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Supplementary Information

Insights into the intramolecular acetate-mediated formation of ruthenium vinylidene complexes: a ligand-assisted proton shuttle (LAPS) mechanism.

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Introduction

This document contains the SCF energies, ZPEs, XYZ coordinates and vibrational frequencies for the stationary points reported in the main section of the publication.

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Explanation of Terms

The nomenclature follows the paper in terms of discrete ground state and transition state points on the potential energy surface. Where more than one isomer is possible, this is designated with an underscore (_) and then the following symbols:

af – derived from $\mathbf{I_{12}}$ where the vacant coordination is opposite the κ^2 acetate
pf – derived from $\mathbf{I_{12}}$ where the vacant coordination is opposite phosphourus
(also the position of the uncoordinated oxygen of the κ^1 acetate is named e, t, and p depending on position relative to the PR_3 ligands)

x or y - denotes the proton of the terminal alkyne and later vinylidene being closest (x) or furthest from the uncoordinated acetate oxygen
m or n - is as above, only the proton is closest or furthest away from the PR_3 ligand.

a or b - is used when the uncoordinated acetate oxygen atom is closest or furthest away to the incoming organic molecule

u or d – found on the TS_{25} point, which informs which way the Carbon-Hydrogen-Carbon three-membered ring is facing

Finally, a green colour represents a ground state, with red inidicating a transition state or intermediate.

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Model i Energies

Molecule	bp86_SV(P) SCF energy (a.u.)	pbe0_tzvpp SCF energy (a.u.)	Zero Point Energy (a.u.)	Entropy (KJ mol^{-1} K^{-1})	Chem Pot (KJ mol^{-1})	H (KJ mol^{-1}) pbe0/TZVPP	G (KJ mol^{-1}) pbe0/TZVPP	G (KJ mol^{-1}) BP86/SV(P)	Rel. E to *Cis 1* (kJ mol-1) pbe0
alkyne	-116.559812	-116.546269	0.053838	0.25762	77.55	-305851	-305915	-305950	
1									
Cis 1	-1237.931459	-1237.728388	0.154607	0.55849	285.59	-3249250	-3249370	-3249903	
+ alkyne						-3555101	-3555285	-3555854	0
Trans 1	-1237.914901	-1237.711602	0.153485	0.58605	276.47	-3249209	-3249335	-3249869	
+ alkyne						-3555060	-3555250	-3555819	35
TS_{12}									
Cis I_{12}_af	-1237.897210	-1237.694553	0.154775	0.55991	285.48	-3249161	-3249282	-3249814	
+ alkyne						-3555012	-3555196	-3555764	89
Cis I_{12}_pft	-1237.910406	-1237.709932	0.155053	0.55790	286.60	-3249200	-3249321	-3249847	
+ alkyne						-3555051	-3555236	-3555797	49
Cis I_{12}_pfp	-1237.909849	-1237.708903	0.154790	0.58449	278.80	-3249198	-3249326	-3249854	
+ alkyne						-3555049	-3555241	-3555804	44
Trans I_{12}	-1237.887886	-1237.683565	0.153813	0.58534	276.96	-3249134	-3249261	-3249798	
+ alkyne						-3554985	-3555176	-3555748	109

2

Cis 2_afx	-1354.516379	-1354.296547	0.211583	0.64325	421.45	-3555150	-3555284	-3555861	1
Cis 2_afy	-1354.513544	-1354.293190	0.211885	0.63530	424.02	-3555140	-3555273	-3555851	12
Cis 2_pfex	-1354.504514	-1354.283078	0.210786	0.65141	418.10	-3555117	-3555252	-3555834	33
Cis 2_pfey	-1354.506240	-1354.284903	0.210883	0.64843	419.01	-3555121	-3555256	-3555837	29
Cis 2_pfpx	-1354.505928	-1354.285143	0.211227	0.64683	420.15	-3555121	-3555255	-3555835	29
Cis 2_pfpy	-1354.507135	-1354.286069	0.211125	0.66448	414.75	-3555124	-3555263	-3555844	22
Cis 2_pftx	-1354.505707	-1354.285382	0.210943	0.64992	418.74	-3555122	-3555258	-3555836	27
Cis 2_pfty	-1354.507819	-1354.289089	0.211174	0.63707	422.69	-3555132	-3555263	-3555838	22
Trans 2_x	-1354.508183	-1354.283971	0.210399	0.65789	415.41	-3555120	-3555257	-3555846	28
Trans 2_y	-1354.508405	-1354.283848	0.210437	0.64607	418.76	-3555120	-3555253	-3555843	31

TS_{24}

Cis TS_{24}_af	-1354.485734	-1354.264384	0.205776	0.65646	409.17	-3555662	-3555212	-3555793	73
Cis TS_{24}_pf	-1354.486600	-1354.264969	0.206782	0.65051	410.28	-3555662	-3555212	-3555794	73
Trans TS_{24}	-1354.470609	-1354.247610	0.205218	0.67936	399.88	-3555624	-3555177	-3555763	108

TS_{25}

Cis TS_{25}_afxu	-1354.444729	-1354.226070	0.207973	0.63964	412.72	-3555549	-3555108	-3555682	177
Cis TS_{25}_afxd	-1354.442440	-1354.223852	0.206970	0.63098	414.98	-3555545	-3555100	-3555674	185
Cis TS_{25}_afyu	-1354.439062	-1354.220920	0.207510	0.62905	414.88	-3555535	-3555092	-3555665	193
Cis TS_{25}_afyd	-1354.436768	-1354.217730	0.207412	0.62231	417.15	-3555529	-3555081	-3555657	203

