.073152	C	-3.490675	-2.061384	0.252656
C	-3.02899	2.212202	-0.474567	C	-2.956606	2.212005	0.500601
O	-2.729977	1.71397	-1.52931	O	-2.834716	1.747989	1.608088
C	-2.865718	3.647128	-0.061745	C	-2.581642	3.595444	0.04995
H	-3.811912	4.049217	0.312765	H	-1.655658	3.545738	-0.535646
H	-2.13609	3.714268	0.75298	H	-3.358248	4.020492	-0.591548
H	-2.518878	4.231343	-0.914128	H	-2.418855	4.227586	0.923516
C	-2.972411	-2.930663	-1.214469	C	-2.922634	-3.410135	0.56042
C	-5.022295	-0.460677	0.401214	C	-5.028213	-0.360591	-0.422311
C	-6.309326	0.24473	0.612594	C	-6.293349	0.338403	-0.79719
H	-7.016063	-0.006695	-0.188971	H	-6.744261	-0.111896	-1.690474
H	-6.773698	-0.100683	1.547063	H	-7.036226	0.265522	0.007327
H	-6.181436	1.327256	0.662386	H	-6.109616	1.395605	-1.001912
C	-4.8954	-1.934162	0.217805	C	-4.947533	-1.82449	-0.071925
H	-1.888448	-3.065571	-1.263435	H	-1.901055	-3.335902	0.942804
H	-3.289461	-2.378673	-2.105482	H	-2.88793	-3.98835	-0.372492
H	-3.44671	-3.916735	-1.229234	H	-3.545281	-3.967019	1.267877
H	-3.003706	-2.768916	0.925114	H	-3.010134	-1.196113	1.27383
Au	-0.732158	-0.444723	0.133199	Au	-0.711343	-0.519544	0.069905
P	1.605429	-0.007448	0.037126	P	1.593057	-0.025998	-0.042049

H	-5.461127	-2.25402	-0.668919	H	-5.225833	-2.483359	-0.909561
H	-5.338609	-2.478617	1.06374	H	-5.613678	-2.104789	0.756431
C	2.488241	-1.250694	-0.979129	C	2.395350	-0.093419	1.601467
C	2.174495	-2.609399	-0.801483	C	1.667363	0.323941	2.728971
C	3.467154	-0.884613	-1.914153	C	3.719611	-0.532152	1.755165
C	2.839121	-3.585557	-1.541805	C	2.262081	0.311342	3.990182
H	1.415016	-2.904193	-0.081179	H	0.638305	0.658471	2.622149
C	4.124874	-1.867171	-2.657815	C	4.306962	-0.546584	3.021509
H	3.714874	0.161022	-2.065991	H	4.289208	-0.866767	0.893685
C	3.813815	-3.214919	-2.472607	C	3.581267	-0.125018	4.137432
H	2.593545	-4.633557	-1.396574	H	1.693596	0.635424	4.856953
H	4.879956	-1.576025	-3.382107	H	5.331031	-0.890136	3.134514
H	4.326596	-3.975794	-3.053721	H	4.041083	-0.140710	5.121279
C	2.389622	-0.03251	1.691897	C	1.854056	1.666516	-0.696621
C	1.679330	0.489579	2.785991	C	1.099753	2.081416	-1.808420
C	3.684445	-0.537329	1.885504	C	2.782502	2.548007	-0.124631
C	2.261567	0.515669	4.052578	C	1.281373	3.356321	-2.343398
H	0.671509	0.873566	2.647571	H	0.375884	1.406411	-2.259095
C	4.260498	-0.512241	3.157093	C	2.955028	3.826489	-0.661022
H	4.239475	-0.953178	1.050359	H	3.366902	2.243094	0.737685
C	3.552289	0.014135	4.239097	C	2.208148	4.231148	-1.768224
H	1.706135	0.919975	4.893795	H	0.700578	3.666703	-3.207306
H	5.262264	-0.906433	3.300716	H	3.674614	4.504153	-0.211052
