

Supporting Information for

Ligand Effect on the Electronic Structure of Cobalt Sulfide Clusters: A Combined Experimental and Theoretical Study

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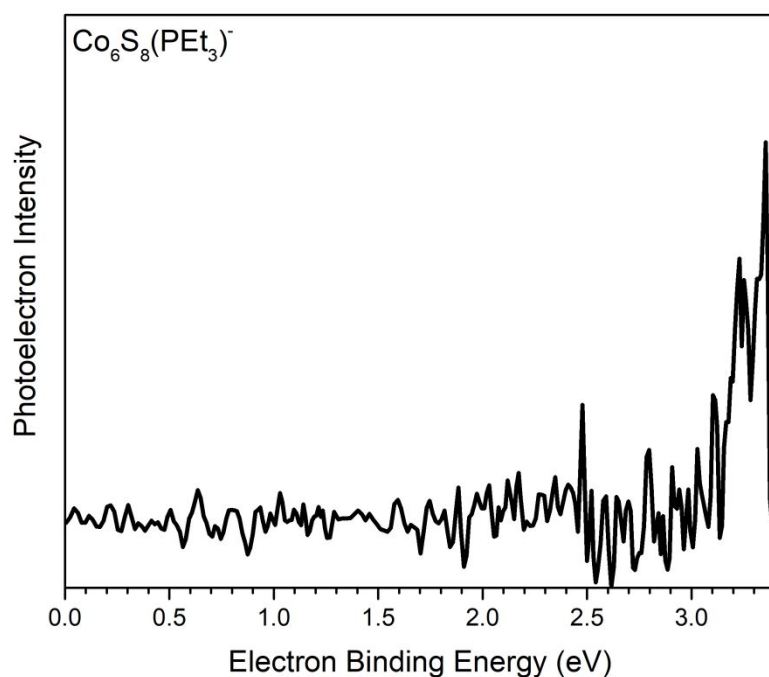


Figure S1. Photoelectron spectrum of $\text{Co}_6\text{S}_8(\text{PEt}_3)^-$ taken with 355 nm photon (3.49 eV).

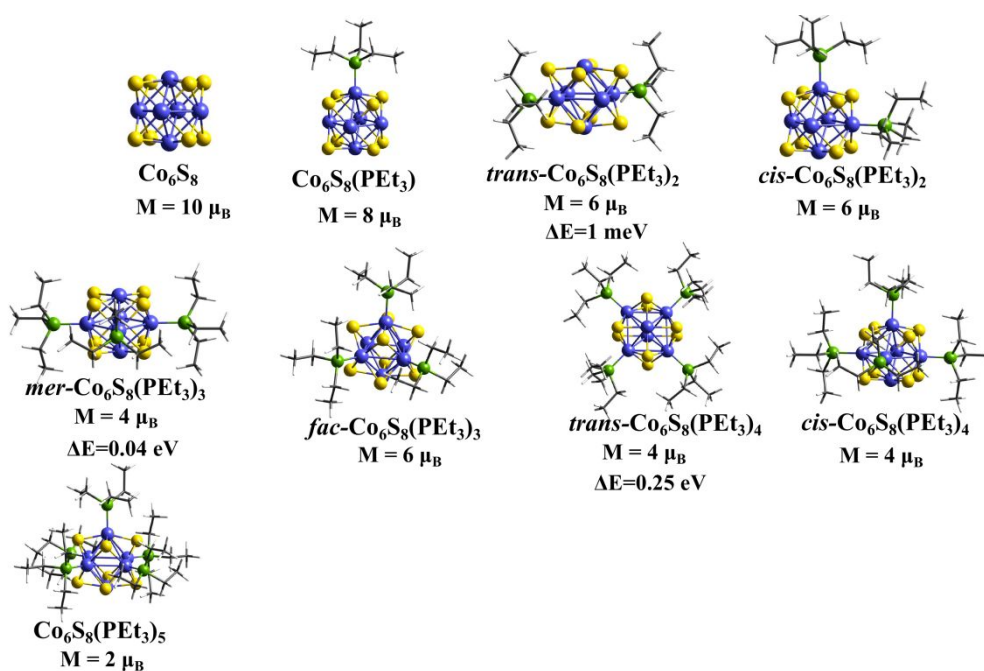


Figure S2. Optimized ground state geometry of neutral $\text{Co}_6\text{S}_8(\text{PEt}_3)_x$ ($x = 0-5$) clusters. The magnetic moment in each case is also shown.

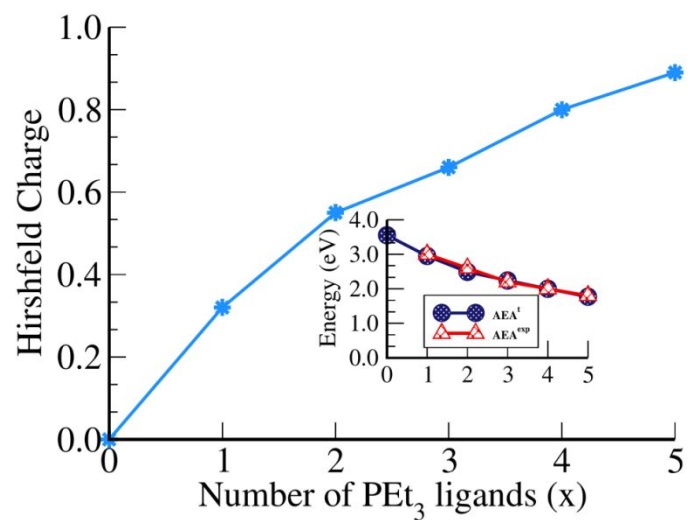


Figure S3. Hirshfeld charge donated by PET₃ ligands to Co₆S₈ core.

Anion	With GGA PBE functional		Grimme corrected PBE functional	
Cluster	AEA (eV)	VDE (eV)	AEA (eV)	VDE (eV)
Co ₆ S ₈	3.55	3.59	3.55	3.55
Co ₆ S ₈ (PET ₃)	2.94	2.98	2.95	2.99
<i>trans</i> -Co ₆ S ₈ (PET ₃) ₂	2.35	2.59	2.30	2.57
<i>cis</i> -Co ₆ S ₈ (PET ₃) ₂	2.49	2.60	2.46	2.59
<i>fac</i> -Co ₆ S ₈ (PET ₃) ₃	2.26	2.32	2.23	2.28
<i>mer</i> -Co ₆ S ₈ (PET ₃) ₃	2.10	2.16	2.06	2.18
<i>trans</i> -Co ₆ S ₈ (PET ₃) ₄	2.03	2.07	1.97	2.09
<i>cis</i> -Co ₆ S ₈ (PET ₃) ₄	2.00	2.11	1.99	2.09
Co ₆ S ₈ (PET ₃) ₅	1.77	1.88	1.78	1.88

Table S1. The absolute values of calculated AEA and VDE with GGA PBE and Grimme corrected PBE functional for anionic Co₆S₈(PET₃)_x (x=0-5) clusters. All the values are given in eV.

Table S2. The absolute values of HOMO and LUMO and HOMO-LUMO gap in anionic and neutral $\text{Co}_6\text{S}_8(\text{PET}_3)_x$ ($x=0-5$) clusters. All the values are given in eV.

	Anion			Neutral		
Cluster	HOMO(eV)	LUMO (eV)	Gap (eV)	HOMO (eV)	LUMO(eV)	Gap(eV)
Co_6S_8	-1.4232	-1.0707	0.3525	-5.3732	-5.3444	0.0288
$\text{Co}_6\text{S}_8(\text{PET}_3)$	-1.0817	-0.8415	0.2402	-4.8606	-4.6315	0.2291
<i>trans</i> - $\text{Co}_6\text{S}_8(\text{PET}_3)_2$	-0.8598	-0.6134	0.2464	-4.2671	-3.9296	0.3375
<i>cis</i> - $\text{Co}_6\text{S}_8(\text{PET}_3)_2$	-0.8467	-0.4896	0.3571	-4.2601	-4.0845	0.1756
<i>fac</i> - $\text{Co}_6\text{S}_8(\text{PET}_3)_3$	-0.6885	-0.511	0.1775	-3.9902	-3.8194	0.1708
<i>mer</i> - $\text{Co}_6\text{S}_8(\text{PET}_3)_3$	-0.6624	-0.4094	0.253	-3.8735	-3.5868	0.2867
<i>trans</i> - $\text{Co}_6\text{S}_8(\text{PET}_3)_4$	-0.6208	-0.2666	0.3542	-3.6769	-3.475	0.2019
<i>cis</i> - $\text{Co}_6\text{S}_8(\text{PET}_3)_4$	-0.5997	-0.2494	0.3503	-3.7327	-3.4896	0.2431
$\text{Co}_6\text{S}_8(\text{PET}_3)_5$	-0.4974	0.0528	0.5502	-3.5078	-3.1778	0.330

Clusters	Moment/ Multiplicity	Neutral	Moment/ Multiplicity	Anion
Co ₆ S ₈	8 /9	-79.87741855	7 /8	-83.32435236
	10 /11	-80.19171292	9 /10	-83.75336918
	12 /13	-79.28992922	11 /12	-82.92695271
	14 /15	-78.37773162		
Co ₆ S ₈ (PEt ₃)	6 /7	-196.2281978	5 /6	-199.14587754
	8 /9	-196.5449686	7 /8	-199.49198659
	10 /11	-196.1962120	9 /10	-199.12051925
<i>trans</i> -Co ₆ S ₈ (PEt ₃) ₂	4 /5	-312.3419827	3 /4	-314.82964744
	6 /7	-312.7348963	5 /6	-315.08427408
	8 /9	-312.3819652	7 /8	-315.00956342
<i>cis</i> -Co ₆ S ₈ (PEt ₃) ₂	4 /5	-312.4497473	3 /4	-314.85481444
	6 /7	-312.7355702	5 /6	-315.22081567
	8 /9	-312.4682895	7 /8	-315.03001445
<i>mer</i> -Co ₆ S ₈ (PEt ₃) ₃	2 /3	-428.5683882		
	4 /5	-428.7804991	3 /4	-430.84500635
	6 /7	-428.6732752	5 /6	-430.88542865
	8 /9	-428.0376680	7 /8	-430.45291377

<i>fac</i> -Co ₆ S ₈ (PEt ₃) ₃	2 / 3	-428.5804907		
	4 / 5	-428.8078555	3 / 4	-430.95339998
	6 / 7	-428.8198340	5 / 6	-431.08202331
	8 / 9	-428.0938831	7 / 8	-430.42785478
<i>trans</i> -Co ₆ S ₈ (PEt ₃) ₄	2 / 3	-544.6793814	1 / 2	-546.67771226
	4 / 5	-544.7485446	3 / 4	-546.77842373
	6 / 7	-544.0981853	5 / 6	-546.21148387
<i>cis</i> -Co ₆ S ₈ (PEt ₃) ₄	2 / 3	-544.8424653	1 / 2	-546.67771226
	4 / 5	-544.9979993	3 / 4	-547.00406608
	6 / 7	-544.3220908	5 / 6	-546.42342123
Co ₆ S ₈ (PEt ₃) ₅	0 / 1	-660.9980408	1 / 2	-662.96923264
	2 / 3	-661.1944330	3 / 4	-662.39523837

Table S3: Total energies of Neutral and anionic Co₆S₈(PEt₃)_x (x=0-5) clusters with spin magnetic moment and spin-multiplicity (2S+1).

	Neutral		Anion	
	S ² (exact)	<S ² > (calculated)	S2 (exact))	<S2> (calculated)
Co ₆ S ₈	30	30.09	24.75	24.83
Co ₆ S ₈ (PEt ₃)	20	20.11	15.75	15.86
<i>trans</i> -Co ₆ S ₈ (PEt ₃) ₂	12	12.12	8.75	8.87
<i>cis</i> -Co ₆ S ₈ (PEt ₃) ₂	12	12.12	8.75	8.89
<i>fac</i> -Co ₆ S ₈ (PEt ₃) ₃	12	12.09	8.75	8.85
<i>mer</i> -Co ₆ S ₈ (PEt ₃) ₃	6	6.12	8.75	8.87
<i>trans</i> -Co ₆ S ₈ (PEt ₃) ₄	6	6.08	3.75	3.89
<i>cis</i> -Co ₆ S ₈ (PEt ₃) ₄	6	6.09	3.75	3.87
Co ₆ S ₈ (PEt ₃) ₅	2	2.04	0.75	0.80

Table S4: Spin contamination (S²) values of neutral and anionic Co₆S₈(PEt₃)_x (x=0-5) clusters.