Cis TS_{25}_pfex	-1354.425206	-1354.205705	0.204991	0.64198	410.57	-3555505	-3555057	-3555633	228
Cis TS_{25}_pfey	-1354.430450	-1354.210525	0.205984	0.63851	412.22	-3555516	-3555068	-3555645	217
Cis TS_{25}_pftx	-1354.425365	-1354.206583	0.205487	0.64099	411.39	-3555504	-3555058	-3555632	227
Cis TS_{25}_pfty	-1354.430969	-1354.212276	0.206761	0.63782	412.43	-3555516	-3555072	-3555646	213
Cis TS_{25}_pftm	-1354.437016	-1354.220298	0.207342	0.63531	413.36	-3555530	-3555092	-3555661	193
Cis TS_{25}_pfpy	-1354.430250	-1354.210610	0.207682	0.65588	407.27	-3555511	-3555073	-3555649	212
Cis TS_{25}_pfpm	-1354.436812	-1354.220277	0.204808	0.64299	410.87	-3555536	-3555094	-3555663	191
Trans TS_{25}_xu	-1354.428700	-1354.226070	0.207134	0.63264	413.02	-3555509	-3555108	-3555640	177
Trans TS_{25}_xd	-1354.427813	-1354.205020	0.207426	0.63222	413.40	-3555506	-3555052	-3555637	233
Trans TS_{25}_yu	-1354.432757	-1354.209972	0.206380	0.63719	411.41	-3555521	-3555067	-3555652	218
Trans TS_{25}_yd	-1354.432682	-1354.209082	0.207142	0.63309	412.71	-3555519	-3555063	-3555650	222
3									
Cis 3_afx	-1354.489354	-1354.268470	0.209421	0.68411	405.38	-3555662	-3555226	-3555806	58
Cis 3_afy	-1354.489098	-1354.266529	0.209716	0.66742	410.80	-3555661	-3555216	-3555800	69
Cis 3_pftx	-1354.485048	-1354.263822	0.209587	0.66752	411.07	-3555650	-3555209	-3555789	76
Cis 3_pfty	-1354.480842	-1354.260986	0.209515	0.67732	408.08	-3555639	-3555204	-3555781	81
Trans 3_x	-1354.481583	-1354.256515	0.208417	0.69574	400.64	-3555644	-3555200	-3555791	85
Trans 3_y	-1354.479999	-1354.255186	0.208423	0.67869	405.00	-3555640	-3555192	-3555782	93
TS_{34}									
Cis TS_{34}_pf	-1354.488244	-1354.264590	0.204913	0.65480	405.15	-3555671	-3555217	-3555804	68

Trans TS_{34}	-1354.480873	-1354.254210	0.204450	0.68338	396.08	-3555653	-3555198	-3555793	87
TS_{35}									
Cis TS_{35}_afx	-1354.474671	-1354.253055	0.207022	0.65874	405.76	-3555630	-3555186	-3555767	99
Cis TS_{35}_afzu	-1354.474635	-1354.253048	0.206567	0.65733	406.26	-3555631	-3555185	-3555767	100
Cis TS_{35}_pftx	-1354.464205	-1354.244432	0.206410	0.67269	400.84	-3555604	-3555168	-3555745	117
Cis TS_{35}_pfty	-1354.461580	-1354.241843	0.206405	0.66233	404.04	-3555597	-3555158	-3555735	127
Trans TS_{35}_y	-1354.461019	-1354.236660	0.205812	0.67674	399.42	-3555597	-3555149	-3555738	136
4									
Cis 4_af	-1354.513598	-1354.300621	0.210531	0.67738	410.65	-3555723	-3555306	-3555865	-21
Cis 4_pf	-1354.498070	-1354.282924	0.209570	0.67724	408.53	-3555684	-3555261	-3555826	24
Trans 4	-1354.495739	-1354.280357	0.209014	0.69078	404.04	-3555680	-3555259	-3555825	26
4h									
Cis 4h_afy	-1354.435044	-1354.201311	0.207769	0.67881	403.23	-3555524	-3555052	-3555666	233
Trans 4h_1	-1354.457672	-1354.223806	0.208038	0.68342	402.51	-3555582	-3555112	-3555726	173
Trans 4h_2	-1354.457789	-1354.223904	0.208173	0.66741	407.26	-3555582	-3555108	-3555722	177
TS_{45}									

Cis TS_{45}_af	-1354.502794	-1354.279074	0.206482	0.65424	405.37	-3555705	-3555254	-3555842	31
Cis TS_{45}_pf	-1354.485438	-1354.259630	0.205513	0.66621	400.38	-3555662	-3555208	-3555801	77
Trans TS_{45}	-1354.491681	-1354.268063	0.206064	0.69903	390.42	-3555677	-3555240	-3555827	45
5									
Cis 5_af_m	-1354.525594	-1354.301852	0.212016	0.65811	418.60	-3555750	-3555301	-3555888	-16
Cis 5_af_n	-1354.525545	-1354.301573	0.211913	0.65278	419.91	-3555750	-3555299	-3555887	-14
Cis 5_pfe_x	-1354.507556	-1354.279669	0.210859	0.66698	414.28	-3555706	-3555247	-3555845	38
Cis 5_pfe_y	-1354.507409	-1354.279832	0.210545	0.68722	407.99	-3555706	-3555254	-3555851	31
Cis 5_pft_x	-1354.507952	-1354.280649	0.211099	0.65927	416.59	-3555706	-3555247	-3555844	38
Cis 5_pft_y	-1354.507997	-1354.280874	0.211107	0.65792	417.05	-3555706	-3555247	-3555844	38
Cis 5_pfp_x	-1354.506061	-1354.278450	0.210982	0.67713	411.43	-3555702	-3555247	-3555844	38
Trans 5_y	-1354.525034	-1354.297225	0.211078	0.68087	410.60	-3555751	-3555297	-3555895	-12
Trans 5_x	-1354.525091	-1354.297310	0.211136	0.66513	415.21	-3555751	-3555292	-3555890	-7
6									
Cis 6_afx	-1354.541581	-1354.320519	0.213444	0.62583	429.67	-3555789	-3555339	-3555919	-54
Cis 6_afy	-1354.543806	-1354.322326	0.213419	0.63215	428.14	-3555794	-3555345	-3555927	-60
Cis 6_pfx	-1354.531931	-1354.308606	0.212761	0.63289	426.45	-3555765	-3555311	-3555897	-26
Cis 6_pfy	-1354.532497	-1354.308606	0.212780	0.64026	424.64	-3555766	-3555313	-3555900	-28
Trans 6_x	-1354.529228	-1354.306985	0.211798	0.66144	417.19	-3555760	-3555316	-3555899	-31
Trans 6_y	-1354.528658	-1354.305485	0.212165	0.64600	422.24	-3555758	-3555307	-3555893	-22