H	4.002913	0.028981	5.227184	H	2.345707	5.225651	-2.182554
C	1.963438	1.630800	-0.698300	C	2.521858	-1.159844	-1.138193
C	1.133885	2.106222	-1.728445	C	2.19493	-2.526127	-1.132572
C	3.056461	2.404004	-0.276954	C	3.563433	-0.701966	-1.959446
C	1.404701	3.332756	-2.335115	C	2.906059	-3.421284	-1.930345
H	0.276499	1.52351	-2.055962	H	1.386323	-2.889088	-0.502924
C	3.318089	3.633059	-0.884915	C	4.268787	-1.602592	-2.760067
H	3.698879	2.052718	0.524683	H	3.821483	0.352308	-1.980147
C	2.495773	4.09697	-1.913929	C	3.942631	-2.95989	-2.74604
H	0.760976	3.691437	-3.133036	H	2.648043	-4.47625	-1.920229
H	4.164287	4.227286	-0.552569	H	5.071962	-1.24097	-3.39538
H	2.702755	5.053919	-2.384257	H	4.491966	-3.65685	-3.372148
10a				(H ₂ O) ₄			
O	4.359768	1.060289	0.190861	O	-1.90725	0.064704	0.048907
C	3.780609	-0.189445	0.078724	H	-1.31096	-0.73456	0.052213
C	2.937696	-0.801390	1.120775	H	-2.39495	-0.00057	-0.78614
C	2.601096	-2.087428	0.720297	H	0.734534	-1.31095	-0.05251
C	3.553479	2.146795	0.416404	O	-0.0647	-1.90728	-0.04891
O	2.347708	2.065469	0.496442	H	0.000577	-2.39447	0.786443
C	4.375666	3.398095	0.546482	H	1.310952	0.734556	0.052237

H	5.068417	3.302804	1.389314	O	1.907256	-0.06471	0.048907
H	4.979886	3.546229	-0.354415	H	2.394936	0.000586	-0.78615
H	3.717849	4.253214	0.701955	H	-0.73453	1.310945	-0.0525
C	3.987504	-1.039336	-0.949938	O	0.064703	1.907279	-0.04891
C	4.76197	-0.801012	-2.204605	H	-0.00059	2.394499	0.786423
H	5.566032	-1.538727	-2.320658				
H	4.118435	-0.889732	-3.089673				
H	5.211201	0.195180	-2.206216				
C	3.263523	-2.326346	-0.629173				
Au	0.708734	-0.593135	0.401386				
P	-1.468529	0.108958	-0.091746				
H	3.965143	-3.169078	-0.532717				
H	2.554338	-2.617774	-1.416095				
H	2.836516	-0.406573	2.127696				
C	2.097203	-3.211778	1.583045				
H	1.362261	-3.831127	1.058868				
H	2.936973	-3.86571	1.855614				
H	1.645340	-2.843473	2.508107				
C	-2.531678	-1.289509	-0.603923				
C	-2.015889	-2.251165	-1.489113				
C	-3.856268	-1.400982	-0.155389				
C	-2.818135	-3.304346	-1.924583				
H	-0.989379	-2.174409	-1.839427				
C	-4.652893	-2.462376	-0.590846				
H	-4.265716	-0.667704	0.532090				
C	-4.136897	-3.412101	-1.473764				
H	-2.413882	-4.043286	-2.610238				
H	-5.67645	-2.544695	-0.237473				
H	-4.758879	-4.237046	-1.808504				
C	-1.515519	1.344424	-1.436870				
C	-0.520129	2.335837	-1.488683				
C	-2.544761	1.337087	-2.391388				
C	-0.565575	3.31127	-2.48451				
H	0.284772	2.348055	-0.758714				
C	-2.577664	2.315017	-3.386884				
H	-3.315343	0.573308	-2.362563				
C	-1.590671	3.301296	-3.434127				
H	0.203896	4.07693	-2.521135				
