Electronic Supplementary Material (ESI) for Dalton Transactions

Carbonylation of Alkyl Halides with $[Fe(CO)_3(NO)]^-$: *In Silico* Identification of a Common Intermediate

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1. Computational Details

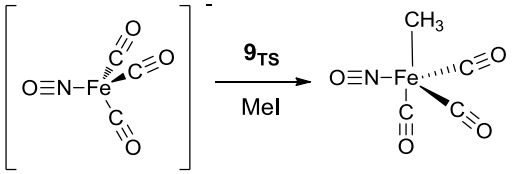
Density functional theory (DFT) calculations were carried out using TURBOMOLE v6.3[1] in combination with the graphical interface TmoleX v3.1 and v3.3.[2] The BP86-functional[3, 4] in combination with the split valence basis set def2-SVP and the triple-ζ basis set def2-TZVP by Ahlrichs[5] was used. Geometries were optimised using the def2-SVP basis set. At these geometries, energies were calculated using the def2-TZVP basis set. An effective core potential (ECP) was used for iodine freezing 28 inner electrons.[6] The multipole-accelerated resolution of identity approach (MARIJ)[7] was used. Solvent effects of THF ($\varepsilon = 7.36$)[8] were approximated by the conductor-like screening model (COSMO).[9] Convergence criteria were set to minimum 10^{-4} Hartree/Bohr for the gradient norm and to 10^{-8} Hartree for the change in energy. Derivatives of quadrature weights have been used in all calculations. Minima were confirmed by the absence of imaginary frequencies and transition states were confirmed by a single imaginary frequency, see below. Visual inspection of the transition modes confirmed a direct connection between reactants and products in all cases. Energies are given as potential energies plus zero-point vibrational energies (ZPE) throughout. All species considered are in their closed-shell configuration. All HOMO-LUMO gaps obtained are > 0.8 eV. Open-shell single point calculations at all stationary points starting with triplet guess MOs resulted in closed-shell singlet states when using Fermi thermal smearing techniques, confirming intersystem crossing to be unlikely. Thus, a spin-restricted treatment was used throughout.

2. Evaluation of Basis Sets

Using the BP86-functional we tested:

(i) Can def2-SVP geometries be used in combination with def2-TZVP energies?
(ii) Are diffuse functions required?

We have calculated ground states **1** and **2** along with the transition state $\mathbf{3}_{TS}$ for a number of different basis sets.* As can be seen from Table S1 it is not sufficient to calculate geometries and energies at the def2-SVP level (Entry 1). However, calculating def2-TZVP basis set energies at the def2-SVP geometries gives values in good agreement with energies obtained at def2-TZVP geometries (Entries 2 and 3).
The use of recent def2-SVPD/def2-TZVPD[10] basis sets containing a small number of diffuse functions have no significant effect on the overall energetics (Entries 4-6).
We therefore decided to utilize def2-SVP basis set for geometry optimizations and then calculated energies at the def2-TZVP for the overall pathway.

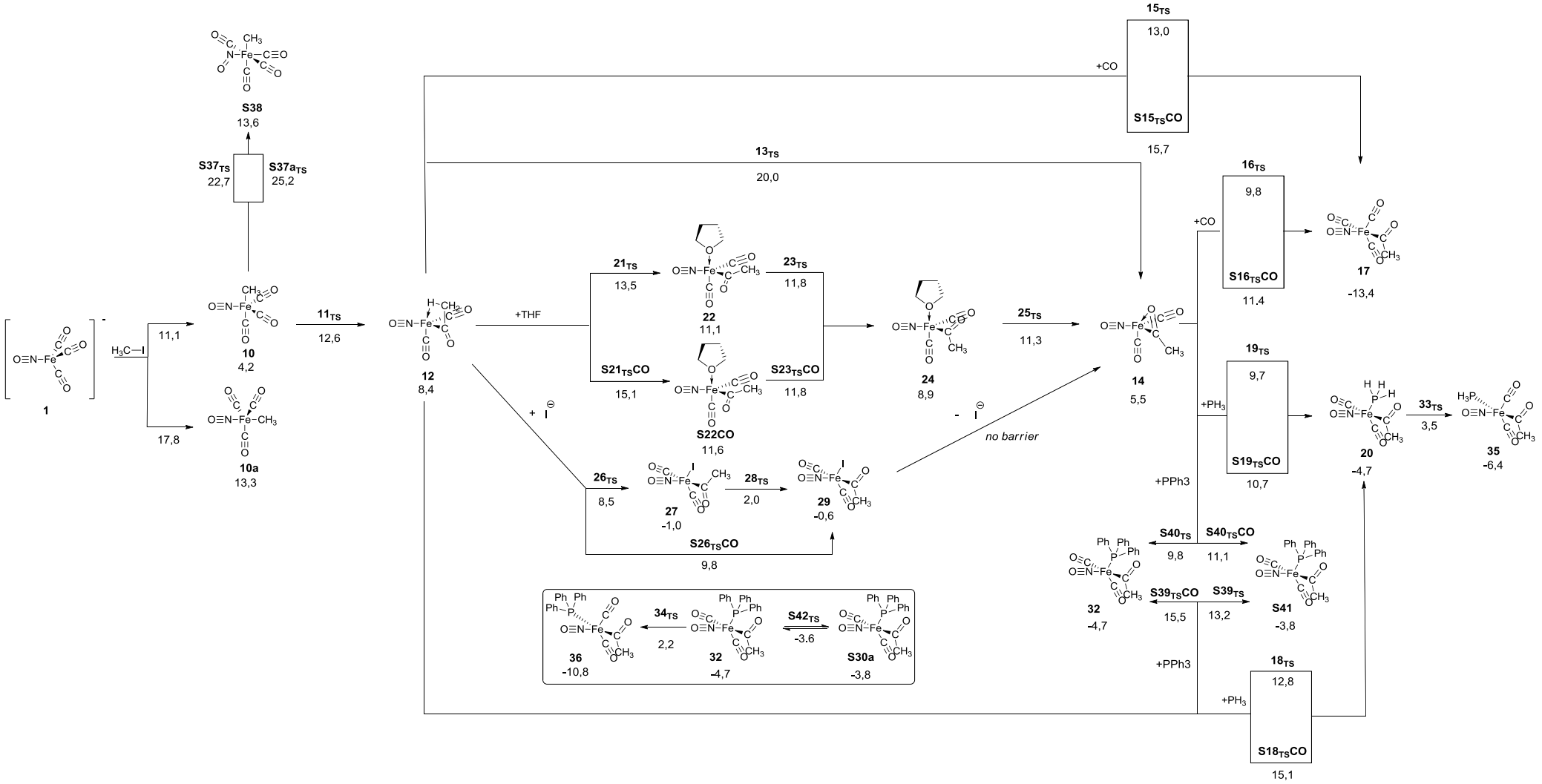


1 **10**

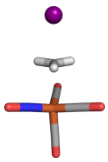
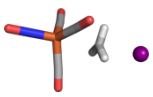
Entry	Basis set used for geo. opt. and ZPE	Basis set used for energy	ΔE($\mathbf{9}_{TS}$) (kcal/mol)	ΔE_{ZPE} ($\mathbf{9}_{TS}$) (kcal/mol)	ΔE(**10**) (kcal/mol)	ΔE_{ZPE}(**10**) (kcal/mol)
1	def2-SVP	def2-SVP	8.64	8.25	1.31	1.89
2	def2-SVP	def2-TZVP	11.48	11.09	3.65	4.23
3	def2-TZVP	def2-TZVP	11.55	11.37	3.76	4.55
4[10]	def2-SVPD	def2-SVPD	10.38	10.35	3.41	4.29
5[10]	def2-SVPD	def2-TZVPD	11.86	11.83	4.12	5.00
6[10]	def2-TZVPD	def2-TZVPD	11.90	11.75	4.18	5.01

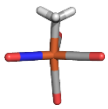
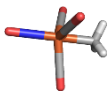
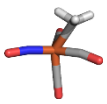
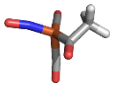
* BP86 functional and COSMO ($\varepsilon = 7.36$) used for all calculations.