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Model ii Energies

Molecule	bp86_SVP SCF energy (a.u.)	pbe_TZVVP SCF energy (a.u.)	Zero Point Energy (a.u.)	Entropy (KJ mol^{-1} K^{-1})	Chem Pot (KJ mol^{-1})	G (KJ mol^{-1}) bp86/SVP	delta H (KJ mol^{-1}) pbe0/TZVPP	delta G (KJ mol^{-1}) pbe/TZVPP	Rel. E to *Cis 1* (kJ mol-1) pbe0
alkyne	-308.169904	-308.123234	0.106497	0.33588	199.28	-808901	-808698	-808778	
1									
Cis 1	-2623.269090	-2622.871217	0.637843	1.12716	1460.63	-6885932	-6884674	-6884888	
+ alkyne						-7694833	-7693372	-7693666	0
Trans 1	-2623.260161	-2622.860837	0.636533	1.18597	1441.27	-6885928	-6884650	-6884880	
+ alkyne						-7694829	-7693348	-7693658	8
TS_{12}									
Cis I_{12}_afb	-2623.234985	-2622.836737	0.636528	1.14474	1453.40	-6885850	-6884587	-6884804	
+ alkyne						-7694751	-7693285	-7693583	83
Cis I_{12}_pfb	-2623.245578	-2622.846758	0.636190	1.15431	1450.42	-6885881	-6884614	-6884834	
+ alkyne						-7694782	-7693312	-7693612	54
Trans I_{12}	-2623.228821	-2622.828918	0.635493	1.19764	1436.93	-6885850	-6884569	-6884800	
+ alkyne						-7694751	-7693267	-7693579	87
2									

Cis 2_afax	-2931.428208	-2930.976889	0.745607	1.26296	1723.81	-7694741	-7693322	-7693556	110
Cis 2_afay	-2931.440177	-2930.990027	0.745042	1.29818	1712.78	-7694783	-7693358	-7693602	64
Cis 2_afbx	-2931.415970	-2930.963741	0.745736	1.26933	1721.82	-7694711	-7693287	-7693523	143
Cis 2_afby	-2931.424993	-2930.973509	0.745762	1.27530	1719.87	-7694736	-7693313	-7693551	115
Cis 2_pfax	-2931.426289	-2930.975269	0.745342	1.28046	1718.09	-7694742	-7693319	-7693557	109
Cis 2_pfay	-2931.433074	-2930.983133	0.745357	1.29080	1715.78	-7694762	-7693339	-7693580	86
Cis 2_pfbx	-2931.422077	-2930.969477	0.745888	1.26484	1723.66	-7694725	-7693302	-7693537	129
Cis 2_pfby	-2931.425187	-2930.974348	0.745378	1.28558	1716.95	-7694740	-7693316	-7693556	110
Trans 2_ax	-2931.445056	-2930.993159	0.744343	1.32971	1702.58	-7694806	-7693368	-7693620	46
Trans 2_ay	-2931.447859	-2930.994899	0.744934	1.31501	1708.11	-7694808	-7693371	-7693619	47
Trans 2_bx	-2931.448816	-2930.996614	0.744861	1.32866	1704.18	-7694815	-7693376	-7693627	39
Trans 2_by	-2931.444562	-2930.992301	0.744888	1.30991	1709.51	-7694798	-7693365	-7693611	55
TS_{25}									
Cis TS_{25}_afay	-2931.344790	-2930.897400	0.741110	1.27529	1708.60	-7694537	-7693125	-7693363	303
Cis TS_{25}_afbx	-2931.324079	-2930.873171	0.741616	1.26277	1712.05	-7694479	-7693060	-7693295	371
Cis TS_{25}_afby	-2931.348080	-2930.900520	0.740342	1.28420	1704.77	-7694550	-7693136	-7693375	291
Cis TS_{25}_pfax	-2931.342518	-2930.893575	0.739945	1.26136	1713.29	-7694526	-7693118	-7693348	318
Cis TS_{25}_pfay	-2931.351546	-2930.904234	0.740720	1.29850	1703.13	-7694560	-7693144	-7693386	280
Cis TS_{25}_pfbx	-2931.334887	-2930.885159	0.739070	1.26514	1711.84	-7694508	-7693099	-7693327	339
Cis TS_{25}_pfby	-2931.347625	-2930.901069	0.739142	1.28707	1705.24	-7694548	-7693140	-7693376	291
Trans TS_{25}_ax	-2931.369085	-2930.918196	0.740966	1.32072	1695.28	-7694614	-7693180	-7693430	236
Trans TS_{25}_ay	-2931.369180	-2930.919420	0.740173	1.30357	1700.44	-7694609	-7693186	-7693428	238