H	-3.374312	2.303397	-4.124859				
H	-1.61837	4.059605	-4.211234				
C	-2.245515	0.867394	1.379921				
C	-2.082998	0.248588	2.631529				
C	-3.012924	2.03738	1.279609				
C	-2.687764	0.790301	3.764183				

H	-1.486993	-0.656582	2.71987				
C	-3.611613	2.577439	2.419919				
H	-3.141663	2.528745	0.320575				
C	-3.45102	1.956663	3.659503				
H	-2.558762	0.306712	4.727998				
H	-4.202022	3.485057	2.336412				
H	-3.916143	2.381663	4.544088				
2b				TS3b			
O	-0.52483	1.171114	-2.848641	O	-1.416489	0.426319	-3.664322
C	-1.040154	1.86662	0.702267	C	-1.396484	0.429276	-1.680498
C	-0.099824	1.928473	-0.105364	C	-0.154657	0.431754	-1.339695
C	0.806485	2.656021	-1.040896	C	0.96985	0.62303	-2.340153
H	0.171483	3.34337	-1.611547	H	0.947587	1.668745	-2.671766
C	0.691122	1.136388	-2.885722	C	-0.425793	-0.14015	-4.150154
O	1.468001	1.784006	-1.983874	O	0.751758	-0.178679	-3.552768
C	1.521512	0.410819	-3.909868	C	-0.454005	-0.82359	-5.484666
H	0.882855	-0.245904	-4.501516	H	-1.480131	-1.07747	-5.753029
H	1.998309	1.141493	-4.573157	H	-0.050815	-0.138852	-6.240574
H	2.32106	-0.159979	-3.428701	H	0.179167	-1.714392	-5.471856
C	1.909082	3.415286	-0.307751	C	2.359635	0.253016	-1.853327
C	-2.227073	1.840104	1.508685	C	-2.814378	0.394204	-1.447468
C	-3.529427	1.573788	0.783147	C	-3.594443	-0.821513	-1.891217
H	-4.350417	1.466946	1.496969	H	-4.640763	-0.739348	-1.586152
H	-3.766045	2.402246	0.10487	H	-3.559368	-0.92124	-2.980814
H	-3.451279	0.665845	0.175796	H	-3.174773	-1.737263	-1.458641
C	-2.126647	2.083881	2.830296	C	-3.365315	1.453105	-0.821787
H	-1.17145	2.279434	3.307381	H	-2.778219	2.322546	-0.544327
H	-3.011598	2.10314	3.459691	H	-4.420835	1.460216	-0.563231
H	2.543826	2.727028	0.257578	H	2.390927	-0.776303	-1.484902
H	1.468527	4.14039	0.382151	H	2.640963	0.91881	-1.03182
H	2.526486	3.949616	-1.035059	H	3.085564	0.370916	-2.662941
Au	0.129618	-0.220356	0.488787	Au	0.166004	0.212221	0.734445
P	0.666059	-2.458453	0.817097	P	0.624159	-0.031815	3.019134
C	1.506995	-3.205775	-0.634464	C	0.367638	-1.732852	3.664014
H	1.709024	-4.266579	-0.451171	H	0.581395	-1.769045	4.737865
H	0.865681	-3.109146	-1.515139	H	-0.665837	-2.048944	3.493959
H	2.452561	-2.690673	-0.827446	H	1.044657	-2.40644	3.131142
C	1.769981	-2.780923	2.248917	C	2.370113	0.360756	3.434527
H	1.300763	-2.41706	3.167596	H	2.551089	0.222418	4.505944
H	1.965439	-3.854108	2.34703	H	3.02302	-0.306365	2.865738
H	2.718979	-2.254084	2.113012	H	2.597843	1.395803	3.163548
C	-0.830383	-3.485029	1.091898	C	-0.385039	1.053514	4.109752
H	-0.556331	-4.541484	1.184962	H	-0.111379	0.903095	5.159671