Ground state	Neutral			Anion		
	$\langle \text{Co-Co} \rangle_{xy}$ (Å)	$\langle \text{Co}_z\text{-Co}_{xy} \rangle$ (Å)	$\langle \text{Co-S} \rangle$ (Å)	$\langle \text{Co-Co} \rangle_{xy}$ (Å)	$\langle \text{Co}_z\text{-Co}_{xy} \rangle$ (Å)	$\langle \text{Co-S} \rangle$ (Å)
Co_6S_8	2.55	2.55	2.25	2.56	2.56	2.25
1PEt_3	2.56	2.66	2.26	2.57	2.65	2.26
<i>cis</i> - 2PEt_3	2.61	2.65	2.26	2.66	2.70	2.26
<i>fac</i> - 3PEt_3	2.69	2.69	2.26	2.72	2.72	2.26
<i>cis</i> - 4PEt_3	2.78	2.73	2.26	2.80	2.75	2.26
5PEt_3	2.86	2.79	2.26	2.90	2.82	2.26

Table S5: Average $\langle \text{Co-Co} \rangle_{xy}$ within xy plane, $\langle \text{Co}_z\text{-Co}_{xy} \rangle$, and $\langle \text{Co-S} \rangle$ bond lengths in ground state of neutral and anionic $\text{Co}_6\text{S}_8(\text{PEt}_3)_x$ ($x=0-5$) clusters

**Cartesian coordinates in angstrom
of optimized anionic $\text{Co}_6\text{S}_8(\text{PEt}_3)_x$
($x=0-5$) clusters**

$\text{Co}_6\text{S}_8(\text{PEt}_3)_5$

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XYZ

S -1.515903 1.615686 -1.572189
S 1.52265 -1.598379 1.572556
S 1.615486 1.516959 -1.574405
S -1.61356 -1.510956 1.561772
S -1.531264 1.626312 1.55572
S 1.536154 -1.625449 -1.575762
S -1.602274 -1.527474 -1.571794
S 1.606798 1.51772 1.563683
Co 0.060875 2.058673 -0.015203
Co -0.051871 -2.055197 -0.006345
Co 0.003932 -0.005781 -2.033645
Co -0.008444 0.009763 1.842507
Co -2.049845 0.058744 -0.017243
Co 2.053875 -0.056117 -0.015021
P -4.172083 0.039344 0.044287
P 4.179111 -0.03105 -0.029961
P -0.07747 -0.011972 -4.167254
P 0.110667 4.182067 -0.030299

P -0.097123 -4.180854 0.069786
C -1.557947 5.005644 -0.061539
C 1.57389 -4.999525 0.04411
C -5.028957 -1.428073 -0.721571
C 5.010053 1.442946 0.750234
C 1.294236 0.85759 -5.083201
C 0.964794 5.013683 1.400891
C -1.017928 -5.070051 -1.285969
C -4.889283 0.108779 1.75965
C 4.954544 -0.103055 -1.720227
C 1.006095 5.000402 -1.44621
C -0.920762 -4.954301 1.551378
C -2.886795 0.181373 -4.640861
C 0.373835 4.74192 -2.812636
C -0.24858 -4.634476 2.885049
C -0.0925 -1.69911 -4.954197
C 0.310164 4.748999 2.755478
C -0.386992 -4.909462 -2.666807
C -5.069178 1.406016 -0.851293
C 5.05137 -1.39257 0.89542
C -1.540557 0.826164 -4.964018
C 2.659005 0.19272 -4.922515
C -4.826865 2.792691 -0.2612
C 4.841779 -2.778503 0.290926
C -4.711653 -2.763571 -0.052228

C	4.703287	2.773508	0.065993	H	-0.986614	-6.042528	1.386133
C	-1.603011	6.533319	-0.067282	H	2.021876	4.578789	-1.417783
C	1.624311	-6.525869	0.101315	H	-1.945743	-4.554326	1.54245
C	-0.156147	-1.777545	-6.479417	H	-3.714299	0.783773	-5.044932
C	-6.41141	0.089076	1.897837	H	-3.016494	0.096622	-3.553375
C	6.480295	-0.090077	-1.810419	H	-2.968208	-0.828732	-5.067196
H	-2.061667	4.585774	-0.94489	H	1.005422	5.145312	-3.618271
H	2.116605	-4.548844	0.888081	H	-0.835674	-5.041915	3.721611
H	-2.091411	4.590209	0.806293	H	-0.617511	5.209294	-2.898442
H	2.064504	-4.612766	-0.861596	H	0.762158	-5.062805	2.944733
H	-6.114348	-1.235158	-0.735474	H	0.251303	3.66249	-2.975521
H	6.095609	1.254709	0.79107	H	-0.160996	-3.548379	3.022514
H	-4.680382	-1.44013	-1.765302	H	0.803529	-2.202551	-4.561416
H	4.633925	1.457559	1.783966	H	-0.946382	-2.215367	-4.491066
H	1.014003	0.947388	-6.145641	H	0.912152	5.181668	3.568332
H	1.317619	1.87221	-4.658682	H	-1.039636	-5.326489	-3.448379
H	1.987264	4.607444	1.392297	H	0.217257	3.669162	2.933118
H	-2.025504	-4.628492	-1.279005	H	-0.221071	-3.847207	-2.886418
H	1.033989	6.094082	1.191514	H	-0.696377	5.187321	2.813837
H	-1.118724	-6.132911	-1.011299	H	0.583535	-5.421709	-2.733411
H	-4.422005	-0.733136	2.291938	H	-4.687252	1.363713	-1.882396
H	4.514274	0.745069	-2.265271	H	4.625964	-1.354818	1.90926
H	-4.451583	1.012098	2.210102	H	-6.144493	1.165286	-0.88539
H	4.530166	-1.004533	-2.18713	H	6.12292	-1.144482	0.971335
H	1.087846	6.080285	-1.239932	H	-1.517002	1.856295	-4.578333

H	-1.370689	0.872878	-6.052315	H	-1.094385	6.955854	-0.945567
H	3.454496	0.818851	-5.353437	H	-1.130647	6.961026	0.82833
H	2.696391	-0.78598	-5.422057	H	-2.644416	6.889365	-0.089711
H	2.881771	0.035569	-3.85953	H	-3.749806	2.981471	-0.168507
H	-3.624809	-2.912815	0.001233	H	-5.272983	2.893556	0.738405
H	3.617103	2.920524	-0.00563	H	-5.26138	3.573925	-0.902767
H	-5.152109	-3.597753	-0.618949				
H	5.131838	3.612022	0.635262	<i>trans</i> -Co ₆ S ₈ (PEt ₃) ₄			
H	-5.104849	-2.809217	0.973263	102			
H	5.115232	2.814052	-0.952566	XYZ			
H	0.702721	-1.281235	-6.953397	S	-1.537368	1.584426	-1.598452
H	-1.069086	-1.311072	-6.875795	S	1.537902	-1.584258	1.598558
H	-0.153214	-2.826419	-6.813667	S	1.648103	1.497323	-1.56393
H	-6.882548	0.938745	1.383063	S	-1.647561	-1.497147	1.564019
H	6.930655	-0.942212	-1.281662	S	-1.568072	1.640666	1.517935
H	-6.704324	0.145743	2.95733	S	1.568612	-1.640499	-1.517831
H	6.806611	-0.146742	-2.860299	S	-1.620872	-1.539394	-1.547409
H	-6.849049	-0.831925	1.487094	S	1.621417	1.539573	1.54751
H	6.907936	0.828606	-1.384646	Co	0.053551	2.037809	-0.030572
H	5.331131	-2.874535	-0.688998	Co	-0.053004	-2.037646	0.030672
H	3.770412	-2.972425	0.152775	Co	0.016746	-0.027104	-1.68175
H	5.252221	-3.559674	0.94795	Co	-0.016205	0.02729	1.681832
H	2.66635	-6.879811	0.07519	Co	-2.142169	0.057419	-0.016083
H	1.101083	-6.987183	-0.748482	Co	2.142714	-0.057253	0.016179
H	1.16976	-6.915871	1.022891	P	-4.264005	0.039296	0.041586

P	4.264554	-0.039168	-0.041482	C	-6.499528	0.099715	1.899061
P	0.096549	4.197325	-0.053505	C	6.5001	-0.099557	-1.898926
P	-0.096008	-4.197152	0.053639	H	-2.071114	4.587072	-0.981247
C	-1.573712	5.013484	-0.097365	H	2.071686	-4.586903	0.981321
C	1.574253	-5.013317	0.097457	H	-2.111186	4.600486	0.769317
C	-5.110175	-1.435906	-0.718273	H	2.111703	-4.60033	-0.769245
C	5.110733	1.435974	0.718484	H	-6.197327	-1.253244	-0.733655
C	0.942062	5.029385	1.380767	H	6.19788	1.253288	0.733906
C	-0.941572	-5.029199	-1.380612	H	-4.760345	-1.447323	-1.761589
C	-4.977865	0.118812	1.757435	H	4.760856	1.447355	1.761784
C	4.978432	-0.118573	-1.75733	H	1.96272	4.618087	1.380584
C	1.001591	4.999316	-1.468759	H	-1.962222	-4.617882	-1.380409
C	-1.001016	-4.999137	1.468921	H	1.018845	6.108874	1.170001
C	0.384033	4.721732	-2.838366	H	-1.018372	-6.108686	-1.169846
C	-0.383416	-4.721571	2.838514	H	-4.50949	-0.719355	2.294867
C	0.276816	4.770599	2.731859	H	4.510119	0.719671	-2.294695
C	-0.276352	-4.770418	-2.731719	H	-4.540024	1.024879	2.202484
C	-5.15023	1.402161	-0.867522	H	4.540546	-1.024574	-2.202469
C	5.150747	-1.402121	0.86752	H	1.078965	6.081741	-1.273853
C	-4.886756	2.793988	-0.297453	H	-1.078407	-6.081559	1.274013
C	4.887188	-2.793899	0.297373	H	2.018278	4.580763	-1.423582
C	-4.780436	-2.766064	-0.043104	H	-2.017702	-4.580576	1.423778
C	4.781054	2.766167	0.043354	H	1.017664	5.130217	-3.639347
C	-1.621839	6.540616	-0.110917	H	-1.017033	-5.130051	3.639508
C	1.622378	-6.540449	0.11102	H	-0.612225	5.176323	-2.934924

H	0.612836	-5.176181	2.935043	H	5.320743	-2.911616	-0.706036
H	0.278265	3.640825	-3.001609	H	3.807022	-2.972495	0.220197
H	-0.277625	-3.640667	3.001763	H	5.321642	-3.570913	0.943613
H	0.87523	5.203149	3.547228	H	2.664005	-6.894978	0.139984
H	-0.874791	-5.202953	-3.547077	H	1.154519	-6.973261	-0.784549
H	0.17836	3.69195	2.912607	H	1.110206	-6.95867	0.989193
H	-0.177882	-3.691769	-2.912464	H	-1.109627	6.958846	-0.989063
H	-0.728062	5.213506	2.782248	H	-1.154024	6.973424	0.784678
H	0.728517	-5.213342	-2.782133	H	-2.663467	6.895138	-0.139927
H	-4.771161	1.338718	-1.89869	H	-3.806601	2.97259	-0.220122
H	4.771722	-1.338727	1.898708	H	-5.320475	2.911794	0.705874
H	-6.22872	1.175302	-0.894529	H	-5.321106	3.570947	-0.943827
H	6.229247	-1.175307	0.894499				
H	-3.692209	-2.90779	0.004288	<i>cis</i> -Co ₆ S ₈ (PEt ₃) ₄			
H	3.692831	2.907916	-0.004089	102			
H	-5.218156	-3.605635	-0.603375	XYZ			
H	5.218756	3.605707	0.603686	S	-1.520798	1.604322	-1.594962
H	-5.168817	-2.808931	0.984425	S	1.539438	-1.634596	1.570454
H	5.169493	2.809072	-0.984151	S	1.666172	1.496286	-1.605008
H	-6.970932	0.947037	1.380793	S	-1.581013	-1.50629	1.548116
H	6.971437	-0.946984	-1.38077	S	-1.487795	1.618439	1.545748
H	-6.79099	0.161087	2.958586	S	1.558326	-1.640429	-1.605653
H	6.791577	-0.160798	-2.958454	S	-1.617318	-1.525157	-1.582323
H	-6.93742	-0.823046	1.492654	S	1.647824	1.520838	1.55535
H	6.938049	0.823117	-1.49238	Co	0.091201	2.036839	-0.035498