Trans TS_{25}_bx	-2931.368595	-2930.921062	0.741100	1.29854	1702.03	-7694606	-7693187	-7693431	235
Trans TS_{25}_by	-2931.364446	-2930.915254	0.741255	1.29800	1701.95	-7694595	-7693172	-7693416	250
3									
Cis 3_afam	-2931.427108	-2930.975998	0.743636	1.30493	1707.43	-7694754	-7693325	-7693570	96
Cis 3_afbx	-2931.414828	-2930.963028	0.743003	1.31578	1703.11	-7694727	-7693293	-7693540	126
Cis 3_afby	-2931.417971	-2930.968169	0.743489	1.31874	1703.04	-7694735	-7693305	-7693554	112
Cis 3_pfay	-2931.412171	-2930.959479	0.743328	1.32165	1702.53	-7694720	-7693283	-7693532	134
Cis 3_pfbx	-2931.411296	-2930.957647	0.743928	1.31627	1705.12	-7694715	-7693276	-7693524	142
Cis 3_pfby	-2931.407143	-2930.954634	0.743453	1.32381	1701.80	-7694708	-7693269	-7693520	146
Trans 3_ax	-2931.448052	-2930.992679	0.742618	1.32741	1698.55	-7694818	-7693372	-7693623	43
Trans 3_ay	-2931.432524	-2930.979537	0.742650	1.34345	1694.60	-7694781	-7693337	-7693592	74
Trans 3_bx	-2931.434754	-2930.980793	0.742985	1.34631	1695.05	-7694787	-7693339	-7693595	71
Trans 3_by	-2931.425571	-2930.971881	0.742534	1.33754	1696.37	-7694761	-7693317	-7693570	96
TS_{34}									
Cis TS_{34}_pf	-2931.423479	-2930.966886	0.740683	1.29035	1701.84	-7694751	-7693309	-7693552	114
Trans TS_{34}	-2931.446138	-2930.989367	0.7405991	1.31983	1694.65	-7694817	-7693368	-7693618	48
TS_{35}									
Cis TS_{35}_afam	-2931.415132	-2930.963902	0.740681	1.30456	1700.98	-7694729	-7693301	-7693545	121
Cis TS_{35}_pfam	-2931.402996	-2930.952783	0.740082	1.30598	1699.58	-7694699	-7693273	-7693517	149

Cis TS_{35}_pfbx	-2931.390671	-2930.938938	0.741073	1.29964	1702.21	-7694664	-7693234	-7693478	188
Cis TS_{35}_pfby	-2931.400075	-2930.949404	0.740584	1.31719	1696.68	-7694694	-7693263	-7693511	155
Trans TS_{35}_ay	-2931.417365	-2930.964124	0.740047	1.34154	1689.08	-7694747	-7693303	-7693557	109
Trans TS_{35}_bx	-2931.417427	-2930.963853	0.739716	1.35050	1686.41	-7694750	-7693303	-7693559	107
Trans TS_{35}_by	-2931.412473	-2930.958027	0.740066	1.32789	1693.60	-7694730	-7693287	-7693537	129
4									
Cis 4_af	-2931.457400	-2931.015579	0.745336	1.32342	1706.24	-7694835	-7693425	-7693675	-9
Cis 4_pf	-2931.435474	-2930.991584	0.745180	1.30533	1710.56	-7694773	-7693362	-7693608	58
Trans 4	-2931.451364	-2931.005786	0.744591	1.34705	1698.16	-7694827	-7693401	-7693658	8
4h									
Trans 4h	-2931.405515	-2930.946404	0.741423	1.37392	1684.27	-7694721	-7693253	-7693516	151
TS_{45}									
Cis TS_{45}_af	-2931.449519	-2930.996933	0.740958	1.30860	1697.75	-7694823	-7693387	-7693635	31
Cis TS_{45}_pf	-2931.430952	-2930.978025	0.740864	1.29746	1700.85	-7694771	-7693338	-7693582	84
Trans TS_{45}	-2931.445842	-2930.993171	0.741137	1.31376	1696.63	-7694814	-7693377	-7693626	40
5									

Cis 5_pfbx	-2931.436111	-2930.978772	0.745656	1.30173	1712.61	-7694773	-7693327	-7693572	94
Cis 5_pfby	-2931.442121	-2930.985863	0.745563	1.29950	1713.24	-7694788	-7693346	-7693590	76
Cis 5_afax	-2931.463150	-2931.008889	0.746046	1.28723	1717.70	-7694839	-7693405	-7693646	20
Cis 5_afay	-2931.466591	-2931.011484	0.745609	1.31816	1707.89	-7694858	-7693413	-7693663	3
Cis 5_afbx	-2931.453061	-2931.000267	0.745208	1.30917	1709.86	-7694820	-7693385	-7693631	35
Cis 5_afby	-2931.462245	-2931.009837	0.745225	1.32267	1706.06	-7694848	-7693410	-7693660	6
Trans 5_ax	-2931.484536	-2931.028269	0.745661	1.33416	1704.11	-7694909	-7693457	-7693711	-45
Trans 5_ay	-2931.483676	-2931.027752	0.745445	1.32390	1706.68	-7694904	-7693456	-7693707	-41
Trans 5_bx	-2931.481618	-2931.025834	0.745359	1.32025	1707.84	-7694897	-7693451	-7693700	-34
Trans 5_by	-2931.481625	-2931.025768	0.745245	1.32691	1705.82	-7694899	-7693452	-7693702	-36
6									
Cis 6_afx	-2931.466806	-2931.016190	0.748290	1.22934	1735.75	-7694830	-7693418	-7693647	19
Cis 6_afy	-2931.483137	-2931.032314	0.748261	1.24968	1730.32	-7694879	-7693461	-7693695	-29
Cis 6_pfx	-2931.467227	-2931.016528	0.748302	1.25751	1729.60	-7694838	-7693419	-7693654	12
Cis 6_pfy	-2931.471512	-2931.020260	0.748340	1.27039	1726.20	-7694852	-7693429	-7693667	-1
Trans 6_x	-2931.482224	-2931.031172	0.747751	1.28160	1722.30	-7694884	-7693459	-7693700	-34
Trans 6_y	-2931.483492	-2931.031632	0.747754	1.29440	1718.68	-7694891	-7693460	-7693705	-39