H	-1.338581	-3.164185	2.005876	H	-0.223696	2.102511	3.844523
H	-1.513917	-3.354191	0.248506	H	-1.447063	0.824026	3.981721
H	-2.957453	-1.089878	-1.956392	H	1.949727	-3.091845	0.652902
O	-2.121181	-0.861998	-1.520641	O	2.517677	-2.467391	1.129867
H	-1.724615	-0.170202	-2.08362	H	3.397876	-2.87511	1.106672
4b				TS5b			
O	-1.093807	-0.312392	-3.509926	O	-3.816032	-1.68782	-0.130055
C	-1.090632	-0.245234	-2.024401	C	-1.594599	-1.750822	0.018619
C	0.016402	0.1479	-1.393146	C	-1.399758	-0.374422	-0.008978
C	1.231728	0.525474	-2.176274	O	-3.61583	0.584065	-0.05583
H	1.551807	1.544498	-1.948519	C	-2.210195	0.687703	-0.058553
C	-0.134724	0.191468	-4.195076	H	-1.623276	-2.282255	-0.932563
O	0.940859	0.650928	-3.684706	C	-4.31443	-0.573258	-0.080826
C	-0.308742	0.276103	-5.672435	C	-5.792768	-0.31412	-0.033304
H	-0.956654	-0.530676	-6.020867	H	-6.05249	0.165478	0.91697
H	-0.79238	1.231865	-5.912878	H	-6.079073	0.372592	-0.836183
H	0.661692	0.245474	-6.170768	H	-6.332845	-1.25596	-0.1317
C	2.402397	-0.443202	-2.083982	C	-1.475798	-2.610689	1.236057
C	-2.426249	-0.658891	-1.554965	C	-1.81622	2.115002	-0.120287
C	-3.020441	-1.911426	-2.160111	C	-2.608676	3.002681	-1.052783
H	-3.981183	-2.143871	-1.693968	H	-2.185589	4.010101	-1.075309
H	-3.187343	-1.79754	-3.237222	H	-2.611783	2.605182	-2.075546
H	-2.354044	-2.773156	-2.026228	H	-3.653948	3.078216	-0.734415
C	-3.061859	0.06868	-0.624009	C	-0.80519	2.577854	0.632444
H	-2.645391	0.992459	-0.235497	H	-0.274453	1.962798	1.353595
H	-4.024854	-0.245611	-0.23139	H	-0.490217	3.614872	0.550833
H	2.089548	-1.460974	-2.338691	H	-1.427988	-2.022005	2.154334
H	2.77593	-0.447368	-1.055835	H	-0.590506	-3.254535	1.163631
H	3.213111	-0.133532	-2.750002	H	-2.347315	-3.275151	1.263322
Au	0.173459	0.280353	0.683643	Au	0.720356	-0.297804	-0.15996
P	0.403689	0.461685	3.021364	P	3.049484	-0.107722	-0.409573
C	-0.539433	-0.793883	3.97602	C	4.012339	-0.703334	1.036503
H	-0.404808	-0.637505	5.051853	H	3.795407	-1.759283	1.223233
H	-1.604588	-0.726796	3.734876	H	5.086068	-0.586066	0.853471
H	-0.167066	-1.784019	3.699703	H	3.719925	-0.11494	1.910821
C	2.136925	0.286381	3.605152	C	3.722438	-1.021619	-1.857283
H	2.186316	0.370238	4.696171	H	4.805943	-0.878624	-1.930094
H	2.506814	-0.693793	3.29401	H	3.50934	-2.089772	-1.755076
H	2.76305	1.06423	3.157939	H	3.251519	-0.661874	-2.77687
C	-0.159848	2.083494	3.688256	C	3.590811	1.631596	-0.649313
H	-0.021201	2.123243	4.774043	H	3.294137	2.220353	0.222637
H	0.409678	2.895439	3.226237	H	4.678626	1.680796	-0.766933
H	-1.219279	2.232323	3.458992	H	3.114424	2.054188	-1.538683

H	0.862652	-2.864272	1.352054	H	2.118741	2.266294	3.193549