Co -0.036422 -2.052241 -0.021504	C 1.540987 -0.817799 4.997753
Co 0.004551 -0.013893 -1.766783	C -2.66368 -0.210527 4.917455
Co 0.025601 0.002898 2.04772	C -4.847853 2.796616 -0.273306
Co -2.042549 0.059479 -0.004983	C -4.727218 -2.754404 -0.053895
Co 1.771445 -0.072741 0.000787	C -1.594546 6.516565 -0.123141
P -4.187999 0.04698 0.034718	C 1.706133 -6.488658 0.043702
P 0.078356 0.011198 4.194245	C 0.119742 1.787823 6.499744
P 0.130653 4.175993 -0.111525	C -6.481457 0.118451 1.827758
P -0.062706 -4.186242 -0.000476	H -2.095949 4.538081 -0.898703
C -1.540604 4.990486 -0.063861	H 2.127619 -4.517692 0.896834
C 1.626715 -4.962393 0.02397	H -2.017007 4.604552 0.849934
C -5.030118 -1.424159 -0.740501	H 2.142681 -4.539765 -0.850751
C -1.296756 -0.865551 5.098079	H -6.114912 -1.231311 -0.778707
C 1.071747 5.052549 1.23521	H -4.658496 -1.442682 -1.775849
C -0.912986 -5.028541 -1.425565	H -1.029459 -0.950967 6.164229
C -4.955955 0.11954 1.728951	H -1.307712 -1.882301 4.677714
C 0.938099 4.940096 -1.603857	H 2.073528 4.598232 1.215494
C -0.941603 -5.011192 1.420059	H -1.943404 -4.64236 -1.404677
C 2.888458 -0.180695 4.66574	H 1.180942 6.11482 0.961385
C 0.253341 4.614725 -2.929939	H -0.960484 -6.110133 -1.216837
C -0.318209 -4.732883 2.786518	H -4.521034 -0.734218 2.269616
C 0.075265 1.701767 4.974402	H -4.522998 1.015874 2.198011
C 0.453277 4.895811 2.622313	H 1.004007 6.028919 -1.442663
C -0.277982 -4.75045 -2.786436	H -1.002697 -6.09365 1.220379
C -5.063427 1.413417 -0.882146	H 1.962969 4.5401 -1.60097

H	-1.965987	-4.610267	1.386011	H	-3.641743	-2.906453	0.018953
H	3.712142	-0.77032	5.094868	H	-5.158615	-3.592891	-0.620867
H	3.034318	-0.127072	3.578558	H	-5.139797	-2.791627	0.964559
H	2.964959	0.840888	5.064985	H	-0.741746	1.288319	6.965558
H	0.82889	5.025911	-3.772379	H	1.030836	1.328731	6.90855
H	-0.941752	-5.149554	3.591586	H	0.106404	2.838018	6.829473
H	-0.760908	5.036134	-2.979321	H	-6.927553	0.977739	1.30713
H	0.683756	-5.176148	2.874959	H	-6.801964	0.170642	2.879649
H	0.172749	3.528114	-3.066466	H	-6.918955	-0.793703	1.397992
H	-0.221087	-3.650708	2.947519	H	2.755378	-6.820416	0.058985
H	-0.817592	2.200011	4.567711	H	1.235127	-6.935548	-0.843374
H	0.932888	2.219657	4.520039	H	1.215984	-6.914441	0.930906
H	1.11623	5.310395	3.396196	H	-1.157672	6.904932	-1.053815
H	-0.878838	-5.196956	-3.592547	H	-1.056497	6.98018	0.716003
H	0.285493	3.834485	2.845517	H	-2.636536	6.86859	-0.078593
H	-0.209088	-3.669383	-2.966656	H	-3.775913	2.989445	-0.138018
H	-0.513907	5.413038	2.698892	H	-5.332946	2.889828	0.708995
H	0.736952	-5.167156	-2.854473	H	-5.259713	3.581554	-0.924828
H	-4.64548	1.378784	-1.89917				
H	-6.136008	1.168321	-0.953086				
H	1.513351	-1.853685	4.627299				
H	1.370335	-0.850423	6.086583				
H	-3.461017	-0.838124	5.342786				
H	-2.713154	0.771005	5.410349				
H	-2.875675	-0.061058	3.851213				
				<i>mer</i> -Co ₆ S ₈ (PEt ₃) ₃			
				80			
				XYZ			
				S	-1.521811	1.591938	-1.613169
				S	1.565382	-1.603247	1.581474
				S	1.630398	1.490954	-1.577988

S	-1.660205	-1.49789	1.622292	C	-0.332076	-4.748975	-2.72255
S	-1.523893	1.626408	1.592922	C	5.169385	-1.369028	0.838661
S	1.564538	-1.647334	-1.532532	C	4.928527	-2.766603	0.272891
S	-1.65935	-1.536471	-1.573173	C	4.759006	2.789087	-0.004414
S	1.633952	1.518282	1.557759	C	-1.712331	6.455446	-0.057226
Co	0.051429	2.025437	-0.012472	C	1.606348	-6.50333	0.093268
Co	-0.075346	-1.98677	0.030437	C	6.489334	-0.058378	-1.940321
Co	0.021509	-0.060805	-1.777865	H	-2.131817	4.485628	-0.913831
Co	0.019684	-0.019293	1.793539	H	2.066827	-4.547582	0.952128
Co	-1.748419	0.058005	0.004866	H	-2.138501	4.502719	0.834161
Co	2.121553	-0.063539	0.002152	H	2.080407	-4.564664	-0.799019
P	4.259087	-0.021993	-0.071381	H	6.186631	1.287812	0.686746
P	0.064253	4.163008	-0.028048	H	4.754267	1.479402	1.72075
P	-0.116462	-4.166898	0.057479	H	1.948847	4.617178	1.372724
C	-1.628098	4.929239	-0.042136	H	-2.001013	-4.573003	-1.35171
C	1.556451	-4.97616	0.076658	H	0.970616	6.086804	1.178952
C	5.098327	1.464153	0.675571	H	-1.068094	-6.072387	-1.145989
C	0.919752	5.006598	1.393475	H	4.484668	0.723181	-2.332232
C	-0.984811	-4.994702	-1.363074	H	4.546428	-1.020179	-2.226771
C	4.96883	-0.102854	-1.790158	H	0.984255	6.068996	-1.252886
C	0.933698	4.986049	-1.453233	H	-1.083563	-6.042369	1.295779
C	-0.998477	-4.960361	1.48956	H	1.962093	4.595764	-1.418306
C	0.312146	4.701206	-2.819016	H	-2.013199	-4.535953	1.461063
C	-0.355572	-4.68713	2.848498	H	0.923887	5.139904	-3.621146
C	0.28742	4.739182	2.757941	H	-0.977089	-5.095383	3.658814

H	-0.699983	5.121902	-2.901157	H	-1.236008	6.901613	0.827321
H	0.640784	-5.144889	2.927426	H	-2.762742	6.783232	-0.063714
H	0.241537	3.619422	-2.993385				
H	-0.244522	-3.607104	3.013554	<i>fac</i> -Co ₆ S ₈ (PEt ₃) ₃			
H	0.892811	5.188566	3.558994	80			
H	-0.945263	-5.177753	-3.528633	XYZ			
H	0.215888	3.659738	2.945698	S	-1.544147	1.658451	-1.597602
H	-0.224035	-3.672441	-2.910496	S	1.534211	-1.589401	1.541891
H	-0.725507	5.160338	2.826802	S	1.667597	1.578902	-1.615278
H	0.666863	-5.203897	-2.783119	S	-1.612294	-1.517431	1.562079
H	4.793993	-1.309081	1.871342	S	-1.499513	1.646602	1.568258
H	6.244333	-1.124808	0.86225	S	1.542962	-1.603407	-1.574521
H	3.670419	2.929408	-0.04365	S	-1.594126	-1.500339	-1.588334
H	5.199858	3.63315	0.546674	S	1.626292	1.531743	1.571334
H	5.138139	2.827331	-1.035557	Co	0.089334	1.79482	-0.028503
H	6.978943	-0.890511	-1.414475	Co	-0.04255	-2.051846	0.002509
H	6.776109	-0.127576	-3.000643	Co	0.03834	0.040223	-1.782173
H	6.912388	0.877217	-1.548022	Co	0.014541	9.1E-05	2.055788
H	5.360506	-2.878778	-0.731792	Co	-1.77145	0.072371	-0.004425
H	3.852037	-2.967344	0.200456	Co	2.064781	-0.029728	-0.017986
H	5.38027	-3.534117	0.918696	P	4.227174	-0.020979	-0.079643
H	2.649115	-6.855354	0.106133	P	0.048277	0.017661	4.194711
H	1.124658	-6.939021	-0.793442	P	-0.080818	-4.194256	0.053975
H	1.109446	-6.919702	0.980897	C	1.588868	-5.015192	0.051982
H	-1.230406	6.884306	-0.947259	C	5.082225	1.43667	0.701123

C	-1.390899	-0.781149	5.0641	H	4.497742	-0.98177	-2.252357
C	-0.974995	-5.035165	-1.345147	H	-1.021878	-6.071644	1.318616
C	4.936698	-0.081465	-1.79678	H	-1.957182	-4.569422	1.487684
C	-0.93992	-4.987923	1.503458	H	3.627797	-0.910417	5.154083
C	2.831992	-0.284673	4.72332	H	2.987413	-0.226192	3.637523
C	-0.279131	-4.703229	2.851424	H	2.94355	0.728878	5.133828
C	0.112655	1.72124	4.937961	H	-0.888476	-5.102053	3.675975
C	-0.343975	-4.801886	-2.716659	H	0.71851	-5.159739	2.921633
C	5.116118	-1.400186	0.804311	H	-0.164864	-3.620579	2.997665
C	1.455607	-0.871753	5.030995	H	-0.752157	2.247983	4.507852
C	-2.735676	-0.109955	4.789126	H	0.994332	2.196013	4.482148
C	4.869707	-2.780065	0.198817	H	-0.969417	-5.237004	-3.509796
C	4.760125	2.783431	0.056658	H	-0.238855	-3.726836	-2.914657
C	1.634761	-6.542554	0.083103	H	0.65343	-5.258775	-2.788928
C	0.139358	1.830703	6.462502	H	4.731266	-1.367587	1.834917
C	6.458222	-0.062291	-1.939632	H	6.192634	-1.166131	0.846143
H	2.11775	-4.58119	0.913708	H	1.396726	-1.905388	4.657821
H	2.099211	-4.61652	-0.837506	H	1.265175	-0.899927	6.11649
H	6.167872	1.24386	0.704892	H	-3.555787	-0.685819	5.242665
H	4.743237	1.43013	1.748331	H	-2.773485	0.908222	5.20149
H	-1.174295	-0.819405	6.144538	H	-2.920032	-0.042654	3.708621
H	-1.404423	-1.817165	4.693296	H	3.675867	2.954747	0.03659
H	-1.99063	-4.61286	-1.319931	H	5.229157	3.603069	0.620994
H	-1.055817	-6.111173	-1.118118	H	5.125696	2.83672	-0.97853
H	4.468474	0.763995	-2.32259	H	-0.754125	1.384637	6.921878