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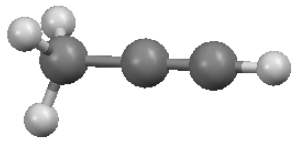
Model i Data

alkyne



bp86_svp SCF energy = -116.5598116785
pbe0_tzvpp SCF energy = -116.5462693163

xyz Coordinates

7

H	0.00027	-2.45879	0.00003
C	-0.00004	-0.15443	-0.00001
C	-0.00001	-1.37681	0.00000
C	-0.00000	1.30657	0.00001
H	-0.51491	1.71202	0.90014
H	1.03702	1.71196	-0.00397
H	-0.52178	1.71204	-0.89618

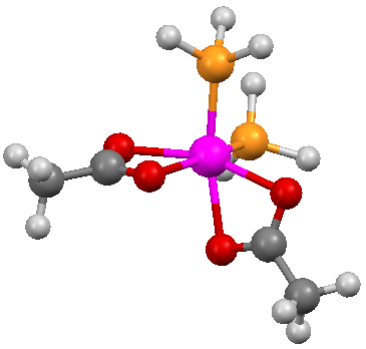
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	337.50	7.76057	YES	YES
8	a	337.64	7.72748	YES	YES
9	a	627.16	41.72245	YES	YES
10	a	627.17	41.75380	YES	YES
11	a	943.48	0.07047	YES	YES
12	a	1022.38	2.82149	YES	YES
13	a	1022.58	2.79831	YES	YES
14	a	1365.96	0.06320	YES	YES
15	a	1414.74	9.75548	YES	YES
16	a	1414.88	9.72704	YES	YES
17	a	2169.85	6.52608	YES	YES
18	a	2933.80	18.89148	YES	YES
19	a	3013.67	4.96288	YES	YES
20	a	3013.92	4.95041	YES	YES
21	a	3387.28	53.58486	YES	YES

$end

* zero point VIBRATIONAL energy : 0.0538377
Hartree *

Cis 1



bp86_svp SCF energy = -1237.9314592950
pbe0_tzvpp SCF energy = -1237.728387502

xyz Coordinates

23

C	-2.07667	1.19314	0.23695
C	-3.23981	2.11525	0.50183
H	-2.87606	3.01243	1.05102
H	-4.00620	1.60951	1.12345
H	-3.68093	2.46157	-0.45573
C	2.07541	1.19264	-0.23469
C	3.23645	2.11433	-0.51001
H	3.67770	2.47112	0.44348
H	2.87035	3.00444	-1.06914
H	4.00304	1.60393	-1.12774
H	-0.42926	-2.04770	-2.57755
H	-2.35696	-1.55400	-1.71925
H	-1.15829	-3.12874	-0.84995
H	0.55607	-3.13143	1.29695
H	2.41452	-2.03205	1.16134
H	0.97866	-1.54092	2.70690
O	-1.83504	0.20114	1.01783
O	-1.28025	1.39176	-0.74511
O	1.29673	1.38167	0.76256
O	1.81845	0.20946	-1.02326
P	-0.99470	-1.75913	-1.28238
P	0.99880	-1.75765	1.28172
Ru	-0.00062	-0.21972	-0.00083

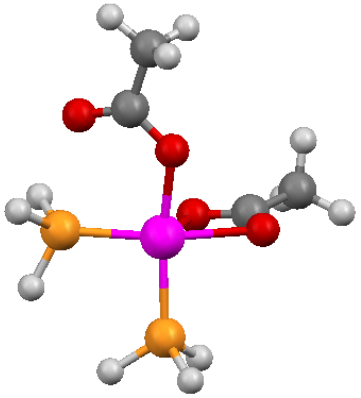
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	37.15	0.03003	YES	YES
8	a	58.88	1.11538	YES	YES
9	a	68.40	2.61367	YES	YES
10	a	72.05	0.92873	YES	YES
11	a	77.03	0.94652	YES	YES
12	a	82.35	1.82046	YES	YES
13	a	105.37	7.05842	YES	YES
14	a	114.81	0.91202	YES	YES
15	a	133.03	2.46980	YES	YES
16	a	139.47	0.50793	YES	YES
17	a	158.00	0.04920	YES	YES
18	a	185.27	0.90430	YES	YES
19	a	194.01	0.34785	YES	YES
20	a	290.42	0.38508	YES	YES
21	a	295.95	13.42836	YES	YES
22	a	311.39	18.55712	YES	YES
23	a	344.72	33.31621	YES	YES
24	a	384.14	21.77195	YES	YES
25	a	391.40	0.12299	YES	YES
26	a	481.40	3.37582	YES	YES
27	a	483.18	8.74037	YES	YES
28	a	571.76	1.22975	YES	YES
29	a	584.84	3.57237	YES	YES
30	a	589.33	11.40966	YES	YES
31	a	595.51	2.25546	YES	YES
32	a	604.12	1.71298	YES	YES
33	a	607.09	1.23719	YES	YES
34	a	671.07	100.96362	YES	YES
35	a	679.34	31.87422	YES	YES
36	a	941.05	29.25767	YES	YES
37	a	942.03	23.04113	YES	YES
38	a	981.32	2.76724	YES	YES
39	a	981.50	0.69072	YES	YES
40	a	1025.84	3.45840	YES	YES
41	a	1026.13	10.77844	YES	YES
42	a	1036.36	262.78208	YES	YES
43	a	1063.09	137.97042	YES	YES
44	a	1084.33	9.84006	YES	YES
45	a	1089.15	7.78967	YES	YES
46	a	1093.80	5.91348	YES	YES
47	a	1099.16	6.13631	YES	YES
48	a	1326.52	2.10673	YES	YES
49	a	1327.39	0.05748	YES	YES
50	a	1396.25	37.46914	YES	YES
51	a	1397.10	46.70170	YES	YES
52	a	1408.92	28.07404	YES	YES
53	a	1409.43	28.26224	YES	YES
54	a	1456.14	337.74845	YES	YES
55	a	1460.71	183.59787	YES	YES
56	a	1527.64	156.45013	YES	YES
57	a	1541.95	26.18927	YES	YES
58	a	2271.83	138.08784	YES	YES
59	a	2283.33	78.20134	YES	YES
60	a	2288.89	84.19137	YES	YES