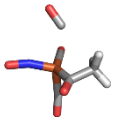
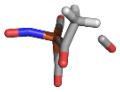
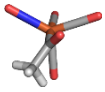
2. Depiction of the Total Pathway

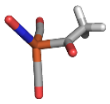
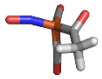
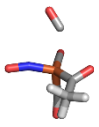


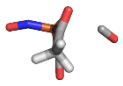
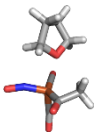
3. XYZ-Coordinates and Energies

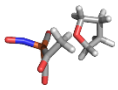
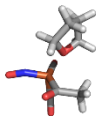
Structure		x	y	z	E[H]	ZPE[H]	E+ZPE[H]	Imag. Freq. [Hz]
1 	Fe	1.15117	0.86639	-1.21437	-1734.3934194	0.0322178	-1734.3612016	
	C	0.89219	1.31175	-2.90742				
	C	2.90925	0.68097	-1.1326				
	N	0.48261	1.87952	-0.09505				
	C	0.58764	-0.8106	-1.16936				
	O	4.08061	0.57694	-1.05431				
	O	0.70372	1.63319	-4.02555				
	O	0.19394	-1.92018	-1.11567				
	O	-0.00115	2.61281	0.7148				
Methyl Iodide 	C	-0.05645	0.03999	-0.01736	-337.7907187	0.0352512	-337.7554675	
	H	0.30421	1.07352	-0.15062				
	H	-0.48404	-0.36531	-0.94951				
	H	-0.76548	-0.03844	0.82356				
	I	1.67242	-1.18491	0.48298				
Iodide	I				-298.0317197			
9_{TS} 	Fe	1.09467	1.27309	-2.01945	-2072.1658364	0.0668434	-2072.0989930	296.41
	C	2.53572	2.00359	-2.74976				
	C	1.93558	0.03653	-1.03963				
	C	-0.9834	-0.10179	-1.01676				
	N	0.2393	2.51364	-1.31946				
	C	0.50346	0.42358	-3.47728				
	O	2.50374	-0.75067	-0.38572				
	O	3.4749	2.51847	-3.21947				
	O	0.11758	-0.106	-4.44718				
	O	-0.32775	3.43375	-0.83947				
	H	-0.71298	0.23597	-0.01382				
	H	-1.66354	0.4943	-1.62932				
	H	-0.618	-1.06329	-1.38547				
	I	-3.16724	-1.41534	0.05849				
$9a_{TS}$ 	Fe	1.0905	1.27746	-2.01442	-2072.1550892	0.0667336	-2072.0883556	260.83
	N	2.36784	2.12874	-2.62321				
	C	1.77106	0.08204	-0.86781				
	C	-1.00808	-0.12084	-1.01364				
	C	0.02531	2.46398	-1.19929				
	C	0.28494	0.49354	-3.40851				
	O	2.28809	-0.66968	-0.13608				
	O	3.27897	2.73586	-3.05706				
	O	-0.18606	0.01555	-4.36639				
	O	-0.6182	3.29606	-0.68804				
	H	-0.82013	0.15898	0.02618				
	H	-1.76478	0.42309	-1.58498				

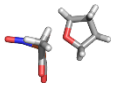
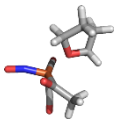
	H	-0.65774	-1.09009	-1.37792				
	I	-3.23997	-1.6076	0.0515				
10	Fe	0.74928	1.07404	-1.85432	-1774.1466016	0.0683954	-1774.0782062	
	C	2.23549	1.76424	-2.61849				
	C	1.68688	-0.11054	-0.8734				
	C	-0.89195	-0.04079	-1.06578				
	N	0.04996	2.44721	-1.22719				
	C	0.21356	0.28388	-3.38187				
	O	2.25653	-0.87277	-0.20888				
	O	3.18724	2.20575	-3.1079				
	O	-0.17659	-0.22149	-4.35112				
	O	-0.44724	3.40443	-0.78381				
	H	-0.89734	0.13034	0.02559				
	H	-1.80735	0.37204	-1.52623				
	H	-0.79933	-1.11837	-1.28792				
10a	Fe	0.90366	0.9966	-1.95705	-1774.1319787	0.0682482	-1774.0637305	
	N	2.22781	1.7503	-2.61633				
	C	1.69692	-0.14424	-0.8079				
	C	-0.83695	0.00553	-1.09069				
	C	0.03922	2.40104	-1.22789				
	C	0.15822	0.26821	-3.4285				
	O	2.21038	-0.87789	-0.06862				
	O	3.15425	2.27764	-3.07786				
	O	-0.31954	-0.19976	-4.37778				
	O	-0.51515	3.30733	-0.75917				
	H	-0.84095	0.1838	-0.0011				
	H	-1.74921	0.42595	-1.54896				
	H	-0.76954	-1.07654	-1.29949				
11_{TS}	Fe	-0.02887	0.12493	0.15243	-1774.1330635	0.0681184	-1774.0649451	273.39
	C	0.4943	0.30531	-1.53311				
	C	1.66943	-0.0903	0.77488				
	C	-0.89654	-1.29446	1.61839				
	N	-0.83939	1.55906	0.4457				
	C	-0.89452	-1.37801	-0.22643				
	O	2.76309	-0.20707	1.14527				
	O	0.80853	0.41534	-2.64537				
	O	-1.42029	-2.29345	-0.75555				
	O	-1.41513	2.57624	0.47693				
	H	-0.57282	-0.51191	2.32818				
	H	-1.99199	-1.40522	1.69722				
	H	-0.36792	-2.23687	1.83913				
12	N	2.79934	0.93587	-2.85801	-1774.1407077	0.0690965	-1774.0716112	
	C	1.54087	0.33493	-0.51338				
	C	0.33202	-0.53498	-0.88775				
	C	1.02116	2.6922	-1.42607				
	C	0.18424	1.44708	-3.62757				
	O	2.22972	0.29553	0.46884				

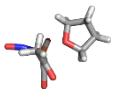
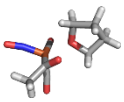
	O	3.87195	1.03348	-3.31707				
	O	-0.49643	1.68297	-4.53541				
	O	0.94082	3.76236	-0.96919				
	H	-0.46555	-0.36686	-0.13893				
	H	-0.12577	-0.32896	-1.89488				
	H	0.65295	-1.59433	-0.89868				
CO	C	0.3958	0.12782	0	-113.3660233	0.0049024	-113.3611209	
	O	-0.1988	1.10218	-0.0001				
15_{TS}	Fe	0.1729	-0.00643	-0.09852	-1887.5003340	0.0750061	-1887.4253279	128.67
	C	0.88657	0.13404	-1.70351				
	C	1.74727	-0.50447	0.73154				
	C	-1.43641	-0.51621	-0.9964				
	N	-0.16285	1.51196	0.48007				
	O	2.76738	-0.7835	1.20222				
	O	1.38585	0.38343	-2.72832				
	O	-0.12105	2.67702	0.61259				
	O	-2.36936	-0.00896	-1.55995				
	C	-1.25008	-1.99485	-0.64994				
	H	-0.30342	-2.23966	-0.11995				
	H	-1.24931	-2.55887	-1.60467				
	H	-2.09491	-2.30713	-0.00215				
	C	-0.98273	-0.71935	2.20854				
	O	-1.0241	-0.24986	3.2542				
$S15_{TS}CO$	Fe	0.8423	0.93917	-1.50713	-1887.4959474	0.0748991	-1887.4210483	150.09
	C	1.71208	0.90634	-3.03193				
	C	2.15788	0.097	-0.53205				
	C	-0.8879	1.13108	-2.35665				
	N	0.83413	2.48296	-0.89342				
	C	0.49746	-1.72784	-2.14384				
	O	3.03847	-0.35884	0.06752				
	O	2.33696	1.02293	-4.0111				
	O	1.12264	-2.48195	-2.74001				
	O	1.14664	3.59899	-0.7178				
	O	-1.38879	1.60892	-3.33741				
	C	-1.59158	0.40213	-1.20994				
	H	-0.92407	0.06723	-0.38368				
	H	-2.08796	-0.4974	-1.62834				
	H	-2.33635	1.10028	-0.77789				
17	Fe	0.22497	-0.09669	-0.15169	-1887.5450120	0.0776608	-1887.4673512	
	C	-0.28854	1.33939	-1.13073				
	C	1.82122	-0.1888	-1.00119				
	C	-1.69022	0.14345	0.82225				
	C	1.00209	0.55236	1.34109				
	N	-0.30396	-1.66464	-0.36354				
	O	2.83748	-0.27259	-1.54989				
	O	-0.62808	2.24206	-1.77354				
	O	-0.60572	-2.78249	-0.52568				

	O	1.54323	0.95445	2.28782				
	O	-2.64296	0.50678	0.1852				
	C	-1.74283	-0.23545	2.28258				
	H	-1.24495	0.56433	2.86896				
	H	-1.1861	-1.17309	2.46919				
	H	-2.79776	-0.32488	2.60954				
13_{TS}	Fe	0.3676	-0.30627	0.09543	-1774.1212797	0.0681726	-1774.0531071	66.86
	C	1.36951	0.94637	-0.81163				
	C	0.15156	-1.75535	-0.92676				
	C	-1.36247	0.49528	-0.20804				
	N	0.17269	-0.47819	1.73842				
	O	0.13121	-2.77404	-1.49655				
	O	2.02986	1.72261	-1.36656				
	O	0.11521	-0.81395	2.86206				
	O	-1.52807	1.57654	0.30343				
	C	-2.3925	-0.20684	-1.07516				
	H	-2.64307	-1.18831	-0.62846				
	H	-1.97059	-0.39656	-2.08087				
	H	-3.29872	0.42462	-1.15359				
14	Fe	0.57297	0.6211	-1.71269	-1774.1455424	0.0693149	-1774.0762275	
	C	1.90166	1.43086	-2.67388				
	N	0.99972	-0.97044	-1.5375				
	C	-1.28869	0.68572	-1.53887				
	C	0.85456	1.55143	-0.25613				
	O	1.49557	-1.96587	-1.15854				
	O	2.72777	1.96438	-3.28773				
	O	1.09623	2.08932	0.754				
	O	-1.31383	1.08745	-2.7003				
	C	-2.42152	0.44204	-0.61158				
	H	-2.30998	1.11769	0.26128				
	H	-2.35154	-0.59201	-0.21905				
	H	-3.39556	0.61033	-1.10958				
16_{TS}	Fe	0.198	-0.05673	0.19574	-1887.5053270	0.0748917	-1887.4304353	115.78
	C	0.32607	-0.45369	-2.42663				
	C	1.79314	0.82854	-0.03353				
	C	-1.69383	0.11994	0.01792				
	C	0.00175	0.47806	1.85188				
	N	0.55242	-1.6799	0.21251				
	O	2.79059	1.40877	-0.12996				
	O	0.99899	-1.04125	-3.14653				
	O	0.91423	-2.72092	0.62312				
	O	-0.06072	0.69782	2.99802				
	O	-1.64747	1.08102	-0.73248				
	C	-2.89416	-0.64093	0.4742				
	H	-2.90423	-0.67287	1.58214				
	H	-2.80734	-1.69052	0.1269				
$S16_{TS}CO$	Fe	0.10392	-0.31382	-0.24079	-1887.5028071	0.0749528	-1887.4278543	127.66