H	1.019179	1.3329	6.894667	Co	-0.039497	0.02261	-2.079483
H	0.174887	2.885705	6.773672	Co	0.024641	-0.020312	2.07961
H	6.930794	-0.913591	-1.428836	Co	-1.768801	0.047764	0.030318
H	6.747518	-0.115639	-3.000126	Co	1.862447	-0.053597	-0.030672
H	6.896516	0.857568	-1.527528	P	-0.104955	-0.024724	-4.191824
H	5.315193	-2.870767	-0.801935	P	0.039686	0.031795	4.193134
H	3.79267	-2.968161	0.104834	C	1.313257	0.792036	-5.071006
H	5.303615	-3.569094	0.830948	C	-1.408127	-0.766217	5.041997
H	2.676145	-6.899095	0.078325	C	-2.906683	0.257977	-4.648906
H	1.13352	-6.985563	-0.789039	C	2.824165	-0.275809	4.716565
H	1.154455	-6.948664	0.984548	C	-0.162382	-1.735549	-4.910365
				C	0.096833	1.743975	4.908684
<i>trans</i> -Co ₆ S ₈ (PEt ₃) ₂				C	-1.539563	0.849017	-4.987193
58				C	1.445189	-0.856361	5.022593
XYZ				C	2.670365	0.137796	-4.818612
S	-1.538497	1.654598	-1.528765	C	-2.75425	-0.105017	4.751179
S	1.560176	-1.640182	1.533578	C	-0.222678	-1.853501	-6.433253
S	1.601864	1.55253	-1.583869	C	0.116145	1.865913	6.432371
S	-1.578093	-1.57153	1.579513	H	1.077855	0.8294	-6.147415
S	-1.507898	1.608936	1.62801	H	-1.200185	-0.795389	6.124299
S	1.526483	-1.594149	-1.635336	H	1.314961	1.825739	-4.6944
S	-1.642627	-1.521765	-1.576851	H	-1.408602	-1.80341	4.675243
S	1.664004	1.504848	1.582783	H	-3.709394	0.872775	-5.081708
Co	0.072746	1.813407	0.0335	H	3.6123	-0.899127	5.163606
Co	-0.029914	-1.82224	-0.033955	H	-3.052011	0.218838	-3.561397

H	2.992663	-0.233688	3.632441	58
H	-3.017815	-0.763058	-5.040613	XYZ
H	2.935125	0.742623	5.114976	S -1.543102 1.609453 -1.575439
H	0.718407	-2.247761	-4.495922	S 1.544972 -1.654878 1.530364
H	-0.767881	2.263045	4.469718	S 1.622013 1.50482 -1.60578
H	-1.028821	-2.21422	-4.430587	S -1.596047 -1.549147 1.569191
H	0.98002	2.213326	4.450742	S -1.498443 1.600095 1.574301
H	-1.473014	1.884151	-4.620401	S 1.540361 -1.658832 -1.640494
H	1.378075	-1.889932	4.651451	S -1.67021 -1.552604 -1.59852
H	-1.369374	0.869741	-6.076245	S 1.655762 1.494157 1.525236
H	1.248651	-0.877719	6.1072	Co 0.069159 2.051514 -0.026899
H	3.473789	0.723691	-5.288451	Co -0.05259 -1.800618 -0.035785
H	-3.57218	-0.679412	5.210215	Co -0.014702 -0.019272 -1.801993
H	2.714018	-0.881004	-5.228747	Co 0.034273 -0.025219 2.052596
H	-2.799677	0.918987	5.147991	Co -1.82651 0.038528 0.001213
H	2.87434	0.076765	-3.741506	Co 1.842301 -0.088168 -0.045425
H	-2.934042	-0.055343	3.669263	P 0.059887 0.020552 4.17178
H	0.654495	-1.399983	-6.916087	P 0.065109 4.1713 -0.062366
H	-0.780362	1.42539	6.891028	C -1.629718 4.924282 0.042176
H	-1.118937	-1.369996	-6.846767	C -1.387293 -0.780652 5.020888
H	0.993782	1.372252	6.873014	C 1.028345 5.049617 1.265566
H	-0.252636	-2.911026	-6.735398	C 0.819907 4.962515 -1.566259
H	0.150778	2.923959	6.732182	C 2.843887 -0.290363 4.699791
				C 0.121256 4.633665 -2.883665
<i>cis</i> -Co ₆ S ₈ (PEt ₃) ₂				C 0.128998 1.714147 4.932357

C	0.458101	4.873828	2.670174	H	1.266488	-0.92441	6.073128
C	1.465533	-0.881617	4.989578	H	-3.549719	-0.673138	5.205913
C	-2.728073	-0.09781	4.754912	H	-2.759066	0.917034	5.176276
C	-1.731439	6.448226	-0.009089	H	-2.915109	-0.021171	3.675694
C	0.139974	1.803228	6.458543	H	-0.764995	1.365105	6.902166
H	-2.197611	4.452241	-0.77311	H	1.008002	1.288087	6.893464
H	-2.063244	4.518381	0.968203	H	0.18733	2.854018	6.782091
H	-1.17035	-0.832899	6.100572	H	-1.343738	6.853525	-0.95423
H	-1.403438	-1.810298	4.63434	H	-1.176728	6.926169	0.811041
H	2.038576	4.617907	1.209084	H	-2.78112	6.766791	0.077091
H	1.1052	6.115205	0.994072				
H	0.858413	6.051048	-1.3947	Co₆S₈(PEt₃)			
H	1.856042	4.592888	-1.583894	36			
H	3.633245	-0.922738	5.131621	XYZ			
H	3.014519	-0.220117	3.617359	S	-1.569213	1.648993	-1.566562
H	2.952465	0.717392	5.125429	S	1.552597	-1.645647	1.51191
H	0.668067	5.077239	-3.728625	S	1.616833	1.562129	-1.613736
H	-0.906575	5.022348	-2.907668	S	-1.591722	-1.559428	1.558859
H	0.072985	3.547685	-3.036647	S	-1.515024	1.605631	1.592284
H	-0.728303	2.253716	4.50367	S	1.531651	-1.623216	-1.648607
H	1.023598	2.183216	4.497246	S	-1.659719	-1.535489	-1.601933
H	1.136253	5.301501	3.423303	S	1.652485	1.517871	1.54525
H	0.323203	3.808508	2.894195	Co	0.053569	1.811208	-0.000806
H	-0.517447	5.368356	2.779275	Co	-0.048687	-1.820849	-0.044958
H	1.403933	-1.907987	4.598825	Co	-0.022797	0.014984	-1.790614

Co	0.031383	-0.017084	2.051558	H	-0.711059	1.428169	6.880143
Co	-1.812946	0.045104	0.007607	H	1.062461	1.362017	6.839287
Co	1.818056	-0.055705	-0.047365	H	0.229296	2.91979	6.711575
P	0.066372	0.032426	4.170074				
C	-1.378631	-0.754921	5.033325	Co₆S₈			
C	2.854786	-0.29429	4.678055	14			
C	0.143832	1.744176	4.886864	XYZ			
C	1.473159	-0.865659	4.9882	S	-1.549482	1.639294	-1.570501
C	-2.721137	-0.077458	4.765775	S	1.549872	-1.639113	1.570536
C	0.182802	1.862566	6.410566	S	1.623256	1.5487	-1.588902
H	-1.15451	-0.790174	6.112277	S	-1.623093	-1.548489	1.58916
H	-1.394702	-1.791201	4.664513	S	-1.531642	1.624808	1.603526
H	3.639579	-0.922866	5.123255	S	1.531796	-1.624689	-1.603256
H	3.022918	-0.253378	3.59391	S	-1.640457	-1.533145	-1.584949
H	2.974268	0.722882	5.077042	S	1.64087	1.533313	1.584952
H	-0.722162	2.271172	4.46002	Co	0.053319	1.810101	0.008313
H	1.025438	2.207917	4.420449	Co	-0.052913	-1.809941	-0.008267
H	1.397166	-1.89939	4.619387	Co	-0.00974	0.008782	-1.810333
H	1.281256	-0.885449	6.073635	Co	0.010112	-0.008614	1.810389
H	-3.538458	-0.644345	5.234789	Co	-1.808796	0.05306	0.011111
H	-2.749007	0.944738	5.168768	Co	1.809221	-0.052896	-0.011047
H	-2.918549	-0.019912	3.687297				

	268.197397	cm-1	274.508873
Neutral	269.382413	-----	286.856080
Co₆S₈	271.671786	163.049836	286.941899
Frequency	272.221186	163.538730	286.989953
cm-1	273.016597	163.766605	307.004175
-----	282.523468	164.916307	307.424659
91.514283	289.121896	166.028323	307.933379
153.828695	289.454181	169.945679	323.860698
154.710957	310.655233	170.200679	369.863547
161.863818	311.996399	170.813700	372.439909
166.499469	312.834080	199.248434	372.781014
167.171489	332.625491	199.430871	373.175865
168.060676	374.567264	220.535097	381.709758
172.299390	376.542287	222.470325	382.284240
201.659814	379.490933	224.461293	382.542087
203.834018	379.825115	239.444329	
220.405575	388.024663	239.569852	Neutral
223.322552	388.530181	239.953093	Co₆S₈(PEt₃)
224.171966	388.881719	262.944978	Frequency
227.809616		270.879035	cm-1
236.549977	Anionic	271.039660	-----
236.651219	Co₆S₈	272.682821	34.940176
242.170624	Frequency	273.770416	53.440642

54.390088	238.074523	367.902288	1223.800613
84.054701	244.494998	376.389152	1229.947097
90.617355	246.273320	378.712511	1232.916104
97.822647	247.672202	385.185688	1247.709932
107.279175	250.198030	385.934316	1356.535085
117.533135	254.651988	425.090381	1360.229920
124.849091	259.493466	600.294422	1362.351939
136.952817	270.234377	633.447496	1387.335205
142.767350	271.430797	684.019746	1399.617811
148.264132	272.520947	695.330767	1404.291911
162.597911	277.749142	733.172799	1440.872305
163.059891	290.054940	736.987660	1441.973314
163.546758	291.689706	947.619302	1445.090659
166.880034	298.367880	953.329441	1447.765592
173.539901	305.271579	954.993877	1449.471619
179.257141	306.391347	973.680872	1450.864438
189.139871	307.097604	982.786104	2947.180542
198.819828	314.626115	990.039637	2950.544434
203.302234	321.032420	1019.420563	2952.135708
207.791485	327.559515	1020.178711	2953.173722
209.868491	356.315673	1044.533116	2954.518590
212.593227	361.329194	1211.896985	2972.000175
236.454585	363.054834	1213.924058	3009.298641

3012.566249	135.410938	266.754269	626.659519
3019.990742	142.521363	269.752884	681.363014
3034.893547	153.514513	275.686688	687.237151
3037.901681	165.885383	276.344989	731.144539
3039.366687	166.867029	289.863722	737.524845
3045.056087	169.741099	290.221665	945.211139
3047.227337	172.279979	293.209967	951.597604
3048.039625	176.890206	295.752919	953.613809
	181.972295	296.138748	972.200478
Anionic	190.323310	299.696715	982.287891
Co₆S₈(PEt₃)	195.657375	311.096398	990.015445
Frequency	200.880591	319.541383	1017.252243
cm-1	204.335171	319.893735	1020.031868
-----	211.800019	353.318143	1044.012084
36.665980	215.197915	355.366910	1209.330833
53.912879	235.908289	359.528441	1213.054585
54.928447	240.205758	366.760429	1223.443116
84.904475	243.553120	367.662110	1227.207516
91.686299	244.952133	369.465190	1229.172259
101.214904	246.540481	377.491699	1245.374644
109.063054	250.831539	378.196560	1349.157848
119.163417	255.141442	426.759480	1355.752073
129.396988	256.758842	597.462968	1357.463269

1387.331701	3040.578361	127.919940	239.948740
1399.190335		138.742277	240.109507
1405.309188	Neutral	139.396716	244.839555
1439.962635	<i>trans</i> -Co ₆ S ₈ (PEt ₃) ₂	145.501243	247.547885
1440.196827	Frequency	150.293054	249.716895
1443.207658	cm-1	154.321282	254.260465
1445.258767		156.956194	255.453489
1448.453511	31.697128	173.364149	268.597656
1450.200464	38.205155	173.870390	269.741148
2934.849586	39.937864	176.076656	282.694096
2937.501079	40.575801	177.476994	283.871599
2939.947166	67.148459	182.093320	285.031282
2940.782189	67.808677	183.565526	288.722927
2941.063770	85.065886	189.396480	289.525722
2967.703874	85.764111	189.775835	289.702749
3001.580246	91.945034	203.462693	292.584727
3004.449161	96.306307	206.343379	293.873462
3011.899627	102.434845	218.348261	294.259620
3015.694642	102.929185	221.131635	305.298965
3021.925815	108.542449	228.024388	318.333613
3022.906178	114.633025	236.115781	319.200577
3033.242121	117.687633	236.292646	333.611235
3040.314304	124.166296	237.016379	356.938633