61	a	2301.03	87.29394	YES	YES
62	a	2309.08	164.67007	YES	YES
63	a	2316.68	75.55176	YES	YES
64	a	2959.75	3.53000	YES	YES
65	a	2959.85	3.22869	YES	YES
66	a	3045.38	2.44813	YES	YES
67	a	3045.53	2.13673	YES	YES
68	a	3077.84	3.16169	YES	YES
69	a	3077.94	2.58645	YES	YES

zero point VIBRATIONAL energy : 0.1546066 Hartree

Cis I_{12}_af



bp86_svp SCF energy = -1237.8972104880
pbe0_tzvpp SCF energy = -1237.694553145

xyz Coordinates

23

C	-1.19070	-0.44389	1.91220
C	-1.54643	-1.05407	3.24019
H	-0.63428	-1.09732	3.87638
H	-1.92970	-2.08688	3.11129
H	-2.29621	-0.42100	3.75726
C	2.62236	0.13481	0.40208
C	3.77563	0.59172	1.29075
H	4.73381	0.17498	0.92228
H	3.60059	0.24881	2.33442
H	3.82690	1.70134	1.32014
H	-3.02970	1.59336	-1.47867
H	-3.43399	-0.33638	-0.61015
H	-2.55678	-0.20230	-2.57992
H	-0.23548	-1.08163	-3.12014
H	1.75822	-0.32707	-2.79093
H	1.07412	-2.15956	-1.77385
O	-0.83141	-1.21567	0.92926
O	-1.18853	0.80595	1.69802
O	1.47754	0.70917	0.69332
O	2.78840	-0.70619	-0.49301
P	-2.33725	0.34509	-1.26151
P	0.65930	-0.81110	-2.00601
Ru	-0.28513	0.33871	-0.28933

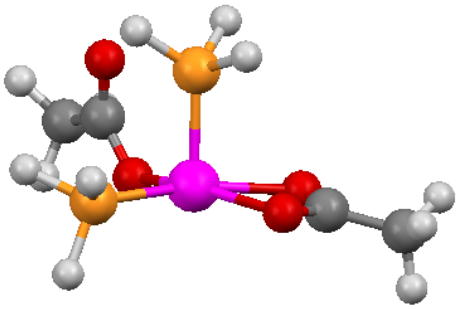
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	37.48	0.29867	YES	YES
8	a	41.96	2.18271	YES	YES
9	a	61.83	0.21758	YES	YES
10	a	69.19	0.54398	YES	YES
11	a	73.90	0.32109	YES	YES
12	a	88.43	0.42973	YES	YES
13	a	100.36	4.00135	YES	YES
14	a	111.32	5.87994	YES	YES
15	a	146.50	1.83837	YES	YES
16	a	166.00	1.39822	YES	YES
17	a	179.10	9.00576	YES	YES
18	a	195.92	7.26808	YES	YES
19	a	206.24	1.14470	YES	YES
20	a	268.47	26.32273	YES	YES
21	a	288.31	28.14532	YES	YES
22	a	336.27	5.93170	YES	YES
23	a	356.15	3.77222	YES	YES
24	a	359.90	1.61034	YES	YES
25	a	374.66	1.68310	YES	YES
26	a	497.34	10.61813	YES	YES
27	a	519.24	5.56962	YES	YES
28	a	546.20	4.89056	YES	YES
29	a	573.40	15.68889	YES	YES
30	a	582.85	6.27845	YES	YES
31	a	594.88	2.09563	YES	YES
32	a	600.54	3.09685	YES	YES
33	a	632.54	10.77761	YES	YES
34	a	668.68	61.00948	YES	YES
35	a	683.29	38.83354	YES	YES
36	a	924.06	2.68004	YES	YES
37	a	938.72	19.62966	YES	YES
38	a	978.41	2.29706	YES	YES
39	a	988.42	24.63128	YES	YES
40	a	1018.38	127.47822	YES	YES
41	a	1022.44	12.04700	YES	YES
42	a	1024.47	12.88036	YES	YES
43	a	1045.19	166.77762	YES	YES
44	a	1079.01	70.61261	YES	YES
45	a	1090.36	13.59919	YES	YES
46	a	1093.60	9.08137	YES	YES
47	a	1115.96	16.30005	YES	YES
48	a	1296.59	307.85923	YES	YES
49	a	1328.63	3.39130	YES	YES
50	a	1342.11	228.12829	YES	YES
51	a	1386.78	86.28798	YES	YES
52	a	1405.67	21.01380	YES	YES
53	a	1407.30	22.53772	YES	YES
54	a	1416.96	11.61994	YES	YES
55	a	1440.38	152.10730	YES	YES
56	a	1551.07	108.49894	YES	YES
57	a	1660.99	220.50795	YES	YES
58	a	2227.56	171.17817	YES	YES
59	a	2280.22	102.79996	YES	YES