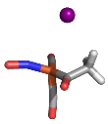
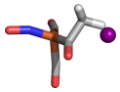
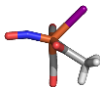
	C	1.86086	0.16532	-0.48704				
	C	-1.79048	-0.10576	-0.49653				
	C	0.08873	-0.03192	1.48609				
	N	0.14923	-1.95799	-0.50993				
	O	2.98739	0.41341	-0.59785				
	O	0.36054	-3.08231	-0.24365				
	O	0.10318	0.03896	2.6531				
	O	-1.66215	0.30897	-1.6355				
	C	-3.04307	-0.28543	0.29001				
	H	-3.02158	0.41494	1.1506				
	H	-3.06422	-1.3084	0.71549				
	H	-3.93894	-0.0988	-0.33308				
	C	0.0388	2.4344	-0.35879				
	O	0.44265	3.28748	0.29322				
THF	O	-0.07	-0.81706	2.44259	-232.5519151	0.1127105	-232.4392046	
	C	1.08621	-1.51415	2.93984				
	H	0.76397	-2.38833	3.55553				
	H	1.67099	-1.90592	2.07973				
	C	-0.22375	0.43246	3.13923				
	H	-1.28952	0.55763	3.4286				
	H	0.04361	1.27797	2.46051				
	C	0.72616	0.37193	4.34258				
	C	1.86486	-0.50099	3.78896				
	H	2.48018	-0.98109	4.57547				
	H	2.5402	0.1054	3.1488				
	H	0.23461	-0.133	5.2011				
	H	1.05746	1.3739	4.68022				
21_{TS}	Fe	0.16627	0.00836	-0.86637	-2006.6853163	0.1826979	-2006.5026184	71.95
	C	0.35583	-0.31435	-2.57498				
	C	1.91135	-0.36968	-0.40655				
	C	-1.383	-1.96297	-0.43915				
	N	0.02558	1.64919	-0.6351				
	C	-1.63801	-0.58833	-1.06787				
	O	3.01818	-0.60849	-0.15636				
	O	0.51852	-0.38049	-3.73202				
	O	-2.70513	-0.15723	-1.42839				
	O	0.12805	2.79118	-0.90784				
	H	-0.33154	-2.1432	-0.12771				
	H	-2.03537	-2.07743	0.44803				
	H	-1.63618	-2.71908	-1.21007				
	O	-0.29704	-0.3217	1.76705				
	C	0.44889	-1.12142	2.71597				
	H	-0.12072	-2.05476	2.93066				
	H	1.42071	-1.40854	2.26345				
	C	-0.83201	0.85109	2.42179				
	H	-1.88213	0.991	2.09214				
	H	-0.2511	1.74804	2.1074				

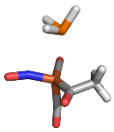
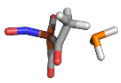
	C	-0.68821	0.58781	3.92311				
	C	0.59813	-0.25389	3.96994				
	H	0.70102	-0.85634	4.89374				
	H	1.49163	0.39977	3.88617				
	H	-1.55103	-0.00064	4.30011				
	H	-0.62646	1.52242	4.51452				
S21$_{TS}$CO 	Fe	0.38689	0.54107	0.06614	-2006.6830748	0.1829900	-2006.5000848	81.16
	C	0.50513	1.12657	-1.5884				
	C	2.12576	-0.02581	0.02777				
	C	-2.34695	0.37208	1.20924				
	N	0.4787	1.70288	1.23716				
	C	-1.64091	0.86935	-0.04889				
	O	3.2537	-0.29842	-0.03879				
	O	0.62006	1.65251	-2.62685				
	O	-2.25398	1.40315	-0.94838				
	O	0.70821	2.69881	1.82699				
	H	-1.82837	-0.4736	1.69236				
	H	-2.35307	1.22173	1.92527				
	H	-3.39709	0.10709	0.97062				
	O	-0.23946	-1.5045	0.11057				
	C	-0.73857	-2.1974	-1.07649				
	H	-1.82014	-1.96407	-1.17074				
	H	-0.21075	-1.79847	-1.96508				
	C	0.26343	-2.46324	1.0823				
	H	0.02112	-2.07814	2.09252				
	H	1.36976	-2.54047	0.98608				
	C	-0.43223	-3.77012	0.71579				
	C	-0.47312	-3.68475	-0.82108				
	H	-1.25152	-4.32943	-1.2729				
	H	0.50643	-3.98251	-1.24819				
	H	-1.45782	-3.79446	1.13885				
	H	0.11674	-4.65652	1.08855				
22 	Fe	0.31344	0.15602	-0.46423	-2006.6900149	0.1834954	-2006.5065195	
	C	0.33099	-0.61133	-2.02423				
	C	2.11157	-0.09989	-0.3067				
	C	-1.76241	-1.95694	-0.14298				
	N	0.16697	1.80162	-0.7257				
	C	-1.61364	-0.49377	-0.53404				
	O	3.25853	-0.29655	-0.32028				
	O	0.37748	-1.03764	-3.11662				
	O	-2.5685	0.21282	-0.78059				
	O	0.31993	2.7902	-1.34959				
	H	-0.91553	-2.33086	0.45939				
	H	-2.72654	-2.11829	0.38136				
	H	-1.77954	-2.53604	-1.09172				
	O	-0.03329	-0.15316	1.63575				
	C	0.78388	-0.94023	2.55562				

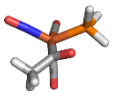
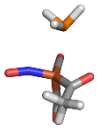
	H	0.44003	-1.99548	2.50076				
	H	1.83952	-0.8943	2.22191				
	C	-0.83422	0.81796	2.37195				
	H	-1.82935	0.8741	1.8907				
	H	-0.34508	1.81411	2.29697				
	C	-0.85283	0.29052	3.8027				
	C	0.55349	-0.32052	3.93616				
	H	0.63023	-1.07042	4.74708				
	H	1.30186	0.4745	4.1327				
	H	-1.63438	-0.48863	3.91963				
	H	-1.05123	1.09174	4.54076				
S22CO 	Fe	0.38689	0.54107	0.06614	-2006.6895226	0.1839205	-2006.5056021	
	C	0.50513	1.12657	-1.5884				
	C	2.12576	-0.02581	0.02777				
	C	-2.34695	0.37208	1.20924				
	N	0.4787	1.70288	1.23716				
	C	-1.64091	0.86935	-0.04889				
	O	3.2537	-0.29842	-0.03879				
	O	0.62006	1.65251	-2.62685				
	O	-2.25398	1.40315	-0.94838				
	O	0.70821	2.69881	1.82699				
	H	-1.82837	-0.4736	1.69236				
	H	-2.35307	1.22173	1.92527				
	H	-3.39709	0.10709	0.97062				
	O	-0.23946	-1.5045	0.11057				
	C	-0.73857	-2.1974	-1.07649				
	H	-1.82014	-1.96407	-1.17074				
	H	-0.21075	-1.79847	-1.96508				
	C	0.26343	-2.46324	1.0823				
	H	0.02112	-2.07814	2.09252				
	H	1.36976	-2.54047	0.98608				
	C	-0.43223	-3.77012	0.71579				
	C	-0.47312	-3.68475	-0.82108				
	H	-1.25152	-4.32943	-1.2729				
	H	0.50643	-3.98251	-1.24819				
	H	-1.45782	-3.79446	1.13885				
	H	0.11674	-4.65652	1.08855				
23_{TS} 	Fe	0.14766	0.08951	-0.70387	-2006.6890870	0.1837219	-2006.5053651	24.21
	C	0.00482	-1.12938	-1.9427				
	C	1.95882	-0.15278	-0.65132				
	C	-2.29923	-1.66044	-0.09947				
	N	0.03373	1.60772	-1.3756				
	C	-1.83838	-0.23091	-0.31844				
	O	3.10241	-0.36008	-0.68979				
	O	-0.05549	-1.85387	-2.86427				
	O	-2.57741	0.71589	-0.13903				
	O	0.14633	2.4474	-2.19417				