363.157331	949.120504	1230.264589	1444.853927
363.951229	954.496504	1230.410221	1447.137316
364.677427	954.575885	1233.605693	1447.244828
370.106601	956.050863	1234.297412	1449.339354
374.874929	956.213007	1248.579033	1449.348056
376.032355	974.288112	1248.748904	1450.883803
378.154737	974.467186	1355.423095	1450.894257
378.605632	983.825647	1355.562241	2946.194804
405.944374	984.755441	1360.281294	2946.434340
414.140202	990.958226	1360.326127	2949.417806
597.768341	990.978906	1362.111932	2949.559906
599.564763	1019.727836	1362.287867	2950.764994
633.113688	1020.217896	1386.448377	2950.806641
633.506361	1020.321848	1386.560494	2951.853403
684.016679	1021.389794	1399.076814	2951.901288
684.233651	1045.288863	1399.231835	2953.152026
693.867839	1045.372532	1404.184200	2953.232018
695.438862	1212.325200	1404.312380	2971.677242
733.298582	1212.444929	1440.213466	2971.796459
733.352000	1214.217752	1440.385736	3009.125956
735.115165	1214.258239	1440.919130	3009.377980
737.537262	1224.408004	1441.067041	3012.320750
949.082266	1224.549874	1444.809827	3012.572163

3019.427702	40.669440	172.665511	280.225571
3019.570825	48.351779	180.151309	291.058895
3032.844123	62.267616	182.980198	295.875526
3032.862662	63.888197	188.277241	296.604506
3035.544501	80.507255	188.411803	300.276441
3035.630531	83.714953	191.714901	301.691527
3037.079859	87.547157	192.606288	305.468290
3037.133767	91.816966	202.237078	311.991463
3043.926402	92.047192	216.003933	315.009963
3043.977493	101.032745	222.838457	319.476927
3047.898098	105.073888	234.651478	320.336800
3047.985529	109.759400	234.733354	321.511932
3048.340704	116.513159	241.488043	336.228957
3048.445288	118.720798	245.307793	341.994464
	122.926880	248.217380	354.524953
Anionic	132.425570	249.063344	355.377412
<i>trans</i>-Co₆S₈(PEt₃)₂	133.616827	249.999452	356.748411
Frequency	135.472969	252.677293	357.354792
cm-1	145.066864	252.844780	365.050031
-----	148.568698	255.401268	367.588304
10.460806	155.234117	272.625281	368.123364
30.814471	167.816785	275.909877	428.368097
36.253941	169.226067	278.404881	430.728847

597.605370	989.913519	1356.591676	2936.788412
598.827990	1016.864421	1356.875831	2938.380478
627.149113	1016.915157	1386.211743	2938.437000
627.187231	1019.306423	1386.331273	2939.805030
680.844963	1020.498382	1398.090063	2939.819951
680.939591	1043.617549	1398.273326	2940.028476
687.107197	1043.697814	1405.391784	2940.078595
688.244104	1208.535366	1405.533554	2966.926565
730.824773	1208.581310	1438.786317	2967.025855
730.942032	1212.491284	1439.082839	3000.907318
735.913042	1212.543774	1439.207802	3000.987380
738.326191	1223.448235	1439.377891	3003.715118
944.730630	1223.546499	1442.444582	3003.831973
944.749374	1227.011056	1442.550201	3011.135870
951.159663	1227.055166	1444.465969	3011.177462
951.201811	1227.730100	1444.594166	3014.909961
953.223613	1228.178262	1447.959211	3014.924583
953.340801	1245.395518	1447.990527	3020.163851
971.285324	1245.447140	1449.689845	3020.446004
971.669539	1347.828583	1449.699073	3021.539342
981.985714	1347.935612	2933.872312	3021.816111
982.677210	1354.578040	2933.894908	3032.733500
989.832200	1354.965039	2936.773460	3032.740411

3039.437721	107.404405	234.635652	319.475382
3039.835965	114.234047	239.230554	331.343262
3040.227319	118.744421	240.822907	354.456813
3040.669670	127.966842	242.643591	358.738943
	131.903655	245.653731	364.506834
Neutral	135.783116	247.676415	366.507408
<i>cis</i> -Co ₆ S ₈ (PEt ₃) ₂	141.367275	251.527482	368.182740
Frequency	150.010451	252.965759	368.955640
cm-1	159.951649	255.770518	373.770815
-----	162.162310	257.430882	379.773260
28.541987	163.586811	263.259106	384.888886
32.761536	168.749342	268.672743	409.339659
38.829524	174.542167	268.904880	417.816087
50.508215	180.885438	273.942893	598.308854
50.931943	183.212273	285.895352	601.517584
59.343315	185.359449	288.963950	631.713960
68.050719	186.692895	291.403962	635.654457
87.490209	192.943839	293.429424	683.464955
88.568600	196.259930	298.307231	686.997011
94.515417	204.375021	299.863010	693.600301
96.412921	207.885404	303.414424	694.864566
99.208442	211.039361	306.924906	732.056011
102.853278	230.403366	317.995359	734.873547

738.058018	1215.402689	1441.038811	3010.839703
739.271604	1221.880724	1443.528496	3011.855635
947.586768	1224.981185	1444.304116	3013.810650
948.769469	1229.478251	1445.020323	3016.984817
953.708312	1231.226162	1447.178685	3019.173249
954.216748	1232.523463	1447.684387	3031.928070
955.855551	1235.914716	1449.059572	3032.086938
956.217430	1246.404602	1449.274676	3034.712591
973.045068	1249.295886	1450.793328	3035.729187
976.773907	1354.942641	1451.027077	3036.724621
983.102158	1355.709344	2945.680642	3037.092804
984.802309	1357.602170	2946.659544	3042.770426
990.149624	1359.453439	2949.383406	3044.975549
991.526237	1361.100486	2949.425675	3045.979302
1018.419969	1361.653215	2950.326896	3046.194028
1018.978621	1387.333741	2951.097847	3048.927031
1021.185695	1387.773432	2951.381689	3054.241818
1021.780557	1399.899821	2952.171759	
1043.748717	1400.598048	2952.968767	Anionic
1046.455992	1405.563347	2953.183306	cis-Co₆S₈(PEt₃)₂
1212.226641	1407.394819	2968.563235	
1213.365972	1439.788549	2969.254906	Frequency
1213.836609	1440.286574	3008.124937	cm-1

-----	160.481490	258.232828	369.165991
28.221181	168.494638	265.162116	373.690388
32.882640	170.424733	265.858039	424.895536
48.910778	176.831531	273.127742	426.567165
51.723149	182.564839	275.981142	596.033808
56.180750	183.313491	291.946669	598.541370
60.287388	184.499803	292.160325	624.676573
84.423606	186.862506	296.252253	626.905302
87.386407	192.540306	297.292139	680.255537
88.718266	198.361680	298.690818	683.932025
95.093523	203.194805	299.962589	685.410426
96.815547	207.654415	309.641222	686.168732
103.315974	212.134663	313.237878	729.747277
105.367680	233.886459	316.150693	734.806642
108.937618	238.505231	318.796473	736.172743
116.768306	240.076072	321.228838	739.031491
118.935898	244.329895	339.491668	943.731334
127.471192	246.461173	341.417436	945.306929
129.798675	248.893963	356.629934	950.737510
138.805986	249.666100	359.644874	951.672561
145.623752	251.862783	360.820102	952.561787
149.229809	253.401471	367.084755	953.831685
155.044065	254.227324	367.593199	970.825187

973.992482	1347.985747	1449.902715	3021.349723
981.734351	1348.427617	2933.339361	3021.546348
983.120789	1351.838521	2934.068031	3031.423372
988.852940	1354.199884	2936.327189	3033.985466
990.777178	1356.034959	2936.626625	3038.706002
1015.645277	1356.146624	2938.014917	3039.359534
1017.410579	1387.051162	2939.388005	3041.840430
1020.188983	1387.266749	2939.547931	3050.423227
1021.000121	1398.795133	2939.922557	
1042.642243	1399.475912	2939.984392	Neutral
1045.394958	1406.330387	2941.297658	<i>fac</i>-Co₆S₈(PEt₃)₃
1208.876302	1409.234386	2964.609932	
1209.647021	1438.499364	2965.027752	Frequency
1212.831827	1439.188412	3000.520012	cm-1
1213.709097	1439.945401	3002.301311	-----
1220.513366	1441.376995	3003.973715	28.473672
1223.830302	1442.632278	3004.870046	31.423350
1226.475347	1442.855187	3009.136010	31.839033
1227.765011	1444.549713	3012.097272	33.240074
1227.954349	1445.279097	3013.757249	36.790617
1230.456609	1447.738973	3013.800856	46.909635
1243.007703	1448.010187	3020.103485	59.581023
1245.853686	1449.812187	3020.661010	60.671639

63.088310	166.606377	245.099267	342.256971
82.642864	168.245098	251.210733	345.715514
84.696138	169.776369	252.395593	348.974316
85.170873	171.603357	252.551289	360.759568
87.833737	173.792083	253.531388	363.617127
88.478826	175.547060	254.559640	364.474815
92.253447	179.755235	255.137667	366.745033
95.298160	182.459679	266.316695	376.695817
98.903003	184.463694	266.440714	378.058553
99.908724	185.263420	268.360412	383.167552
100.687870	187.469045	290.945454	402.296658
105.051421	189.241467	293.028182	403.063511
109.607049	190.209521	297.389015	412.052470
116.153891	205.437038	300.795138	595.861926
118.156594	206.506336	300.959266	596.875048
121.223787	227.607290	305.354219	598.523093
127.661240	232.777324	306.788490	631.420677
131.475293	234.480002	312.840349	631.688864
132.806384	236.551554	315.000720	634.742781
145.267830	236.858893	317.066619	680.099481
151.046977	238.239889	317.915684	680.957780
154.343562	241.695968	318.567931	683.956485
160.217124	243.847366	323.494715	689.671312

690.661902	989.863632	1229.932666	1405.532486
692.688484	990.540842	1231.728685	1407.779162
731.322365	991.377932	1232.301778	1439.652074
732.065111	1017.137508	1234.029185	1440.246392
732.770676	1017.666527	1246.009016	1440.440492
734.100571	1018.008067	1246.905679	1441.396526
736.025670	1019.137303	1247.752288	1441.744929
738.311844	1020.110016	1353.318624	1443.235398
946.335976	1022.768667	1353.829090	1443.784406
946.406059	1043.286045	1354.708335	1444.072402
946.955836	1044.180663	1355.294874	1444.114091
953.875006	1045.410929	1356.450575	1446.578850
954.023844	1212.011265	1356.497652	1446.990728
954.500454	1212.621030	1358.835725	1447.279470
954.761304	1212.825567	1359.448143	1449.217846
955.043260	1214.151407	1359.649598	1449.357585
955.389264	1214.626552	1388.394497	1449.494749
973.075302	1214.968331	1388.711877	1449.870789
973.293646	1222.482572	1389.191732	1450.543907
974.703308	1223.577354	1400.300732	1450.710918
980.603223	1224.267170	1400.450604	2943.571821
981.965477	1228.812872	1401.400883	2943.928464
983.926890	1229.377764	1404.903279	2945.079885