O	1.453848	-2.727841	2.107733	O	1.954482	1.409114	2.769374
H	1.899277	-3.580535	2.232769	H	1.616262	0.849639	3.485724
6b				TS7b			
O	-1.576387	1.009151	-1.73126	O	-2.172051	1.32356	-0.92487
C	-1.773476	1.243536	1.849966	C	-2.178643	0.981106	0.413614
C	-0.757138	1.274812	0.988163	C	-1.010266	0.790168	1.144422
O	-0.241532	2.678123	-0.91335	C	-1.170215	0.95514	2.536129
C	0.043549	2.19606	0.33038	C	-3.344646	0.334336	2.376279
H	-2.144685	0.280788	2.197695	C	-2.240842	0.32112	-1.87087
C	-1.143319	2.126156	-1.82933	O	-2.239356	-0.848455	-1.56745
C	-1.407531	3.113511	-2.926115	C	-2.294875	0.900754	-3.25448
H	-1.860673	4.019293	-2.508505	H	-1.385433	1.479777	-3.44837
H	-0.466831	3.40917	-3.40211	H	-2.386149	0.095179	-3.98315
H	-2.076156	2.667344	-3.662388	H	-3.141831	1.588185	-3.34475
C	-2.479647	2.456023	2.398741	C	-0.351308	0.261747	3.579603
C	1.284516	2.800292	0.855855	C	-3.413058	0.91412	1.110639
C	2.169292	3.570006	-0.096502	C	-4.673849	1.517766	0.557277
H	3.05637	3.933773	0.427153	H	-5.167002	0.793627	-0.10515
H	2.498623	2.94137	-0.931952	H	-5.380232	1.748531	1.359658
H	1.646616	4.430857	-0.526361	H	-4.474866	2.420365	-0.02655
C	1.549889	2.696263	2.172043	H	-4.102749	0.559135	3.124735
H	0.910719	2.136433	2.847079	H	-2.800022	-0.588191	2.540882
H	2.423169	3.176643	2.602022	H	0.549593	0.859852	3.778409
H	-2.044912	3.390627	2.033093	H	-0.032838	-0.73474	3.262386
H	-2.441163	2.457207	3.495186	H	-0.898312	0.194085	4.52558
H	-3.541477	2.431782	2.122387	H	-1.661858	1.870719	2.869294
Au	0.176531	-0.547515	0.292073	Au	0.760077	0.133844	0.267799
P	0.909617	-2.69777	-0.283199	P	2.720312	-0.714171	-0.72972
C	2.665769	-3.067225	0.117306	C	3.250012	-2.298262	0.034396
H	2.835717	-2.947255	1.191268	H	2.426668	-3.011701	-0.05263
H	2.915606	-4.093661	-0.172487	H	4.136707	-2.694413	-0.47204
H	3.323458	-2.375445	-0.417042	H	3.480707	-2.146546	1.093016
C	-0.075121	-3.988445	0.572906	C	4.187997	0.391194	-0.62037
H	0.242567	-4.986635	0.252887	H	4.42096	0.599052	0.428194
H	0.05075	-3.901555	1.656057	H	5.057876	-0.076618	-1.09396
H	-1.128812	-3.840073	0.322946	H	3.977777	1.341042	-1.121
C	0.716259	-3.059215	-2.072572	C	2.534389	-1.097591	-2.51639
H	1.326669	-2.370636	-2.664294	H	3.46759	-1.507852	-2.91737
H	1.024544	-4.088134	-2.28848	H	1.729218	-1.830072	-2.62433
H	-0.336453	-2.923982	-2.335979	H	2.277206	-0.190331	-3.07146
H	-2.231502	-0.912288	-1.440561	H	-0.375709	-3.697513	-1.19348
O	-2.314738	-1.846553	-1.186073	O	-0.029243	-2.792098	-1.1792

H	-3.269304	-2.011785	-1.143022	H	-0.811013	-2.226364	-1.30755
12c				TS13c			
C	1.343314	0.446253	-1.999475	C	-2.336641	0.431382	-0.328453