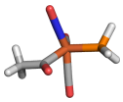
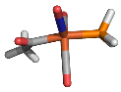
	H	-1.52095	-2.26713	0.40064				
	H	-3.24962	-1.68094	0.4714				
	H	-2.46423	-2.11517	-1.09926				
	O	0.05041	-0.07132	1.43961				
	C	0.66825	-1.10405	2.26594				
	H	-0.00361	-1.98827	2.26119				
	H	1.63703	-1.39438	1.81191				
	C	-0.23152	1.1191	2.23127				
	H	-1.17939	1.54913	1.85582				
	H	0.58763	1.85624	2.07826				
	C	-0.28338	0.60539	3.66601				
	C	0.81148	-0.47763	3.65791				
	H	0.6911	-1.22649	4.46439				
	H	1.81231	-0.0128	3.77064				
	H	-1.27772	0.16274	3.88216				
	H	-0.0941	1.40769	4.40523				
S23$_{TS}$CO 	Fe	0.19302	0.71074	0.07974	-2006.6891785	0.1837680	-2006.5054105	22.4
	C	0.17553	1.41886	-1.5266				
	C	2.00572	0.45975	0.01277				
	C	-2.51631	0.32849	1.2679				
	N	0.09475	1.82138	1.30142				
	C	-1.83999	0.48896	-0.08788				
	O	3.15982	0.36067	-0.07905				
	O	0.17399	2.01815	-2.53195				
	O	-2.46136	0.37649	-1.1239				
	O	0.17926	2.83079	1.90855				
	H	-1.90058	-0.2666	1.96766				
	H	-2.62105	1.34087	1.71175				
	H	-3.52022	-0.12529	1.14289				
	O	-0.07721	-1.41305	0.1292				
	C	-0.25481	-2.2188	-1.08045				
	H	-1.32981	-2.17995	-1.35078				
	H	0.33316	-1.75806	-1.89856				
	C	0.43909	-2.2323	1.2139				
	H	-0.01082	-1.86627	2.15757				
	H	1.54412	-2.10917	1.2743				
	C	0.04274	-3.65374	0.82903				
	C	0.21899	-3.62605	-0.70065				
	H	-0.36173	-4.41279	-1.21974				
	H	1.28775	-3.76072	-0.96555				
	H	-1.01493	-3.84734	1.10321				
	H	0.67432	-4.41499	1.32661				
24 	Fe	-0.31767	0.43723	-0.29197	-2006.6942037	0.1842983	-2006.5099054	
	C	-0.04067	1.34983	1.18328				
	C	-2.09296	0.19276	0.09617				
	C	2.49214	1.70031	-0.5913				
	N	-0.44206	1.29588	-1.69258				

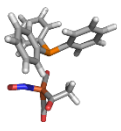
	C	1.72495	0.39618	-0.5039				
	O	-3.21931	0.08696	0.35303				
	O	0.09288	2.07679	2.09342				
	O	2.27617	-0.6822	-0.60765				
	O	-0.60302	2.13192	-2.5087				
	H	2.0571	2.34687	-1.37941				
	H	2.39187	2.25334	0.36475				
	H	3.56289	1.50827	-0.80295				
	O	-0.1932	-1.66624	0.04928				
	C	-0.0482	-2.61311	-1.05068				
	H	-1.06777	-2.85766	-1.41955				
	H	0.52695	-2.12597	-1.86127				
	C	0.29085	-2.24169	1.29113				
	H	-0.38365	-1.90469	2.1027				
	H	1.31851	-1.86685	1.48757				
	C	0.27419	-3.74769	1.04031				
	C	0.66751	-3.8246	-0.44657				
	H	0.36609	-4.77385	-0.93068				
	H	1.76475	-3.71029	-0.55725				
	H	-0.74448	-4.15807	1.20165				
	H	0.97456	-4.29146	1.70391				
25_{TS} 	Fe	-0.18458	-0.19251	-0.92386	-2006.6888690	0.1827084	-2006.5061606	63.04
	C	-0.38305	1.53522	-1.06272				
	C	-1.70716	-0.43896	0.07776				
	C	2.71554	0.69799	-1.84616				
	N	-0.4999	-0.95592	-2.35983				
	C	1.72642	-0.13653	-1.0961				
	O	-2.68694	-0.56964	0.6854				
	O	-0.57223	2.67404	-1.26605				
	O	1.97295	-1.05082	-0.32581				
	O	-0.9379	-1.08468	-3.44707				
	H	2.44846	0.70331	-2.92181				
	H	2.63528	1.74732	-1.49501				
	H	3.74831	0.32524	-1.70152				
	O	0.34177	-0.00222	1.79559				
	C	0.58063	-1.15893	2.6298				
	H	-0.26157	-1.8801	2.51321				
	H	1.50929	-1.65291	2.28078				
	C	-0.05667	1.12416	2.60911				
	H	-0.94426	1.60597	2.14832				
	H	0.77033	1.87081	2.62288				
	C	-0.32647	0.55735	4.0075				
	C	0.65804	-0.62357	4.06275				
	H	0.38974	-1.38793	4.8185				
	H	1.68396	-0.26342	4.28819				
	H	-1.3722	0.19193	4.08231				
	H	-0.16793	1.30589	4.80853				

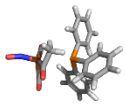
26_{TS} 	Fe 0.110395 1.293682 -0.132114 N 1.760502 1.306326 -0.104324 C -0.337845 1.175397 1.709926 C -1.526686 0.234063 1.460576 C -0.574839 2.903588 -0.135864 C -0.291790 0.881786 -1.895826 O 0.062073 1.538128 2.790673 O 2.879754 1.660734 -0.197184 O -0.524834 0.772413 -3.026681 O -0.885008 4.034420 -0.168273 H -2.432502 0.735534 1.859637 H -1.705853 -0.019470 0.393009 H -1.337741 -0.718107 1.995898 I 0.060756 -2.337020 -0.850196	-2072.1719161	0.0688617	-2072.1030544	48.48
$S26_{TS}CO$ 	Fe 1.358309 -0.056968 -0.153478 N 2.986237 -0.262355 0.026315 C 0.910918 -0.368963 1.682776 C 0.316321 -1.753769 1.385648 C 0.839080 1.610756 -0.072725 C 1.038747 -0.211360 -1.967394 O 1.008872 0.140074 2.772563 O 4.141916 -0.031631 0.103713 O 1.019717 -0.239796 -3.128464 O 0.616385 2.759310 -0.025140 H -0.745072 -1.751346 1.705268 H 0.332338 -2.044832 0.311636 H 0.901750 -2.499481 1.961565 I -2.180572 -0.605991 -1.167713	-2072.1697988	0.0687211	-2072.1010777	61.25
27 	Fe 0.323313 0.738264 -0.419513 N 1.871320 1.271909 -0.131019 C -0.234920 0.237279 1.482535 C -1.722212 0.087529 1.793321 C -0.797915 2.061048 -0.292972 C 0.227634 0.739542 -2.231639 O 0.593715 0.081352 2.363162 O 2.772000 2.041870 -0.123311 O 0.122865 0.795422 -3.391956 O -1.456343 3.036082 -0.236604 H -2.104850 1.103396 2.033991 H -2.291782 -0.292135 0.926042 H -1.868688 -0.561408 2.681572 I -0.136920 -1.972521 -0.771291	-2072.1877300	0.0694691	-2072.1182609	
28_{TS} 	Fe -0.846049 0.044543 -0.208428 N -1.555693 1.530739 -0.116334 C -0.791797 -0.025049 1.866023 C -2.134576 -0.007641 2.588534 C -1.878697 -1.361321 -0.140312 C -0.593129 -0.129401 -1.995209 O 0.246263 -0.008791 2.495627 O -2.337141 2.423128 -0.141719 O -0.527550 -0.222204 -3.155609 O -2.663822 -2.238565 -0.139542 H -2.766875 0.819900 2.209386 H -2.679619 -0.949596 2.374086 H -1.985453 0.094785 3.682938 I 1.854625 -0.615849 -0.340303	-2072.1831209	0,0695845	-2072.1135364	15.42

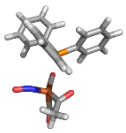
29 	Fe 0.221690 0.014038 1.306767 C 1.732650 -0.092754 0.307480 N 0.167002 -1.483843 2.012687 C -1.633901 0.617339 1.932343 C 0.890822 1.247355 2.342714 O 0.450199 -2.387592 2.729421 O 2.733083 -0.142344 -0.289232 O 1.376241 1.991732 3.111042 O -1.939684 1.719500 2.353584 C -2.685086 -0.495323 1.878201 H -2.527781 -1.137933 2.771049 H -2.566772 -1.132104 0.982946 H -3.704636 -0.059447 1.923648 I -0.885414 0.743049 -1.119238	-2072.1871605	0.0695390	-2072.1176215	
PH_3 	P 0.07617 -0.1146 -0.18609 H -1.32296 0.06229 0.09753 H 0.38287 1.2648 0.0832 H 0.37524 -0.52275 1.1605	-343.1983750	0.0230512	-343.1753238	
18_{TS} 	Fe 0.1861 0.00178 -0.24261 C 0.35303 -0.24315 -1.97191 C 1.85202 -0.65144 0.20084 C -1.68193 -0.3491 -0.50701 N 0.25761 1.62575 0.09694 P -0.3564 -0.13042 2.76731 O 2.9096 -1.06144 0.43754 O 0.52244 -0.26062 -3.12863 O 0.5151 2.7629 -0.06154 O -2.66923 0.26335 -0.82921 C -1.64776 -1.80507 -0.02684 H -0.64243 -2.1778 0.25951 H -2.01643 -2.43296 -0.86451 H -2.32195 -1.89851 0.84958 H -1.20663 1.00351 2.98489 H -0.6983 -0.77864 4.00862 H 0.82274 0.49999 3.28365	-2117.3333372	0.0934871	-2117.2398501	117.61
$S18_{TS}CO$ 	Fe 0.20988 0.33945 0.1485 C 0.23948 0.00625 -1.57125 C 1.80849 -0.49385 0.50632 C -1.71855 0.55682 0.19732 N 0.49544 1.94054 0.47195 P -0.50627 -2.76147 0.19299 O 2.84844 -0.97212 0.69334 O 0.31978 -0.07646 -2.73507 O 0.8568 3.04808 0.31692 O -2.61119 0.9236 -0.52178 C -1.86694 0.0921 1.65177 H -0.91664 -0.20354 2.14562 H -2.55538 -0.77782 1.66928 H -2.30315 0.93593 2.22499 H 0.61326 -3.33392 -0.4957	-2117.3296957	0.0934211	-2117.2362746	117.67