2945.131882	3014.871280	28.759399	118.959168
2945.662236	3028.165169	31.342249	125.516644
2946.623106	3029.102860	31.674112	129.496442
2947.109578	3029.211419	33.323218	130.168007
2947.450354	3029.957025	35.653092	135.230385
2948.890786	3031.302264	45.466463	144.448881
2949.085919	3031.411816	58.110814	145.464390
2949.549208	3033.840671	58.479687	161.836849
2950.368337	3034.305925	61.254043	161.948222
2950.515990	3034.327236	81.892929	163.934032
2950.822524	3039.211018	83.781282	169.889033
2951.018779	3039.436537	85.907758	171.190404
2963.980890	3040.287019	86.299020	179.405993
2967.955324	3040.503416	87.716984	181.393611
2968.121708	3042.169921	91.666863	183.086124
3002.910676	3044.999185	94.109937	185.105172
3003.149603	3046.198752	95.999653	186.101178
3006.379538	3047.530033	97.592721	186.902922
3006.576784	3051.453021	101.950202	189.519023
3007.744311		104.707532	190.208340
3010.435785	Anionic	110.862926	190.629903
3013.679122	<i>fac</i> -Co ₆ S ₈ (PEt ₃) ₃	116.216135	205.613581
3014.870238		117.216253	207.789807

233.787807	304.314255	594.499852	952.345856
235.454794	305.608033	624.003166	952.943500
235.919673	310.895687	624.127138	969.885044
237.317920	313.866130	626.047107	970.286951
240.160916	316.005496	677.226785	971.712059
242.906425	317.007933	678.184467	978.852048
243.757266	317.925130	680.569322	980.253986
245.012865	318.214884	681.290822	981.990024
249.305520	333.891759	682.108447	988.784030
251.157078	339.023481	683.885022	989.015157
252.466582	343.921782	729.316163	990.131089
252.840830	353.342041	729.597708	1014.717433
254.303181	361.784787	732.326138	1014.819559
255.524015	363.394381	733.358701	1015.913155
256.728284	366.238203	734.060925	1017.807184
266.270080	368.499025	738.301587	1019.033304
269.301002	369.357286	942.760534	1021.317549
275.605979	374.358968	942.863518	1042.325694
291.744983	403.319555	943.633781	1042.406962
292.912374	408.875043	950.617605	1044.071445
294.584408	416.990296	951.093208	1207.953784
298.293469	591.467502	951.719561	1208.790408
301.981523	592.572834	951.818099	1208.867401

1212.647156	1355.481031	1447.815602	2994.344569
1213.188859	1387.401910	1448.028681	2996.295876
1213.596452	1387.946759	1448.836343	2997.491503
1221.056014	1388.199081	1449.467887	2999.128102
1222.004500	1398.750419	1449.554914	2999.682872
1222.751643	1399.210443	2930.573236	3002.143697
1225.798645	1399.962536	2931.764550	3006.952859
1226.328852	1404.964900	2931.863403	3007.445946
1226.528803	1406.022396	2933.441379	3008.146610
1227.064192	1408.605874	2934.315021	3011.380854
1227.361149	1438.273981	2934.435730	3011.716586
1228.386057	1439.044466	2935.151012	3011.822827
1242.919511	1439.108574	2935.509328	3017.026631
1243.621635	1439.567775	2936.627627	3017.593724
1244.731568	1439.708965	2937.391842	3018.107489
1346.716279	1440.802583	2937.583620	3019.080757
1346.947326	1441.829915	2937.833188	3019.330077
1347.377806	1441.938425	2938.168726	3019.865818
1350.056340	1442.325088	2938.393709	3029.792423
1351.352407	1443.881273	2939.496824	3030.185699
1351.740889	1444.244538	2960.230380	3031.309683
1353.673691	1444.528484	2962.817658	3034.379877
1354.658662	1447.797933	2964.238665	3034.861533

3037.591479	82.742855	174.533995	253.778821
3037.698924	85.107712	175.383582	254.353385
3039.825543	89.860342	180.086104	257.270502
3045.780812	91.674681	182.075322	261.376369
	94.228059	183.855505	271.418192
	96.712508	185.301204	275.044353
Neutral	97.733613	185.805073	275.915574
<i>mer</i>-Co₆S₈(PEt₃)₃	101.637434	186.468290	287.521875
	105.035636	189.608277	292.006486
Frequency	110.505825	202.965298	295.567248
cm-1	115.202345	208.557168	296.004779
-----	116.262951	213.212315	297.591027
26.430653	120.763063	229.392337	304.552141
29.958239	123.475841	233.827085	305.609730
31.944318	125.916416	235.339855	308.351095
36.996382	134.703242	235.606108	316.568343
37.866186	143.714485	238.460126	317.176247
46.599689	148.336707	239.636537	318.275138
52.445503	151.423437	242.146591	322.666178
62.923451	151.593998	245.809321	327.853630
65.203531	156.410265	248.752168	336.658606
68.811295	158.193295	251.512886	344.327315
78.095493	168.323362	252.652664	350.927454

358.489576	731.239185	1018.621417	1235.298804
360.823353	733.211541	1018.746033	1247.023509
364.373066	734.742536	1019.304557	1247.764387
367.030517	737.492711	1020.349390	1249.086229
367.680251	738.941858	1021.363484	1353.661531
368.709378	947.407635	1022.984252	1353.911969
374.229659	947.752852	1044.124898	1354.818482
409.912413	948.074886	1044.349049	1355.000505
416.356643	954.273414	1046.704357	1357.332310
423.361114	954.425803	1211.941893	1358.508158
598.433765	954.739463	1212.259171	1358.651756
599.133295	955.050861	1212.623370	1359.896969
601.037586	955.503052	1213.842199	1360.071514
629.894222	955.838662	1214.214330	1386.010853
631.806867	973.710358	1215.432402	1387.163536
635.492086	974.059601	1222.245216	1387.978260
680.620859	976.547656	1224.042316	1398.525294
681.763736	982.291575	1225.108364	1399.723816
686.470671	984.089806	1229.470031	1400.568019
691.137596	985.294449	1229.956321	1404.527186
692.817507	990.400095	1231.079932	1405.902062
694.453500	990.539421	1232.601974	1408.291310
730.992068	992.107749	1232.957897	1438.363046

1439.889701	2948.219128	3031.062492	Frequency
1440.089179	2949.448962	3032.502251	cm-1
1440.693072	2949.816477	3032.810168	-----
1441.267604	2949.845759	3033.781446	27.509641
1443.248519	2950.005016	3034.031373	29.305365
1443.664540	2950.536940	3034.109268	32.576922
1443.739066	2951.505977	3034.512123	35.682664
1444.046973	2951.628350	3040.004836	35.924599
1446.364305	2951.731967	3042.300410	44.029635
1446.759723	2967.651646	3042.339188	51.094012
1447.013274	2968.069689	3043.970260	60.676605
1449.074953	2970.792152	3046.591536	65.086888
1449.200407	3005.981067	3046.921385	75.808376
1449.354470	3007.322921	3047.391713	78.321758
1449.464128	3009.366618	3047.893930	83.582346
1449.803787	3009.864626	3052.514448	84.775762
1450.722449	3010.597928		87.744201
2944.716314	3012.714887		89.887880
2945.044116	3014.777167		93.808645
2945.672760	3017.882128		97.197730
2947.301658	3018.028997		98.231068
2947.579321	3029.281883	Anionic	102.090298
2948.189357	3029.910444	mer-Co₆S₈(PEt₃)₃	102.246381

111.484215	199.304614	287.358514	416.995863
114.474007	202.612450	291.210883	591.060759
116.068604	206.587123	291.312279	592.237171
121.212741	207.574636	299.638144	594.955259
123.164219	226.609833	302.800008	622.645945
123.501284	234.018799	305.531677	625.010954
132.566044	234.378015	311.984047	630.316678
141.160598	236.583206	313.430299	677.448481
143.104739	237.131583	315.719260	678.310708
147.658222	239.452836	317.379257	680.353286
149.486665	241.362854	318.724993	681.034550
151.815486	244.830000	321.466375	684.234353
158.403870	247.143507	334.597203	685.344073
166.518290	248.287151	344.057049	729.066897
171.192520	249.895737	353.354120	729.180622
173.631106	251.270329	355.113000	732.807233
179.860348	253.022414	361.292392	733.350881
180.683800	254.614328	361.922729	734.070147
183.518081	268.032981	364.269864	737.913430
185.975871	269.510401	365.453873	943.108709
186.144927	277.165289	371.545349	944.057797
186.577721	279.817836	393.300712	944.135408
188.966343	286.448984	412.036214	951.179878

951.904707	1208.640353	1353.684850	1444.076240
952.110304	1208.882602	1354.038314	1444.439378
952.210011	1209.045620	1354.929195	1447.624175
952.638700	1212.844948	1355.283955	1447.731405
953.319464	1213.021490	1386.369232	1447.894196
970.504503	1213.881297	1387.091552	1448.428135
971.273969	1221.979881	1389.113316	1448.683102
971.736342	1222.756197	1398.121081	1449.242637
979.887074	1223.101537	1398.675531	2930.659921
981.237679	1226.522719	1400.480265	2932.143875
982.646573	1226.782932	1405.246467	2932.250289
989.284449	1227.020327	1406.133674	2933.507012
989.466849	1227.292986	1408.326668	2934.315512
989.912050	1227.527347	1437.998200	2935.304923
1015.505165	1228.777009	1438.943698	2936.039090
1015.651441	1244.043002	1439.088978	2936.539485
1016.069807	1244.186217	1439.361122	2937.460921
1018.136462	1245.216398	1439.495165	2937.714993
1018.895560	1346.564765	1440.606906	2937.819139
1021.513217	1346.705410	1441.707609	2938.108974
1042.605206	1347.169106	1442.232353	2938.360196
1043.239798	1350.114612	1442.343872	2938.671066
1043.841231	1351.610770	1443.837152	2939.178226

2960.198685	3031.461490	34.525953	110.570589
2962.779671	3035.382206	40.796633	114.714422
2964.326486	3037.898030	46.840799	116.818312
2996.444590	3038.166392	46.871989	122.059416
2997.044229	3038.915332	57.219304	126.803286
2999.092888	3039.389656	63.423065	127.345068
2999.441395	3044.690692	68.892393	129.209782
2999.571768		79.938762	130.643748
3001.485032		80.949511	132.639791
3007.063837		81.609757	133.510124
3007.271996		83.780601	143.628510
3008.943554		86.369315	144.389541
3011.123779		86.794367	157.643782
3011.808855		89.048855	160.974934
3013.349813	<i>trans</i> -Co ₆ S ₈ (PEt ₃) ₄	91.949513	164.210526
3017.634599	Frequency	94.695152	165.966770
3018.190167	cm-1	95.697936	171.277285
3018.805860	-----	96.908440	171.733564
3019.282665	22.602580	98.420588	177.274878
3019.301910	28.937753	99.662563	178.743896
3019.839156	30.213094	101.266039	181.559672
3029.795477	32.619556	104.037556	181.657971
3031.435997	33.668764	108.223571	185.324566

185.790238	258.603849	354.693023	689.473917
186.191651	261.900519	358.160347	689.644696
190.279183	270.095048	359.446799	691.334103
190.615858	289.040554	364.112045	692.516141
195.974852	289.611202	365.111304	731.210381
207.948613	293.906917	366.559494	731.438660
213.353023	295.747147	367.921284	733.158972
220.872186	297.408269	402.520758	734.213183
234.996342	299.080629	405.856729	734.825320
235.068039	305.932892	417.197196	736.071292
238.487547	306.030998	419.015677	736.373604
238.615945	309.542042	596.962957	739.395143
238.984791	312.453244	597.236150	946.628958
240.415149	313.788259	598.011325	946.681658
245.350812	316.682116	599.052272	947.235890
247.429668	317.103633	630.268708	947.299981
248.030077	317.180203	630.307002	954.315725
250.510065	320.182928	634.779577	954.422514
250.751440	320.462410	634.789181	954.451455
253.684642	329.571579	681.479085	954.510228
254.461928	344.641016	681.535733	954.672093
254.997248	347.482395	684.207020	954.725056
257.387113	349.929913	684.419810	955.317740