C	1.306326	0.475159	-0.581091	C	-1.282942	-0.58312	-0.44415
C	2.702187	0.477412	-0.078687	C	-1.915736	-1.8244	-0.542308
H	2.791918	-0.565799	0.318098	H	-1.681105	-1.946001	0.896865
O	2.573981	-2.437405	0.923335	O	-1.638792	-2.290143	2.074249
C	3.014452	1.43685	1.083291	C	-1.284385	-3.105476	-1.051149
C	2.645474	0.505009	-2.478502	C	-3.582446	-0.113358	-0.450542
C	3.121695	0.472797	-3.889716	C	-4.932991	0.534663	-0.390369
H	2.786125	1.374786	-4.417662	H	-5.082847	1.199667	-1.249188
H	4.211149	0.42296	-3.941295	H	-5.727026	-0.216455	-0.403109
H	2.692545	-0.373758	-4.436447	H	-5.050063	1.1509	0.506456
C	3.587288	0.612191	-1.32826	C	-3.415971	-1.592665	-0.652478
H	2.355858	1.237867	1.93375	H	-0.212805	-3.131851	-0.826965
H	2.882778	2.482815	0.784731	H	-1.392676	-3.184909	-2.140094
H	4.049481	1.302125	1.41247	H	-1.757385	-3.996033	-0.618996
Au	-0.33773	0.386733	0.631881	Au	0.746714	-0.21869	-0.430352
P	-2.204373	0.28882	2.094272	P	3.073288	0.215355	-0.470715
H	4.10493	1.583742	-1.372104	H	-3.784524	-1.885554	-1.648147
H	4.379191	-0.146255	-1.404955	H	-4.023176	-2.163813	0.065382
H	1.64233	-2.683873	1.132439	H	-0.896331	-1.775919	2.590215
H	3.077707	-2.675757	1.715993	H	-1.406168	-3.235522	2.109525
H	-0.607947	-3.030729	0.696608	H	0.47729	-0.218039	3.157629
O	-0.068994	-3.136509	1.516133	O	0.223754	-1.150013	3.396821
H	-0.12302	-4.079893	1.738182	H	0.069578	-1.155756	4.354851
C	-2.95738	-1.379609	2.236603	C	3.914766	-0.048549	1.143435
H	-3.774389	-1.370541	2.965801	H	4.975433	0.216813	1.077996
H	-3.336359	-1.69215	1.259613	H	3.426504	0.566237	1.904586
H	-2.18579	-2.092534	2.540206	H	3.824749	-1.098372	1.438535
C	-1.792531	0.775286	3.81994	C	4.013696	-0.818431	-1.66886
H	-1.399839	1.796387	3.83681	H	3.624763	-0.660163	-2.679187
H	-2.681185	0.72363	4.45809	H	5.078254	-0.561586	-1.65126
H	-1.027003	0.102711	4.218179	H	3.897567	-1.877018	-1.417778
C	-3.587644	1.402094	1.611396	C	3.490361	1.946654	-0.935184
H	-4.419365	1.310163	2.318107	H	4.575529	2.09496	-0.940984
H	-3.244446	2.440891	1.596547	H	3.092735	2.169267	-1.929836
H	-3.939183	1.141083	0.608836	H	3.038124	2.641281	-0.221348
C	0.101418	0.3104	-2.838196	C	-2.020142	1.870333	-0.088682
F	-0.397161	-0.962555	-2.752863	F	-1.469847	2.050704	1.167409
F	0.325051	0.549205	-4.14004	F	-3.09513	2.668533	-0.142314
F	-0.878187	1.135204	-2.428258	F	-1.105358	2.351354	-0.957239

H	-2.004164	-3.452997	-1.250626	H	0.875751	2.088424	3.345659
O	-1.692108	-2.710776	-0.709042	O	0.898038	1.384805	2.676582
H	-1.343024	-2.061282	-1.340869	H	0.251708	1.650895	1.998244
12d				TS13d			