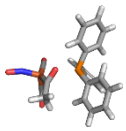
	H	-0.90442	-3.99604	0.8197				
	H	-1.4076	-2.89425	-0.91496				
20	Fe	0.14085	-0.37489	0.08725	-2117.3645273	0.0968422	-2117.2676851	
	P	2.21265	0.4893	-0.2911				
	C	0.57383	-0.48928	1.833				
	C	-0.16608	0.08784	-1.92578				
	C	-1.01039	0.94238	0.39122				
	N	-0.28519	-1.94308	-0.2238				
	O	0.84815	-0.56478	2.96057				
	O	-0.66252	-3.04988	-0.34331				
	O	-1.81365	1.7599	0.62143				
	O	0.72031	0.51996	-2.64037				
	C	-1.54922	-0.20246	-2.47746				
	H	-2.31963	0.34439	-1.89846				
	H	-1.77502	-1.28238	-2.36585				
	H	-1.60153	0.08297	-3.5471				
	H	3.05155	-0.21452	-1.20579				
	H	2.32064	1.79785	-0.84597				
	H	3.14065	0.62884	0.78812				
19_{TS}	Fe	-0.22266	-0.00762	0.19776	-2117.3380621	0.0931895	-2117.2448726	110.49
	P	2.7458	0.10071	-0.57521				
	C	0.402	0.51442	1.84291				
	C	-0.62142	0.55803	-1.59405				
	C	-1.89402	0.33396	0.56071				
	N	0.00858	-1.64993	0.1231				
	O	0.7666	0.86063	2.88714				
	O	-0.20523	-2.79513	0.30026				
	O	-3.02777	0.41637	0.84161				
	O	0.01147	1.60236	-1.63478				
	C	-1.38519	-0.07047	-2.71984				
	H	-2.4395	-0.21025	-2.40573				
	H	-0.97787	-1.08207	-2.9197				
	H	-1.33395	0.5539	-3.63318				
	H	2.85236	-0.71277	-1.75312				
	H	3.87556	0.92853	-0.91009				
	H	3.50031	-0.80012	0.249				
$S19_{TS}CO$	Fe	0.20766	-0.30681	0.31152	-2117.3366321	0.0934001	-2117.2432320	104.05
	P	0.04487	2.72646	-0.89296				
	C	0.33412	0.86213	1.72577				
	C	0.25168	-0.7932	-1.55475				
	C	-1.53132	-0.45286	0.4119				
	N	1.01177	-1.64896	0.84659				
	O	0.38998	1.55658	2.65258				
	O	1.20325	-2.66749	1.40478				
	O	-2.677	-0.6509	0.55071				
	O	1.06966	0.01763	-1.96488				
	C	-0.45063	-1.8337	-2.37075				

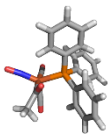
	H -1.53902 -1.61811 -2.36453 H -0.32242 -2.82469 -1.89107 H -0.07122 -1.85097 -3.41108 H 1.24822 3.26535 -1.45939 H -0.64592 2.63269 -2.14643 H -0.51121 4.00738 -0.54958				
33_{TS} 	Fe -0.041949 -0.136194 0.248137 P 1.416288 0.676486 1.696543 C -1.451594 -0.650935 1.189831 C 0.258279 0.275758 -1.807269 C -0.752856 1.479637 -0.027382 N 0.696177 -1.575493 -0.171746 O -2.372710 -1.073381 1.772267 O 1.228999 -2.591954 -0.439542 O -1.233504 2.538939 -0.163254 O 1.263905 0.830069 -2.167020 C -0.832667 -0.239390 -2.709980 H -1.782029 0.279975 -2.468576 H -1.005434 -1.315542 -2.510683 H -0.565555 -0.075993 -3.773685 H 2.639192 1.264696 1.237902 H 1.029319 1.710237 2.601992 H 1.978477 -0.233740 2.644341	-2117.3505914	0.0958742	-2117.2547172	64.70
35 	Fe 0.105201 -0.353258 0.134777 P 0.529812 -0.259926 2.361914 C -1.648222 -0.253654 0.477915 C -0.330414 -0.079260 -1.879306 C 0.873499 1.255686 -0.078604 N 0.843966 -1.812737 -0.136868 O -2.789212 -0.251840 0.729263 O 1.345293 -2.858500 -0.310734 O 1.399881 2.290159 -0.208354 O 0.296966 -0.689493 -2.717679 C -1.440042 0.883433 -2.268755 H -1.399157 1.815669 -1.674228 H -2.416302 0.401450 -2.052536 H -1.382692 1.103931 -3.353492 H 1.890241 -0.269598 2.795754 H 0.067853 0.867103 3.103977 H 0.025849 -1.300612 3.199952	-2117.3670296	0.0965835	-2117.2704461	
$S37_{TS}$ 	Fe -0.08726 -0.05813 0.23113 C 1.72245 0.0208 0.05205 C -0.20689 -1.89029 0.62021 C -2.19117 -0.18057 0.00222 N -0.14908 0.43489 1.93174 C -0.02276 -0.85691 -2.20041 O -0.31813 -3.01569 0.83755 O 2.87245 0.09848 -0.0498 O -0.11773 -0.29649 -3.19878 O -0.10847 1.50581 2.42632 H -2.65544 0.73088 0.4236 H -2.45165 -0.26694 -1.06935 H -2.58205 -1.06152 0.5438	-1887.4825147	0.0726474	-1887.4098673	129.44

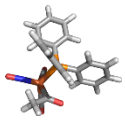
	C	-0.38084	1.53468	-0.51443				
	O	-0.59871	2.55164	-1.03185				
S37a$_{TS}$	Fe	-0.05015	0.04814	0.13341	-1887.4788667	0.0730344	-1887.4058323	218.91
	C	1.7087	-0.02323	-0.29687				
	C	-0.04635	-2.24194	0.64662				
	C	-2.12783	0.20864	0.54952				
	N	0.19353	0.4529	1.88906				
	C	-0.63735	-0.68934	-1.48239				
	O	-0.01308	-3.31405	0.23387				
	O	2.8304	-0.02154	-0.58482				
	O	-1.04481	-0.87426	-2.55201				
	O	0.31338	1.42213	2.55601				
	H	-2.2879	0.98585	1.31936				
	H	-2.72267	0.44453	-0.35135				
	H	-2.41196	-0.78291	0.94525				
	C	-0.24974	1.71199	-0.38517				
	O	-0.39123	2.81577	-0.71509				
S38	Fe	0.68476	1.0178	-1.91426	-1887.4993270	0.0749432	-1887.4243838	
	C	2.28141	1.79271	-2.20185				
	C	1.30851	-0.35805	-0.91294				
	C	-1.20684	0.19403	-1.41027				
	N	0.44655	1.99494	0.0233				
	C	0.61168	0.08123	-3.46273				
	O	1.68029	-1.27354	-0.30857				
	O	3.31109	2.29006	-2.39137				
	O	0.55796	-0.52067	-4.45055				
	O	1.28149	2.71445	0.41901				
	H	-1.44937	0.62444	-0.41928				
	H	-1.97883	0.47464	-2.15079				
	H	-1.16285	-0.90937	-1.34981				
	C	-0.31939	2.40532	-2.50699				
	O	-0.98779	3.25572	-2.9213				
S39$_{TS}$	Fe	-2.42683	-0.06594	0.82078	-2810.7613628	0.3353793	-2810.4259835	62.28
	C	-4.17742	-0.07933	0.97133				
	O	-5.31848	-0.04062	1.22232				
	C	-2.28863	1.65017	0.15579				
	O	-2.24484	2.73105	-0.25919				
	P	0.76784	-0.13618	-0.26465				
	C	1.31685	-0.51959	-1.9926				
	C	2.35335	-1.42663	-2.3053				
	H	2.92153	-1.91225	-1.49771				
	C	2.66778	-1.71382	-3.64569				
	H	3.47787	-2.42423	-3.8732				
	C	1.95806	-1.09615	-4.68982				
	H	2.2075	-1.32199	-5.73807				
	C	0.92322	-0.19145	-4.38906				
	H	0.35919	0.29459	-5.20023				