955.398670	1045.820417	1245.809731	1406.156674
972.920816	1045.916043	1248.293520	1406.261784
973.149594	1211.574531	1248.394679	1408.113831
975.080585	1211.609947	1352.884535	1408.130297
975.149093	1212.719357	1353.015850	1439.285863
982.091202	1212.726629	1353.290351	1439.342099
982.183754	1213.390146	1353.732627	1439.826422
983.625356	1213.450774	1354.177949	1440.040543
985.170483	1215.416731	1354.315894	1440.795574
990.181701	1215.536170	1356.296211	1440.920073
990.200822	1221.789757	1356.520313	1443.240781
991.896207	1222.103275	1357.923249	1443.308424
991.919162	1224.985650	1357.936383	1443.539543
1017.575731	1225.012000	1359.294083	1443.607634
1017.632297	1228.424961	1359.463314	1443.745029
1018.154514	1228.529408	1387.558314	1443.795438
1018.584708	1230.414517	1387.612240	1446.392198
1020.579453	1230.583733	1389.121188	1446.622394
1020.892826	1230.904976	1389.216241	1446.902222
1021.021374	1231.353605	1399.687668	1446.954323
1023.799907	1233.274586	1399.723650	1448.827155
1043.308179	1234.496705	1400.886877	1448.959968
1043.407399	1245.696645	1401.275207	1449.156449

1449.353281	2949.801695	3030.603572	cm-1
1449.637588	2949.906237	3030.897549	-----
1449.758121	2965.416544	3030.921914	21.869196
1450.617914	2965.447163	3031.781988	28.005204
1450.653294	2966.945346	3031.802010	28.450849
2943.873653	2966.971820	3032.080935	30.115957
2943.879105	3005.144885	3032.101384	30.977587
2943.997688	3005.157453	3038.494781	32.258816
2944.011352	3005.877991	3038.497339	37.017416
2945.721545	3005.888617	3040.573554	43.840156
2945.732630	3008.076730	3040.659236	46.188079
2945.939393	3008.119858	3042.446716	55.034507
2946.332666	3008.850410	3042.501439	58.389385
2946.574327	3008.910630	3042.788608	63.306162
2946.638248	3013.354817	3042.816512	73.194296
2947.305703	3013.365816	3043.440577	75.814345
2947.379295	3014.470047	3043.487121	79.088998
2947.504037	3014.489505	3050.858595	82.024418
2947.532533	3026.733330	3050.946723	83.014710
2948.937837	3026.909300		84.323351
2948.987904	3026.915872	Anion	85.735040
2949.276836	3026.993350	trans-Co₆S₈(PEt₃)₄	88.573316
2949.507159	3030.552691	Frequency	89.061043

90.580047	173.850174	248.420594	316.194229
95.591514	179.304656	249.483171	317.773560
98.742566	181.096545	251.457165	320.784753
99.663517	181.519370	253.889392	322.311997
102.587408	182.563471	254.207881	328.860419
104.786451	186.211393	254.522941	337.984301
111.600192	186.301171	257.822140	339.431490
114.113179	186.900098	259.119501	343.687803
115.962221	188.880836	270.459975	350.130184
121.130155	189.401171	271.454547	352.766715
122.416004	189.627200	284.354857	363.088569
128.296976	191.696763	286.824975	364.023651
129.477263	203.987720	289.748975	366.921679
130.214227	215.531378	297.928635	367.972799
136.280855	234.026304	299.124604	405.749391
140.266771	234.709151	302.616900	408.463886
144.563635	236.899729	305.717296	421.065885
147.151397	237.277993	307.675664	424.716670
148.772430	237.489826	308.869353	592.749802
156.065706	240.092690	310.637148	592.880226
157.984414	242.206323	311.671941	593.522734
166.490914	244.971082	313.956372	595.180078
170.858063	247.311313	315.394029	622.872046

623.003049	950.888981	1015.789617	1226.225064
626.763377	950.903324	1018.812706	1226.435196
628.252683	951.201119	1019.042812	1226.650380
678.978463	951.477167	1019.497422	1227.002126
679.128393	951.811899	1021.636830	1227.170849
679.909879	952.231228	1042.208403	1228.095970
680.351538	952.333743	1042.497925	1242.787604
681.152932	952.473042	1044.008257	1243.057879
681.573307	969.643476	1044.129671	1244.364650
683.117998	969.985788	1208.298851	1244.504771
684.216591	971.073769	1208.323898	1345.948970
729.100594	971.479908	1208.388191	1346.211528
729.318116	980.083997	1208.423399	1346.411870
732.633204	980.339648	1212.640692	1346.851546
733.240088	981.257079	1212.851215	1349.902098
733.475779	982.531109	1213.300043	1350.074495
733.668929	988.778169	1213.460320	1351.391834
735.269137	989.132827	1220.610482	1351.827090
739.605277	989.993948	1221.059600	1353.273079
942.627380	990.151676	1222.996461	1353.681407
942.933297	1014.589210	1223.032104	1354.587893
943.094902	1014.771355	1225.905737	1354.946796
943.214847	1015.620880	1225.974246	1386.703108

1386.798659	1443.724717	2936.511622	3007.848033
1388.316521	1443.990145	2936.665521	3007.942134
1388.467923	1444.448422	2936.763027	3010.492565
1398.343170	1444.543577	2936.775504	3010.577373
1398.381323	1447.360878	2936.868196	3010.837435
1399.606574	1447.557348	2937.195395	3011.338777
1399.987089	1447.658387	2937.301657	3016.975738
1406.266754	1447.814437	2938.161572	3017.048969
1406.380571	1448.344233	2938.419823	3017.484010
1408.325748	1448.543351	2961.054648	3017.654593
1408.623030	1449.037408	2961.229570	3017.692188
1438.004395	1449.191832	2962.769727	3017.952462
1438.182773	2930.724744	2962.856740	3018.089434
1438.663765	2931.053456	2996.628418	3018.464012
1439.129376	2931.127942	2996.870826	3029.307389
1439.299283	2931.218654	2997.136387	3029.382959
1439.642271	2933.325858	2997.175701	3031.067510
1440.349391	2933.425884	2999.238481	3031.104142
1440.441413	2933.547807	2999.522403	3033.796521
1441.771626	2933.819177	2999.778813	3034.122155
1441.861291	2934.908763	2999.905915	3036.991227
1442.075319	2935.047638	3006.775060	3037.279801
1442.162435	2936.504605	3006.798895	3037.974432

3038.257207	67.019873	135.582312	222.131599
3042.920441	77.427182	138.848837	235.603980
3044.091111	82.817392	144.320659	237.086222
	84.705039	151.572424	237.524903
	86.372391	157.154546	238.833178
	88.170037	158.476733	241.491261
	91.230510	162.525441	243.599328
Neutral	92.706713	166.368119	244.156369
cis-Co₆S₈(PEt₃)₄	94.968048	173.831889	244.911454
Frequency	97.107223	174.331010	247.635811
cm-1	98.429810	178.358125	251.479261
-----	99.012240	181.460050	252.037843
27.872181	101.963197	182.352138	253.734808
28.679707	104.513269	184.135949	257.146877
29.475906	105.094852	186.560096	258.268831
30.678947	106.250761	187.079588	259.389330
36.437086	114.998154	187.654992	259.666332
36.607228	117.108495	189.274523	261.051697
45.897953	118.329905	190.084318	264.129431
47.101944	123.327900	191.632687	265.406106
51.203318	128.287291	192.202868	278.717651
59.187510	128.904753	211.181687	293.506164
64.964362	131.299117	214.561525	297.106782

298.409128	379.066127	733.595980	982.047063
302.850119	408.030084	734.214827	983.366633
307.882065	408.960867	735.190907	984.852560
308.125070	411.270911	736.219699	990.347874
310.304814	417.135008	737.222279	990.846020
310.540007	597.565933	739.822749	991.029237
314.524008	597.861749	945.176961	991.436390
316.846478	598.041008	945.894074	1017.325447
317.778351	599.684795	946.881164	1017.507073
318.764639	629.982961	947.288287	1017.947937
319.364126	630.633243	952.926259	1018.273147
321.044913	632.002039	953.111097	1020.212443
323.714087	634.021140	953.886438	1020.393113
337.542076	680.444983	954.059685	1021.017910
340.434261	683.289277	954.418409	1023.409962
343.679820	684.219864	954.731020	1044.362181
354.835129	685.397478	955.406812	1044.608780
358.959994	688.304689	955.863032	1044.888205
365.499675	688.708951	973.765725	1045.589124
367.303908	691.155078	973.991259	1211.635824
367.727872	692.386140	974.608804	1211.934018
368.142060	730.923468	975.061967	1212.365896
375.184905	733.027380	980.895526	1212.760742

1214.010554	1353.555782	1439.969888	2944.234486
1214.043956	1353.897223	1440.439188	2944.651861
1214.895572	1354.887162	1440.897155	2944.796547
1214.998928	1355.179380	1442.948779	2945.222699
1221.139386	1356.211044	1443.069231	2945.496787
1221.987632	1356.462057	1443.208948	2946.182212
1222.422532	1359.069389	1443.352932	2946.218776
1224.232008	1359.300166	1443.673086	2946.602892
1227.910498	1359.679534	1443.949372	2946.697642
1229.138770	1387.397079	1444.219103	2946.787521
1229.630264	1388.677865	1445.972093	2948.307299
1230.180145	1388.799327	1446.787171	2948.376314
1231.880557	1389.578890	1446.987188	2948.397585
1232.254477	1399.441302	1447.132042	2948.557383
1232.816480	1400.630042	1448.696247	2949.233464
1234.138592	1401.056084	1448.907331	2949.347168
1244.517216	1402.167880	1449.135721	2949.921275
1246.151818	1405.027247	1449.219089	2950.150899
1246.804312	1407.290590	1449.610031	2950.360585
1247.727650	1408.605680	1450.765472	2964.788848
1352.240102	1409.236826	1450.821179	2964.887961
1352.437735	1439.114750	1451.394693	2965.459126
1352.956816	1439.695821	2943.217833	2968.400422

3004.144107	3032.600869	30.454171	105.805433
3004.985206	3039.025654	35.280260	115.083814
3006.904734	3039.773577	36.022236	116.868611
3007.546654	3040.569051	44.985746	118.607822
3007.767862	3040.763072	45.506120	123.279894
3008.567592	3041.067070	49.680459	127.221245
3009.823457	3041.310951	57.727841	127.429314
3010.435356	3043.496291	63.628474	131.025510
3014.309884	3046.222239	64.186371	135.471790
3014.437413	3046.317225	77.602150	138.521396
3014.679701	3049.717812	83.104646	144.891504
3014.939369	3049.753597	84.505447	150.390414
3025.973846	3051.419090	85.141264	156.559903
3026.373021		86.930922	157.084547
3026.532913	Anionic	89.896597	163.713036
3028.385365	<i>cis</i> -Co ₆ S ₈ (PEt ₃) ₄	91.145879	166.824519
3029.593391		95.829673	171.266225
3029.960144	Frequency	96.189202	175.601497
3030.139346	cm-1	97.895696	178.608926
3030.440964	-----	98.423175	180.546629
3030.595408	28.230145	102.022571	181.597043
3030.905270	28.856414	103.817222	183.742995
3032.253885	29.365743	105.003013	186.318778

187.616497	258.345384	337.512339	679.645883
189.368541	259.117832	348.888745	680.636031
189.511162	260.669141	353.850697	681.414562
190.447090	262.106244	354.975407	682.326345
191.965614	274.120590	364.611929	683.151276
192.258209	279.735824	366.377164	684.215423
210.021603	293.225626	367.150138	728.613547
213.253435	295.974370	367.369933	731.940554
219.387446	298.870056	370.137197	732.849777
234.552721	301.718043	410.032749	733.014353
236.640466	304.844785	412.198441	733.456400
237.252936	305.372880	413.573631	734.422611
238.065026	306.731585	419.964145	735.195484
241.927671	308.619594	591.958898	739.796414
243.561584	314.052192	592.822968	941.989718
243.805469	315.681497	593.756351	942.567770
244.720826	317.287712	595.500812	943.540794
248.644458	318.208031	622.545846	943.859188
251.186249	318.837000	623.048510	950.790360
252.007966	319.249346	624.473183	950.858448
253.871224	320.021638	626.116242	951.030161
256.245095	326.403605	677.412915	951.177748
257.587629	334.224140	679.182711	951.631543