60	a	2294.64	48.94594	YES	YES
61	a	2300.96	185.27104	YES	YES
62	a	2356.70	73.18432	YES	YES
63	a	2394.06	25.29371	YES	YES
64	a	2958.57	9.16273	YES	YES
65	a	2962.09	1.25202	YES	YES
66	a	3039.75	5.60398	YES	YES
67	a	3048.61	1.15613	YES	YES
68	a	3078.62	9.90368	YES	YES
69	a	3079.98	1.54870	YES	YES

zero point VIBRATIONAL energy : 0.1547746 Hartree

Cis $I_{12}1$_pfp



bp86_svp SCF energy = -1237.9098490170
pbe0_tzvpp SCF energy = -1237.708903082

xyz Coordinates

23

C	0.13152	-2.60209	0.70730
C	0.16277	-4.01810	1.22386
H	1.22040	-4.34881	1.33010
H	-0.34772	-4.70099	0.51534
H	-0.30823	-4.07103	2.22703
C	0.14475	2.47897	0.95828
C	0.81320	3.62112	1.71737
H	0.29523	4.57630	1.49560
H	1.89255	3.69733	1.47314
H	0.72356	3.42841	2.81017
H	-2.50586	1.17328	-0.98133
H	-2.49067	0.45924	1.12377
H	-2.65493	-0.94982	-0.53724
H	0.30590	2.12376	-2.41542
H	1.75852	0.58452	-2.87222
H	-0.33029	0.27116	-3.33446
O	-0.01074	-2.35901	-0.54533
O	0.27880	-1.60487	1.50328
O	0.93640	1.47575	0.69537
O	-1.06533	2.52520	0.66711
P	-1.87112	0.20608	-0.14128
P	0.47650	0.70176	-2.21914
Ru	0.28090	-0.24465	-0.19975

Vibrational Spectrum

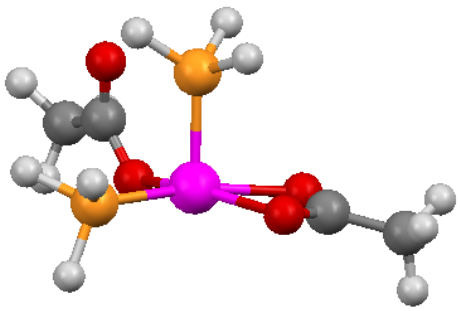
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.67	0.43434	YES	YES
8	a	34.59	0.22374	YES	YES
9	a	35.91	0.91417	YES	YES
10	a	44.52	0.00630	YES	YES
11	a	63.79	0.79990	YES	YES
12	a	76.88	3.77671	YES	YES
13	a	89.28	0.86974	YES	YES
14	a	105.20	3.28218	YES	YES
15	a	128.84	13.03821	YES	YES
16	a	144.87	8.95014	YES	YES
17	a	168.22	2.97677	YES	YES
18	a	185.40	0.66316	YES	YES
19	a	224.81	4.37824	YES	YES
20	a	277.51	4.03213	YES	YES
21	a	301.97	14.76564	YES	YES
22	a	327.36	38.47013	YES	YES
23	a	350.68	1.36329	YES	YES
24	a	382.59	21.99042	YES	YES
25	a	418.29	21.03774	YES	YES
26	a	473.70	4.99619	YES	YES
27	a	516.79	1.84497	YES	YES
28	a	552.70	1.61047	YES	YES
29	a	591.00	0.80853	YES	YES
30	a	593.25	3.95383	YES	YES
31	a	597.71	1.40794	YES	YES
32	a	617.81	2.61291	YES	YES
33	a	635.31	5.84049	YES	YES
34	a	675.44	97.50835	YES	YES
35	a	677.23	31.92011	YES	YES
36	a	933.39	8.61320	YES	YES
37	a	940.00	26.63217	YES	YES
38	a	979.95	1.77354	YES	YES
39	a	991.56	6.30727	YES	YES
40	a	1020.35	22.37854	YES	YES
41	a	1023.25	124.23935	YES	YES
42	a	1026.77	16.02447	YES	YES
43	a	1048.16	134.38384	YES	YES
44	a	1067.92	81.24850	YES	YES
45	a	1080.58	5.90062	YES	YES
46	a	1101.52	14.57551	YES	YES
47	a	1116.20	15.77598	YES	YES
48	a	1314.13	114.55525	YES	YES
49	a	1327.60	1.52634	YES	YES
50	a	1347.88	219.26035	YES	YES
51	a	1395.15	41.79972	YES	YES
52	a	1409.17	33.76189	YES	YES
53	a	1409.74	27.46835	YES	YES
54	a	1420.10	18.19784	YES	YES
55	a	1455.60	294.85600	YES	YES
56	a	1520.73	80.58673	YES	YES
57	a	1640.98	200.02617	YES	YES
58	a	2244.98	159.06339	YES	YES
59	a	2280.81	78.89667	YES	YES
60	a	2304.97	70.58748	YES	YES
61	a	2309.69	119.48103	YES	YES

62	a	2376.70	48.71289	YES	YES
63	a	2390.82	25.27555	YES	YES
64	a	2957.89	11.14257	YES	YES
65	a	2960.16	2.74003	YES	YES
66	a	3043.28	7.30941	YES	YES
67	a	3045.67	2.11693	YES	YES
68	a	3075.41	7.22081	YES	YES
69	a	3081.39	2.19730	YES	YES