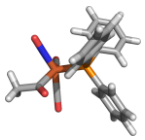
	C	0.59715	0.08515	-3.05172				
	H	-0.22459	0.78574	-2.82941				
	C	1.50242	1.53477	0.06411				
	C	2.24141	2.26941	-0.88858				
	H	2.44649	1.83726	-1.87946				
	C	2.72511	3.55366	-0.57976				
	H	3.30162	4.11212	-1.33377				
	C	2.48229	4.11886	0.68347				
	H	2.86323	5.12352	0.92356				
	C	1.74848	3.39353	1.64011				
	H	1.55264	3.82738	2.63302				
	C	1.25527	2.11617	1.33137				
	H	0.68049	1.56265	2.09017				
	C	1.81509	-1.24823	0.78608				
	C	3.12792	-0.91481	1.19082				
	H	3.57044	0.0448	0.88286				
	C	3.87362	-1.80081	1.98668				
	H	4.89504	-1.52845	2.29506				
	C	3.31944	-3.02992	2.38759				
	H	3.9044	-3.72147	3.01353				
	C	2.01353	-3.36905	1.99293				
	H	1.56998	-4.32566	2.30952				
	C	1.26303	-2.48075	1.20349				
	H	0.23461	-2.75143	0.91777				
	N	-1.71306	-0.00266	2.31392				
	O	-1.57489	0.19149	3.46672				
	C	-2.52727	-1.92578	0.44139				
	C	-2.33719	-1.7327	-1.06878				
	O	-2.59293	-2.98131	1.02172				
	H	-1.42093	-2.27151	-1.3844				
	H	-2.24999	-0.67509	-1.40002				
	H	-3.23042	-2.16262	-1.56724				
S39$_{TS}$CO	Fe	1.01893	0.46851	2.34304	-2810.7575746	0.3353756	-2810.4221990	75.1
	C	0.8842	2.12226	1.78299				
	O	0.87016	3.26322	1.5279				
	C	2.44461	0.04816	1.27151				
	O	3.38867	-0.17517	0.63224				
	P	-0.16816	-0.25909	-0.7811				
	C	0.08601	1.21757	-1.87201				
	C	-0.93528	1.7818	-2.66803				
	H	-1.9382	1.32985	-2.68055				
	C	-0.68009	2.92096	-3.45207				
	H	-1.48727	3.3481	-4.06735				
	C	0.59668	3.50787	-3.45634				
	H	0.79415	4.39957	-4.07112				
	C	1.62059	2.95177	-2.6684				
	H	2.62371	3.40548	-2.6627				

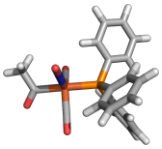
	C	1.36605	1.82129	-1.87607				
	H	2.17747	1.40251	-1.26156				
	C	0.65525	-1.6274	-1.72099				
	C	0.99782	-1.53748	-3.08861				
	H	0.7673	-0.62208	-3.65436				
	C	1.63332	-2.61271	-3.73363				
	H	1.89618	-2.52913	-4.79968				
	C	1.93009	-3.7899	-3.02423				
	H	2.42911	-4.62984	-3.53178				
	C	1.59312	-3.88843	-1.66239				
	H	1.8275	-4.80446	-1.09841				
	C	0.96827	-2.81094	-1.01328				
	H	0.72197	-2.89326	0.05761				
	C	-1.97484	-0.62585	-0.97582				
	C	-2.47142	-1.69892	-1.74807				
	H	-1.77591	-2.34555	-2.30376				
	C	-3.85421	-1.94697	-1.8151				
	H	-4.22597	-2.78813	-2.42077				
	C	-4.75743	-1.12569	-1.11893				
	H	-5.83933	-1.32179	-1.17383				
	C	-4.27218	-0.05377	-0.34733				
	H	-4.97178	0.59308	0.20429				
	C	-2.89154	0.18898	-0.26776				
	H	-2.52549	1.02289	0.35264				
	N	1.59878	0.37779	3.89464				
	O	2.13727	0.7065	4.88803				
	C	-0.83526	0.37597	2.88162				
	C	-0.94968	-1.13587	2.63741				
	O	-1.71152	1.09252	3.29415				
	H	-1.77193	-1.31619	1.91646				
	H	-1.18736	-1.60965	3.61177				
	H	-0.023	-1.61199	2.24917				
S40$_{TS}$	Fe	-2.48964	-0.26461	0.21683	-2810.7668710	0.3354505	-2810.4314205	54.49
	C	-4.19358	-0.22025	-0.16247				
	O	-5.35943	-0.20911	-0.26981				
	C	-2.27937	1.55793	0.24476				
	O	-2.17856	2.7132	0.24321				
	P	0.83177	0.11763	0.01014				
	C	1.63263	0.73822	-1.54293				
	C	2.88719	0.28849	-2.01265				
	H	3.4513	-0.46309	-1.43958				
	C	3.42163	0.7945	-3.2104				
	H	4.39994	0.4343	-3.5653				
	C	2.71359	1.75739	-3.95143				
	H	3.13358	2.15091	-4.89006				
	C	1.46404	2.21109	-3.49231				
	H	0.90041	2.9602	-4.06978				

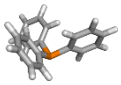
	C	0.92362	1.69827	-2.30128				
	H	-0.06308	2.04758	-1.9585				
	C	1.48765	1.25784	1.31526				
	C	2.4468	2.26425	1.06636				
	H	2.88123	2.37238	0.0611				
	C	2.85443	3.13144	2.09561				
	H	3.6028	3.91135	1.88467				
	C	2.31494	3.00284	3.38709				
	H	2.63639	3.68222	4.19166				
	C	1.35827	2.00424	3.64551				
	H	0.92705	1.89832	4.65315				
	C	0.93949	1.14598	2.61601				
	H	0.18018	0.37721	2.82915				
	C	1.73967	-1.46839	0.33122				
	C	2.69818	-1.6336	1.35491				
	H	2.97173	-0.78186	1.99565				
	C	3.31211	-2.88242	1.56205				
	H	4.05741	-2.99447	2.36507				
	C	2.98372	-3.97879	0.74677				
	H	3.46664	-4.95469	0.90989				
	C	2.03132	-3.82307	-0.27766				
	H	1.76671	-4.67699	-0.92071				
	C	1.40671	-2.58184	-0.47779				
	H	0.65169	-2.47128	-1.27273				
	N	-2.2482	-0.76992	1.77542				
	O	-2.46547	-1.01422	2.90806				
	C	-2.35177	-1.82896	-0.85623				
	C	-2.80112	-3.25026	-0.73499				
	O	-1.64054	-1.35094	-1.73187				
	H	-2.51148	-3.83984	-1.62668				
	H	-3.89901	-3.27841	-0.58771				
	H	-2.34824	-3.69026	0.17726				
S40$_{TS}$CO	Fe	-0.35799	0.1105	2.65118	-2810.7650496	0.3356872	-2810.4293624	61.55
	C	-1.87195	0.93692	2.38788				
	O	-2.88894	1.51582	2.32397				
	C	0.6826	1.55602	2.21873				
	O	1.32433	2.50053	2.00811				
	P	0.17531	0.18677	-0.69641				
	C	-0.03649	1.68877	-1.76515				
	C	-0.93451	1.76129	-2.8532				
	H	-1.53919	0.88427	-3.1282				
	C	-1.06215	2.94961	-3.59477				
	H	-1.76649	2.98862	-4.44043				
	C	-0.29296	4.07848	-3.26476				
	H	-0.39456	5.00745	-3.84686				
	C	0.60563	4.01577	-2.18399				
	H	1.2108	4.89559	-1.91539				

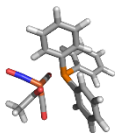
	C	0.72773	2.83426	-1.43543				
	H	1.42594	2.80464	-0.58467				
	C	1.78926	-0.51196	-1.28336				
	C	2.38027	-0.17008	-2.52063				
	H	1.87165	0.53206	-3.19864				
	C	3.61907	-0.72094	-2.89202				
	H	4.06973	-0.44533	-3.85829				
	C	4.27971	-1.62014	-2.03605				
	H	5.25087	-2.04869	-2.32856				
	C	3.69796	-1.96572	-0.8031				
	H	4.21168	-2.66578	-0.12595				
	C	2.46425	-1.41021	-0.42407				
	H	2.01333	-1.67608	0.54423				
	C	-1.08905	-0.9884	-1.36642				
	C	-0.76253	-2.12234	-2.14079				
	H	0.28593	-2.32139	-2.40888				
	C	-1.77024	-3.00196	-2.57526				
	H	-1.49927	-3.88266	-3.17836				
	C	-3.115	-2.75836	-2.24794				
	H	-3.90218	-3.44727	-2.59132				
	C	-3.45025	-1.63014	-1.47687				
	H	-4.50111	-1.43077	-1.21523				
	C	-2.44472	-0.75764	-1.03023				
	H	-2.71965	0.11711	-0.41911				
	N	-0.0485	-0.13671	4.26066				
	O	-0.14099	0.01365	5.42539				
	C	-1.07746	-1.63802	2.30537				
	C	-2.36411	-2.34004	2.60227				
	O	-0.11436	-2.10078	1.71141				
	H	-2.33263	-3.39544	2.2689				
	H	-3.19193	-1.80264	2.09676				
	H	-2.56638	-2.28024	3.69063				
32	Fe	-0.35578	0.32613	1.76075	-2810.7906367	0.3375890	-2810.4530477	
	C	-2.05677	0.76476	1.97814				
	O	-3.15407	1.10388	2.20587				
	C	0.09672	2.06567	1.64141				
	O	0.36861	3.1964	1.67039				
	P	-0.02196	0.06139	-0.53022				
	C	-0.09834	1.61636	-1.54939				
	C	-1.19192	1.9365	-2.38188				
	H	-2.03166	1.23535	-2.49228				
	C	-1.21587	3.15078	-3.09191				
	H	-2.07619	3.38211	-3.73884				
	C	-0.14862	4.05733	-2.98413				
	H	-0.16796	5.0056	-3.54301				
	C	0.94769	3.74387	-2.16054				
	H	1.79229	4.44445	-2.07166				