951.639838	1043.143804	1228.749474	1399.577528
952.149637	1043.478881	1241.631866	1400.670060
953.252249	1043.650124	1242.582070	1405.130512
970.720845	1044.237600	1243.334142	1407.933880
970.994604	1207.959492	1244.732158	1408.751067
971.191707	1208.300327	1345.756310	1409.667814
972.106716	1208.657677	1346.171432	1437.887314
979.275857	1209.146430	1346.404083	1438.256951
980.307115	1212.617941	1346.821115	1438.464952
981.520116	1212.940142	1349.351363	1438.866485
982.721331	1213.377505	1350.254702	1439.036608
989.266390	1213.623034	1350.831670	1440.237320
989.573671	1219.667823	1351.052566	1440.700409
989.732729	1220.321072	1351.363429	1440.852331
990.012110	1220.990105	1354.821784	1441.149700
1015.267702	1222.754530	1355.141442	1442.002214
1015.342788	1225.416577	1355.922074	1442.311871
1015.687690	1226.231626	1386.610600	1442.714196
1015.858110	1226.732564	1387.492237	1443.428850
1018.660923	1226.981596	1388.044834	1444.156994
1018.717261	1227.089486	1388.389855	1444.461977
1019.615184	1227.225480	1398.145454	1444.624445
1021.626030	1227.922815	1399.212650	1447.299032

1447.440912	2937.446737	3012.007154	
1447.649567	2937.997543	3016.112639	Neutral
1447.794395	2938.150238	3016.313524	Co₆S₈(PEt₃)₅
1448.212378	2938.634496	3016.959605	
1449.542785	2960.168249	3017.181658	Frequency
1449.671805	2960.291411	3017.606794	cm-1
1449.964007	2961.417880	3017.674673	-----
2930.907739	2964.258687	3018.157671	22.516747
2931.321345	2995.635337	3018.505115	27.787902
2931.675298	2996.360140	3030.539053	29.624010
2931.684334	2998.592518	3030.601150	31.120309
2933.434473	2999.029605	3030.721978	31.818780
2933.454635	2999.101984	3030.946490	33.503818
2934.012901	2999.498776	3033.403758	35.716418
2934.070973	3001.408510	3035.037194	40.525272
2934.483576	3001.924913	3035.765101	45.352677
2935.190967	3007.316506	3038.021323	47.886222
2935.337898	3007.396092	3038.339391	48.629110
2936.592038	3007.859496	3044.302433	52.678211
2936.721283	3008.457413	3044.509785	63.864911
2936.937962	3009.785797	3045.443015	67.632390
2936.969871	3010.044683		68.455649
2937.317450	3010.683489		72.283359

81.849734	126.293675	190.217261	260.175100
82.953317	129.777641	191.085031	262.092827
85.588719	131.047657	191.215916	265.982127
87.117738	135.716274	192.763559	268.203540
88.038337	136.759731	196.356021	270.418993
89.021567	138.923602	217.799093	272.698310
91.698914	143.699561	220.750333	286.429897
92.118316	148.296789	236.533698	300.173585
93.908678	152.684507	237.610184	301.424321
95.456884	155.310860	238.378341	304.162824
96.534498	160.704261	238.715923	306.675900
97.411715	166.851525	239.251888	307.092617
100.101037	170.397500	240.682957	308.484434
100.871056	173.117934	241.163475	311.597603
102.784161	179.131184	243.920403	313.020805
104.080737	179.900811	244.954658	315.033467
106.938389	180.862659	246.837659	316.494017
110.690158	181.279238	248.517132	318.088655
113.439802	181.440358	251.492659	318.574883
114.708603	182.734368	253.554817	319.293525
118.116757	186.259896	255.399018	320.697884
119.105434	188.137476	256.579961	321.519986
122.559087	188.659073	257.635387	322.800467

325.646750	627.110878	737.657660	982.123552
330.073652	627.733146	740.828504	982.622398
341.804101	629.371127	945.104443	983.519541
344.573136	630.795638	946.082823	985.296472
347.092771	631.373560	946.272270	990.363587
348.116297	680.347947	946.440751	990.560409
351.001867	683.293474	946.917522	991.096044
362.187233	683.793793	953.013531	991.419676
367.258745	684.060759	953.394963	991.655561
368.195445	684.854457	953.875854	1017.055572
368.768684	686.168596	953.968210	1017.206017
369.476303	687.649817	954.043608	1017.554045
370.726454	687.923360	954.186259	1017.895859
410.727285	689.137526	954.356319	1017.961100
412.182571	690.497884	954.396263	1020.512742
413.745097	730.349037	954.928596	1021.015435
418.424823	732.744972	955.076300	1021.108469
421.115222	733.377330	973.291453	1021.490224
596.503008	733.619048	974.182311	1024.082117
597.313696	734.359022	974.497004	1043.491151
598.359374	735.035993	974.756977	1044.617825
598.411120	736.142505	974.897140	1044.764322
599.797333	736.958794	981.124285	1045.391572

1045.686200	1232.612425	1386.677477	1442.672233
1211.299521	1233.213356	1387.213109	1442.774512
1211.694974	1234.129763	1387.985051	1442.967093
1211.822482	1244.362926	1388.494729	1443.110228
1212.084073	1245.419310	1388.858320	1443.321271
1212.148253	1245.741559	1399.311081	1443.372559
1213.851434	1246.312249	1399.880855	1443.863846
1214.286319	1247.211646	1400.312647	1445.811650
1214.476118	1351.734106	1400.554568	1446.335878
1214.668172	1351.930452	1401.654003	1446.536605
1215.129877	1352.130257	1406.287586	1446.601598
1221.070741	1352.303912	1407.839265	1446.705488
1221.371457	1352.841951	1408.968290	1448.695114
1221.717494	1353.302682	1409.798394	1448.871925
1221.985044	1353.455300	1409.958879	1448.954396
1223.693156	1353.998879	1438.468161	1449.041350
1227.875422	1354.166061	1438.884158	1449.386052
1228.529457	1354.945612	1438.952372	1449.804298
1228.852715	1355.537253	1439.276747	1450.347950
1229.341675	1355.762424	1439.544703	1450.839572
1229.926227	1356.164387	1440.190727	1450.909346
1231.498636	1358.386284	1442.310192	1451.034098
1232.449334	1358.884252	1442.620940	2942.452523

2943.250462	2949.629013	3024.878583	3045.091539
2943.487030	2964.197009	3025.064773	3049.088966
2943.693378	2964.795121	3025.295057	3050.465930
2943.773406	2964.999375	3026.743358	3050.749526
2943.985896	2965.046934	3028.183249	3052.205245
2944.023690	2967.389409	3028.431884	
2944.656932	3004.239119	3028.688065	Anionic
2944.750035	3004.830410	3028.880079	Co₆S₈(PEt₃)₅
2944.771304	3006.105165	3029.068893	
2944.945852	3006.132756	3029.177929	Frequency
2945.051493	3007.352407	3029.230310	cm-1
2945.133973	3007.738735	3030.367742	-----
2945.531619	3007.845522	3030.593826	27.505026
2946.576861	3009.160122	3037.511247	29.011137
2946.822353	3009.374229	3038.093929	30.594755
2947.087379	3010.345846	3038.289188	30.658117
2947.297502	3012.951858	3039.097815	32.417141
2948.316885	3013.381034	3039.317956	34.119744
2948.483968	3014.008281	3039.513735	35.445777
2948.777994	3014.385754	3040.084341	38.920699
2948.907584	3014.460197	3040.405417	46.300385
2948.941270	3023.894938	3041.071535	46.603976
2949.105586	3024.467423	3044.604484	47.056351

52.348944	116.124350	182.995483	254.071282
62.351389	116.722512	184.197456	254.525778
64.911799	118.279158	187.669065	254.967078
65.866016	121.459902	189.354472	256.090601
76.455535	124.521827	189.903988	262.675518
81.972468	125.909848	190.010965	265.054547
83.854159	130.243557	191.181901	267.464783
84.792100	131.418932	192.515775	269.692583
86.429702	136.675065	194.014354	272.950513
86.756963	139.092624	195.234398	273.315520
90.105605	140.918938	220.338053	275.166392
90.589732	145.383614	222.737923	293.474344
92.605976	154.238145	235.974770	301.348759
94.132321	155.919982	237.403110	303.962657
95.262274	159.671717	237.656460	306.362308
95.821017	165.444692	237.940194	306.808789
99.031321	168.152191	238.707824	308.721416
100.680692	170.496866	240.520240	310.940067
101.078685	173.153932	243.271329	311.324054
102.447705	178.695803	245.018778	313.092921
105.828204	180.355541	245.291008	314.315472
106.910310	181.190843	247.044087	315.163784
113.612304	182.153067	251.916395	316.522852

318.050237	593.183610	732.417483	971.074055
318.700699	593.723997	733.003523	971.112208
319.144358	594.124316	733.563381	971.519577
319.509581	594.618350	733.648170	971.951051
319.847950	596.114521	734.501379	979.528637
320.728194	620.681262	734.872000	979.984716
327.621815	620.980256	740.447574	980.568171
334.197534	622.284139	942.087776	981.569561
337.129296	622.695795	942.506432	982.955042
339.992745	623.107507	942.695983	988.630766
341.271347	677.632126	943.015920	989.326996
345.296611	678.702497	943.173916	989.526558
346.982987	679.506316	950.436108	990.004165
368.157902	680.060597	950.692755	990.231337
368.514400	680.287306	950.832097	1014.376793
368.616927	681.231344	950.900576	1015.198820
369.353997	681.413640	951.004981	1015.294441
369.487056	681.594963	951.093339	1015.512754
415.749505	682.231940	951.326373	1015.868602
418.077661	682.794567	951.568376	1018.595487
419.535305	728.522430	951.852677	1018.959635
420.207737	731.683272	952.420499	1019.186381
424.334165	732.273177	969.902415	1019.571034

1021.736474	1225.943902	1350.567254	1437.683663
1042.018111	1226.299133	1351.208929	1438.097199
1043.254067	1226.441240	1351.970217	1438.547292
1043.503653	1227.093206	1353.501999	1439.544922
1044.060913	1227.439485	1354.261457	1439.687560
1044.120026	1227.583140	1385.963053	1440.045808
1207.557333	1228.105765	1386.267755	1440.203549
1207.734483	1228.684076	1386.598781	1440.629358
1208.093629	1241.779992	1386.797845	1441.046656
1208.128545	1242.198777	1387.188783	1441.320237
1208.348820	1242.319886	1397.687647	1441.688791
1212.363503	1242.989454	1398.268339	1442.202469
1212.590360	1244.163558	1398.444388	1443.103027
1212.782406	1345.209090	1398.452745	1443.608569
1212.917349	1345.483446	1399.697848	1443.832101
1213.136333	1345.762249	1406.487500	1444.040858
1219.336139	1345.819072	1408.394932	1444.103607
1219.658334	1346.353936	1409.160017	1447.122892
1220.048617	1348.509898	1409.228494	1447.317839
1220.172148	1349.259120	1409.894050	1447.416851
1222.071738	1349.658313	1436.662312	1447.446311
1225.448953	1349.801013	1437.122448	1447.757896
1225.630808	1350.248470	1437.359022	1448.227265

1448.934227	2936.983689	3007.872521	3033.550378
1449.268485	2937.360090	3007.939150	3033.776692
1449.570187	2937.668827	3008.100804	3033.851336
1449.630050	2937.782161	3009.481762	3034.666204
2930.930303	2938.102313	3009.618341	3036.567047
2931.020738	2938.212321	3009.943359	3036.730159
2931.175790	2960.589669	3009.980918	3044.488502
2931.305279	2961.144569	3010.214921	3044.834050
2931.540692	2961.182669	3014.834681	3045.326508
2932.719225	2961.545425	3015.772912	3045.619073
2933.108077	2963.054486	3016.084378	
2933.123478	2996.359844	3016.141050	
2933.182316	2997.628736	3016.480925	
2933.489485	2998.010202	3017.102886	
2933.668397	2998.035603	3017.147950	
2933.897424	2999.231082	3017.182766	
2934.343618	2999.481276	3017.205030	
2934.361595	3000.580447	3017.288030	
2935.482424	3000.716308	3028.987342	
2935.615753	3000.816218	3030.375879	
2936.562625	3001.675640	3030.446505	
2936.773066	3006.975563	3030.594412	
2936.828711	3007.526605	3030.690533	