C	0.981880	0.407569	-1.851515	C	-1.961682	-0.664594	0.474982
C	0.973565	0.433987	-0.426187	C	-0.863914	0.271620	0.701381
C	2.365145	0.392627	0.039076	C	-1.415662	1.433496	1.272017
H	2.441096	-0.713239	0.314853	H	-1.512882	2.013500	0.037141
O	2.562908	-2.467632	0.752517	O	-1.704775	2.715154	-1.047815
C	2.750202	1.184044	1.294181	C	-0.631358	2.472624	2.054548
C	2.269667	0.497712	-2.354578	C	-3.137701	-0.205191	1.002765
C	2.721970	0.491359	-3.775894	C	-4.502210	-0.824638	0.996507
H	3.803363	0.624415	-3.848358	H	-5.217351	-0.199722	1.537371
H	2.448567	-0.45214	-4.264186	H	-4.871773	-0.967788	-0.025434
H	2.224175	1.282906	-4.3468	H	-4.487232	-1.815729	1.462000
C	3.229665	0.587333	-1.217267	C	-2.872832	1.136323	1.61971
H	2.110504	0.903856	2.136099	H	0.362723	2.616536	1.620371
H	2.655264	2.263686	1.132133	H	-0.500756	2.160562	3.098185
H	3.786566	0.968560	1.571647	H	-1.144753	3.440480	2.060836
Au	-0.680317	0.386829	0.779191	Au	1.106668	-0.062779	0.207629
P	-2.590558	0.375426	2.181142	P	3.385641	-0.491036	-0.264501
H	3.718015	1.574822	-1.228487	H	-3.003339	1.079101	2.711857
H	4.037075	-0.15213	-1.3269	H	-3.596138	1.889163	1.272655
H	1.878975	-2.812429	0.139178	H	-1.760763	2.043200	-1.789625
H	3.417264	-2.659579	0.312134	H	-2.589196	3.167379	-0.981287
H	5.173585	-3.30132	-1.276499	H	-4.821756	3.756717	-1.34146
O	5.014384	-2.545466	-0.688975	O	-4.145400	3.833691	-0.649516
H	5.775870	-2.539017	-0.087084	H	-4.142547	4.771614	-0.398969
C	-4.181973	0.189436	1.276991	C	3.669418	-1.867978	-1.452575
H	-5.027209	0.202939	1.973314	H	4.741077	-2.031628	-1.608539
H	-4.296433	1.006769	0.558739	H	3.219152	-2.787164	-1.066096
H	-4.187893	-0.755482	0.725598	H	3.199708	-1.633367	-2.412452
C	-2.596472	-0.971300	3.434755	C	4.307101	0.934617	-0.976918
H	-1.711728	-0.886830	4.072697	H	4.265318	1.78318	-0.287551
H	-3.495262	-0.914294	4.058003	H	5.35475	0.669944	-1.15566
H	-2.567709	-1.944354	2.935644	H	3.848796	1.237743	-1.922986
C	-2.782432	1.923767	3.155835	C	4.351775	-0.965149	1.228519
H	-3.675469	1.873243	3.787791	H	5.397569	-1.160698	0.968514
H	-1.903009	2.073905	3.788981	H	4.310334	-0.159261	1.967259
H	-2.870215	2.779070	2.479343	H	3.919519	-1.864538	1.677017
C	-0.285216	0.270516	-2.648375	C	-1.758467	-1.94891	-0.263258
F	-0.909614	-0.914767	-2.351895	F	-1.338389	-1.70647	-1.558376
F	-0.073619	0.276299	-3.974083	F	-2.874678	-2.686991	-0.361011

F	-1.168305	1.244748	-2.364231	F	-0.800274	-2.717555	0.289072
H	0.087102	-2.552748	-1.595846	H	-1.754499	-0.071787	-2.536953
O	0.609962	-3.241384	-1.155262	O	-1.911011	0.811253	-2.916193
H	-0.029256	-3.924467	-0.9017	H	-1.324638	0.872675	-3.686361