	C	0.97215	2.53571	-1.44689				
	H	1.84174	2.30485	-0.81236				
	C	1.65473	-0.58996	-0.98043				
	C	2.14197	-0.50001	-2.30529				
	H	1.53004	-0.03154	-3.09124				
	C	3.41497	-0.99896	-2.62671				
	H	3.78447	-0.92309	-3.66106				
	C	4.2154	-1.58738	-1.63073				
	H	5.21492	-1.97374	-1.88355				
	C	3.73826	-1.6746	-0.31178				
	H	4.36188	-2.12862	0.47369				
	C	2.46409	-1.17768	0.01269				
	H	2.08989	-1.24402	1.04422				
	C	-1.22789	-1.06471	-1.38123				
	C	-0.82148	-2.12458	-2.21787				
	H	0.24716	-2.31363	-2.39331				
	C	-1.77775	-2.95755	-2.82515				
	H	-1.44354	-3.78408	-3.47119				
	C	-3.1488	-2.74241	-2.60625				
	H	-3.89528	-3.39593	-3.08336				
	C	-3.56201	-1.69323	-1.76642				
	H	-4.6333	-1.51961	-1.58158				
	C	-2.60845	-0.86656	-1.14911				
	H	-2.94923	-0.0626	-0.47914				
	N	0.60234	-0.09938	3.04726				
	O	1.16705	-0.2752	4.06575				
	C	-0.88518	-1.70706	1.76878				
	C	-2.01951	-2.14551	2.67261				
	O	-0.23516	-2.50425	1.12656				
	H	-2.04144	-3.25064	2.75516				
	H	-2.97724	-1.79022	2.2395				
	H	-1.92644	-1.6783	3.67226				
S41	Fe	-1.67254	-0.04622	0.31414	-2810.7919432	0.3374875	-2810.4544557	
	C	-3.05034	0.19457	-0.76963				
	O	-4.01786	0.35072	-1.40824				
	C	-1.68489	1.70915	0.6755				
	O	-1.75411	2.8547	0.88114				
	P	0.64114	0.07015	0.08113				
	C	1.26171	0.67322	-1.5486				
	C	2.59693	0.46757	-1.96608				
	H	3.29664	-0.10136	-1.3353				
	C	3.03967	0.98518	-3.1949				
	H	4.08136	0.82107	-3.51095				
	C	2.15619	1.70747	-4.01713				
	H	2.50501	2.10981	-4.98075				
	C	0.82553	1.90634	-3.61051				
	H	0.12626	2.46067	-4.25505				

	C 0.37796 1.38625 -2.38482 H -0.66909 1.51865 -2.07362 C 1.40796 1.20678 1.33601 C 2.49494 2.05359 1.02887 H 2.91264 2.07654 0.01217 C 3.04763 2.88658 2.01718 H 3.89022 3.54657 1.75933 C 2.5284 2.88068 3.32296 H 2.96396 3.53381 4.09469 C 1.44354 2.04373 3.63612 H 1.0233 2.03716 4.65352 C 0.88006 1.21945 2.64802 H 0.0169 0.58651 2.90206 C 1.54721 -1.52921 0.35614 C 2.01101 -1.88435 1.64218 H 1.89958 -1.18788 2.48612 C 2.63291 -3.12625 1.85747 H 2.99236 -3.38423 2.86555 C 2.80159 -4.02841 0.79341 H 3.29214 -4.99928 0.96267 C 2.34195 -3.68222 -0.48928 H 2.47102 -4.38006 -1.33098 C 1.71454 -2.44487 -0.70903 H 1.35359 -2.19456 -1.71675 N -2.07806 -0.78311 1.74471 O -2.55029 -1.08536 2.78096 C -1.45036 -1.62048 -1.02856 C -1.85497 -2.96584 -0.44848 O -1.05555 -1.51234 -2.1731 H -1.74435 -3.76371 -1.21046 H -2.90349 -2.91612 -0.09232 H -1.22578 -3.19015 0.43611				
34_{TS} 	Fe -1.711267 0.059618 0.502744 C -2.204797 1.057837 -0.888111 O -2.526914 1.727290 -1.793542 C -1.731097 1.507780 1.532888 O -1.834939 2.424959 2.247401 P 0.485858 -0.118271 -0.017208 C 1.039031 0.611593 -1.627081 C 1.673286 -0.152230 -2.629877 H 1.880942 -1.219451 -2.463889 C 2.045803 0.444399 -3.848063 H 2.537122 -0.165213 -4.622128 C 1.798650 1.808507 -4.074242 H 2.093163 2.273990 -5.027421 C 1.171936 2.577658 -3.076561 H 0.975345 3.647854 -3.243956 C 0.787535 1.983282 -1.864992 H 0.296204 2.598499 -1.095255 C 1.589539 0.712873 1.225659 C 2.750964 1.424674 0.854705	-2810.7806422	0.3372336	-2810.4434086	48.43

	H 3.020791 1.529090 -0.206491 C 3.572320 2.005403 1.837800 H 4.471212 2.563720 1.533625 C 3.250751 1.871597 3.199040 H 3.894919 2.327107 3.966885 C 2.100950 1.154632 3.576464 H 1.841720 1.043658 4.640639 C 1.272089 0.585629 2.596616 H 0.370714 0.033490 2.903301 C 1.169753 -1.844593 -0.052984 C 2.393938 -2.178812 0.567698 H 2.975659 -1.410674 1.097555 C 2.878784 -3.497436 0.516115 H 3.832137 -3.744298 1.008579 C 2.152651 -4.493696 -0.158373 H 2.533903 -5.525912 -0.196304 C 0.935582 -4.165920 -0.781727 H 0.359975 -4.940264 -1.312336 C 0.441207 -2.852017 -0.725208 H -0.514684 -2.603698 -1.210695 N -1.978212 -1.166025 1.607307 O -2.131279 -2.058530 2.362852 C -2.932468 -1.166150 -0.741295 C -4.395915 -1.125092 -0.373984 O -2.479312 -1.849978 -1.626843 H -4.990780 -1.721587 -1.094592 H -4.759119 -0.080178 -0.333802 H -4.516680 -1.540560 0.647812				
36 	Fe 0.385997 -1.715373 0.064940 C 1.352612 -1.747869 -1.442084 O 2.009512 -1.798181 -2.403301 C -1.341980 -1.871526 -0.376108 O -2.476433 -1.983903 -0.637812 P 0.234634 0.573426 -0.032610 C 0.125111 1.292815 -1.731539 C 1.105071 2.173396 -2.236310 H 1.952291 2.480842 -1.605879 C 1.004843 2.665544 -3.550231 H 1.776819 3.350910 -3.932588 C -0.072462 2.287339 -4.367860 H -0.149089 2.674158 -5.395633 C -1.053392 1.410123 -3.869208 H -1.900993 1.108517 -4.503505 C -0.953881 0.909462 -2.562262 H -1.728044 0.222060 -2.189187 C -1.226091 1.280338 0.853835 C -1.867593 2.460913 0.417825 H -1.522486 2.976802 -0.490748 C -2.954916 2.981452 1.140960 H -3.450552 3.899967 0.790827 C -3.407701 2.332638 2.302802 H -4.261065 2.741197 2.865638 C -2.772997 1.156446 2.740292 H -3.126920 0.639960 3.645666 C -1.691698 0.628047 2.016819 H -1.210671 -0.303168 2.352939 C 1.687971 1.425131 0.735463 C 1.551417 2.653652 1.418918	-2810.8017405	0.3374799	-2810.4642606	

	H 0.562076 3.122496 1.526531 C 2.679196 3.284658 1.971016 H 2.559582 4.239872 2.505025 C 3.950970 2.699309 1.844845 H 4.832514 3.195001 2.279711 C 4.092665 1.475365 1.167871 H 5.084177 1.007438 1.069970 C 2.967065 0.836190 0.622624 H 3.085188 -0.129344 0.108352 N 1.087659 -1.791833 1.565095 O 1.636929 -1.822484 2.608915 C 0.304953 -3.791779 -0.053618 C -0.279481 -4.473669 1.173494 O 0.702846 -4.428441 -1.005212 H -0.378145 -5.562501 0.990901 H -1.260463 -4.034944 1.440691 H 0.393388 -4.303023 2.038553				
PPh_3 	P 10.31702 1.26603 3.85944 C 11.378 1.93358 2.48776 C 11.37096 1.44172 1.16386 H 10.72586 0.59033 0.89807 C 12.18288 2.03268 0.17887 H 12.1648 1.6392 -0.84965 C 13.01624 3.11712 0.50393 H 13.6509 3.57824 -0.26869 C 13.03023 3.61529 1.81979 H 13.67518 4.46871 2.0814 C 12.20987 3.03485 2.80093 H 12.21251 3.44378 3.82485 C 11.45741 0.0669 4.7045 C 12.69827 -0.35781 4.18038 H 13.03277 0.00663 3.19701 C 13.51331 -1.24475 4.90676 H 14.47927 -1.56533 4.48588 C 13.09778 -1.72345 6.16157 H 13.73761 -2.41743 6.72848 C 11.86373 -1.30599 6.69306 H 11.5338 -1.67093 7.6783 C 11.05513 -0.40999 5.97471 H 10.09855 -0.07263 6.40683 C 9.14748 0.14105 2.95443 C 9.34206 -1.24876 2.79537 H 10.24801 -1.72577 3.19959 C 8.38504 -2.03085 2.12385 H 8.54976 -3.11382 2.00968 C 7.22553 -1.43509 1.59758 H 6.47749 -2.04924 1.07259 C 7.02167 -0.05141 1.75116 H 6.1129 0.42204 1.34778 C 7.97012 0.72829 2.43323	-1036.6279333	0.2659080	-1036.3620253	

	H	7.79335	1.80842	2.56626				
S42$_{TS}$ 	Fe	-0.38018	0.70175	1.7576	-2810.7903097	0.3376187	-2810.452691	15.23
	C	-1.63879	-0.3075	2.48859				
	O	-2.49073	-0.90066	3.02966				
	C	-1.6435	1.82786	1.1421				
	O	-2.48584	2.57215	0.84346				
	P	0.0266	-0.06201	-0.40418				
	C	-1.10025	0.58812	-1.7365				
	C	-2.00746	-0.21667	-2.45688				
	H	-2.0667	-1.29745	-2.26382				
	C	-2.83937	0.35239	-3.4392				
	H	-3.54053	-0.291	-3.99301				
	C	-2.77183	1.7271	-3.71719				
	H	-3.42201	2.16956	-4.48756				
	C	-1.86556	2.53578	-3.00688				
	H	-1.80153	3.61425	-3.21883				
	C	-1.03909	1.97215	-2.02346				
	H	-0.33232	2.6185	-1.47918				
	C	1.67382	0.43062	-1.1036				
	C	1.95566	0.23754	-2.47607				
	H	1.20205	-0.21495	-3.1388				
	C	3.19483	0.63042	-3.00764				
	H	3.40316	0.47301	-4.0772				
	C	4.16101	1.22908	-2.17885				
	H	5.13007	1.54151	-2.59781				
	C	3.8819	1.43438	-0.81704				
	H	4.62991	1.9099	-0.16406				
	C	2.64431	1.03715	-0.28172				
	H	2.42585	1.2053	0.78231				
	C	-0.08203	-1.90106	-0.60956				
	C	0.96662	-2.67826	-1.14306				
	H	1.90213	-2.19918	-1.4647				
	C	0.83117	-4.07315	-1.25362				
	H	1.66098	-4.66684	-1.66741				
	C	-0.35018	-4.70778	-0.83371				
	H	-0.45332	-5.80033	-0.92156				
	C	-1.39655	-3.94069	-0.29177				
	H	-2.32358	-4.42799	0.04761				
	C	-1.26002	-2.54774	-0.17087				
	H	-2.0816	-1.96416	0.27166				
	N	0.54458	1.77283	2.61946				
	O	1.06556	2.56561	3.31758				
	C	0.96665	-0.77651	2.40444				
	C	0.94418	-1.11601	3.88343				
	O	1.777	-1.27767	1.65287				
	H	1.78257	-1.797	4.13166				
	H	-0.01877	-1.60215	4.13961				

	H	1.00615	-0.19202	4.49178		

5. Vibrational Frequencies of 36

Complex **36** was reoptimised using the BP86 functional and a def2-TZVP basis set in combination with the COSMO solvation model (ε = 7.36).

```
$vibrational spectrum
#  mode     symmetry     wave number    IR intensity    selection rules
#                         cm**(-1)        km/mol          IR      RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              5.58         1.30852       YES     YES
     8        a             11.22         3.40403       YES     YES
     9        a             13.88         0.17943       YES     YES
    10        a             29.90         0.16239       YES     YES
    11        a             40.43         0.68305       YES     YES
    12        a             41.07         0.10862       YES     YES
    13        a             45.38         0.52567       YES     YES
    14        a             50.24         0.56096       YES     YES
    15        a             54.53         0.06011       YES     YES
    16        a             59.34         0.73913       YES     YES
    17        a             67.62         0.23376       YES     YES
    18        a             74.26         0.25464       YES     YES
    19        a             90.27         0.06116       YES     YES
    20        a            101.19         0.40918       YES     YES
    21        a            103.63         0.40752       YES     YES
    22        a            118.92         1.46917       YES     YES
    23        a            120.78         0.44458       YES     YES
    24        a            167.97         0.85142       YES     YES
    25        a            174.26         2.18826       YES     YES
    26        a            186.64         0.73715       YES     YES
    27        a            210.99         1.51551       YES     YES
    28        a            213.14         0.83964       YES     YES
    29        a            242.53         2.38853       YES     YES
    30        a            254.18         0.45845       YES     YES
    31        a            255.47         0.40305       YES     YES
    32        a            273.00         1.55624       YES     YES
    33        a            286.29         9.12238       YES     YES
    34        a            350.89         0.13064       YES     YES
    35        a            388.52         0.46611       YES     YES
    36        a            388.80         0.32607       YES     YES
    37        a            393.17         0.91259       YES     YES
    38        a            419.28        53.99801       YES     YES
    39        a            426.73        16.01966       YES     YES
    40        a            428.49        17.76961       YES     YES
    41        a            456.11         9.70586       YES     YES
    42        a            460.42         1.66143       YES     YES
    43        a            474.39        20.86067       YES     YES
    44        a            492.75        27.61563       YES     YES
    45        a            499.87        74.00068       YES     YES
    46        a            503.32       263.95352       YES     YES
    47        a            515.56        49.82165       YES     YES
    48        a            517.57       128.69148       YES     YES
    49        a            539.71        45.25080       YES     YES
    50        a            549.60        92.43552       YES     YES
    51        a            609.48         0.66466       YES     YES
    52        a            609.72         0.61220       YES     YES
    53        a            610.05         2.69718       YES     YES
    54        a            629.11       182.53208       YES     YES
    55        a            641.27       232.02658       YES     YES
    56        a            671.21       100.94200       YES     YES
    57        a            676.46         2.92971       YES     YES
    58        a            685.94        51.99559       YES     YES
```

59	a	686.40	54.88789	YES	YES
60	a	687.42	59.50396	YES	YES
61	a	692.92	37.47904	YES	YES
62	a	693.72	39.95310	YES	YES
63	a	734.50	19.74869	YES	YES
64	a	736.52	23.97384	YES	YES
65	a	737.33	22.85423	YES	YES
66	a	828.27	0.11418	YES	YES
67	a	829.11	0.14216	YES	YES
68	a	830.76	0.13057	YES	YES
69	a	901.36	118.52626	YES	YES
70	a	907.35	0.50956	YES	YES
71	a	907.87	0.48402	YES	YES
72	a	908.42	0.53074	YES	YES
73	a	949.81	0.08698	YES	YES
74	a	950.37	0.02883	YES	YES
75	a	950.86	0.08342	YES	YES
76	a	967.31	9.32983	YES	YES
77	a	970.60	0.09068	YES	YES
78	a	970.88	0.23808	YES	YES
79	a	971.17	0.38454	YES	YES
80	a	987.50	6.13230	YES	YES
81	a	987.64	5.00663	YES	YES
82	a	988.48	1.55177	YES	YES
83	a	1019.02	4.09455	YES	YES
84	a	1019.54	4.39679	YES	YES
85	a	1019.73	3.66661	YES	YES
86	a	1042.07	229.26024	YES	YES
87	a	1073.45	35.52370	YES	YES
88	a	1074.53	25.42336	YES	YES
89	a	1076.25	11.00729	YES	YES
90	a	1077.23	25.58716	YES	YES
91	a	1077.38	10.31924	YES	YES
92	a	1079.82	15.21198	YES	YES
93	a	1160.24	0.20981	YES	YES
94	a	1160.45	0.09739	YES	YES
95	a	1160.75	0.23679	YES	YES
96	a	1172.92	10.57058	YES	YES
97	a	1173.75	9.69708	YES	YES
98	a	1176.00	4.20743	YES	YES
99	a	1292.11	19.82685	YES	YES
100	a	1295.61	5.91384	YES	YES
101	a	1297.06	4.89378	YES	YES
102	a	1304.39	47.79295	YES	YES
103	a	1328.76	0.24273	YES	YES
104	a	1329.47	0.29580	YES	YES
105	a	1330.67	0.43572	YES	YES
106	a	1401.82	17.20133	YES	YES
107	a	1403.05	9.89499	YES	YES
108	a	1424.18	46.16480	YES	YES
109	a	1425.86	16.25790	YES	YES
110	a	1426.00	17.54761	YES	YES
111	a	1467.48	4.96124	YES	YES
112	a	1468.10	10.45469	YES	YES
113	a	1469.25	10.26919	YES	YES
114	a	1565.30	4.43472	YES	YES
115	a	1566.66	0.51868	YES	YES
116	a	1566.91	0.15096	YES	YES
117	a	1575.61	0.59648	YES	YES
118	a	1575.97	0.35960	YES	YES
119	a	1577.03	1.13590	YES	YES
120	a	1666.74	1201.94865	YES	YES
121	a	1731.84	1460.92331	YES	YES
122	a	1907.21	1923.77024	YES	YES
123	a	1974.96	510.67364	YES	YES
124	a	2966.98	23.48085	YES	YES
125	a	3051.64	4.29540	YES	YES
126	a	3057.05	38.70579	YES	YES
127	a	3101.46	0.55890	YES	YES
128	a	3101.50	0.12284	YES	YES

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   129        a             3102.42          0.48707       YES     YES
   130        a             3108.21          2.13490       YES     YES
   131        a             3108.24          1.85437       YES     YES
   132        a             3109.81          3.14473       YES     YES
   133        a             3114.97          6.85977       YES     YES
   134        a             3115.14         12.02904       YES     YES
   135        a             3116.96          8.53762       YES     YES
   136        a             3121.82         19.57407       YES     YES
   137        a             3122.05         18.07387       YES     YES
   138        a             3122.76         23.20692       YES     YES
   139        a             3127.00         30.72913       YES     YES
   140        a             3127.40         32.84621       YES     YES
   141        a             3128.00         20.93143       YES     YES
$end
```

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