$end

* zero point VIBRATIONAL energy : 0.1547897 Hartree *

Cis I_{12}_pft



bp86_svp SCF energy = -1237.9104055200
pbe0_tzvpp SCF energy = -1237.709931926

xyz Coordinates

23

C	-0.09406	-0.53751	2.70679
C	-0.11754	-0.90994	4.16770
H	-1.13902	-1.25418	4.44505
H	0.14569	-0.03628	4.79699
H	0.57966	-1.75225	4.35865
C	-0.08152	-0.89248	-2.51400
C	-0.52779	-1.86178	-3.60400
H	0.19219	-2.70965	-3.64981
H	-0.50698	-1.35209	-4.58937
H	-1.53618	-2.27560	-3.40061
H	2.56130	-0.75345	-0.76055
H	2.69271	0.52977	1.00794
H	2.35102	1.43730	-0.95251
H	0.34399	2.77401	-1.45146
H	-1.50957	1.86949	-2.12938
H	-1.46686	3.00547	-0.28565
O	-0.14698	0.69053	2.33690
O	-0.05232	-1.44165	1.79562
O	-0.67588	-1.07030	-1.36126
O	0.80006	-0.03985	-2.72573
P	1.86094	0.34596	-0.16205
P	-0.71538	1.95198	-0.92756
Ru	-0.26862	0.09491	0.26285

Vibrational Spectrum

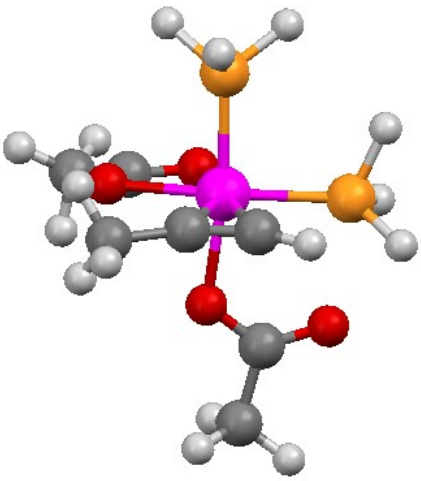
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	33.90	1.46857	YES	YES
8	a	50.87	1.47252	YES	YES
9	a	53.63	1.09237	YES	YES
10	a	62.60	0.43676	YES	YES
11	a	73.58	4.01776	YES	YES
12	a	93.96	0.32796	YES	YES
13	a	108.28	1.76885	YES	YES
14	a	119.17	11.28378	YES	YES
15	a	157.81	4.75610	YES	YES
16	a	166.28	1.39111	YES	YES
17	a	181.67	1.11912	YES	YES
18	a	197.37	0.95615	YES	YES
19	a	227.53	2.67636	YES	YES
20	a	254.59	0.47439	YES	YES
21	a	277.68	2.11251	YES	YES
22	a	304.47	15.46633	YES	YES
23	a	329.20	35.08227	YES	YES
24	a	381.91	26.12840	YES	YES
25	a	430.45	21.76749	YES	YES
26	a	474.38	4.12521	YES	YES
27	a	514.93	2.34402	YES	YES
28	a	582.97	7.80422	YES	YES
29	a	585.94	0.07132	YES	YES
30	a	587.83	3.20553	YES	YES
31	a	601.17	1.46547	YES	YES
32	a	608.20	1.81866	YES	YES
33	a	636.08	5.89567	YES	YES
34	a	675.06	96.60013	YES	YES
35	a	678.38	33.56388	YES	YES
36	a	930.03	7.68763	YES	YES
37	a	940.29	26.82349	YES	YES
38	a	980.57	2.04868	YES	YES
39	a	989.02	9.79348	YES	YES
40	a	1021.23	3.65266	YES	YES
41	a	1026.60	7.71928	YES	YES
42	a	1030.98	197.14441	YES	YES
43	a	1050.64	35.35603	YES	YES
44	a	1059.95	60.17918	YES	YES
45	a	1073.32	24.81208	YES	YES
46	a	1096.26	17.10412	YES	YES
47	a	1105.05	18.49479	YES	YES
48	a	1306.38	206.67657	YES	YES
49	a	1328.25	1.79343	YES	YES
50	a	1340.94	155.85946	YES	YES
51	a	1395.09	45.97593	YES	YES
52	a	1409.82	31.33930	YES	YES
53	a	1411.01	23.49251	YES	YES
54	a	1420.05	16.73158	YES	YES
55	a	1454.54	296.94560	YES	YES
56	a	1521.00	84.27930	YES	YES
57	a	1638.98	181.27527	YES	YES
58	a	2273.60	141.51468	YES	YES
59	a	2293.25	69.77775	YES	YES
60	a	2304.56	137.06305	YES	YES
61	a	2326.97	59.22664	YES	YES

62	a	2357.94	57.32018	YES	YES
63	a	2363.93	26.32222	YES	YES
64	a	2957.27	11.21230	YES	YES
65	a	2960.41	2.84477	YES	YES
66	a	3042.17	6.74725	YES	YES
67	a	3044.72	1.94541	YES	YES
68	a	3074.81	7.09410	YES	YES
69	a	3080.80	2.45270	YES	YES

$end

* zero point VIBRATIONAL energy : 0.1550529 Hartree *

Cis 2_afx



bp86_svp SCF energy = -1354.5163790240
pbe0_tzvpp SCF energy = -1354.296547473

xyz Coordinates

30

C	-0.82904	-0.48024	2.21275
C	-0.97094	-0.70540	3.69579
H	-0.05735	-0.32795	4.20726
H	-1.07244	-1.78711	3.91796
H	-1.84147	-0.14352	4.09268
C	2.61762	0.20907	0.31790
C	3.79462	0.76403	1.11843
H	4.75266	0.51047	0.62225
H	3.78861	0.31471	2.13642
H	3.70266	1.86356	1.24197
H	-3.07305	0.21211	-1.88816
H	-3.43237	-0.81170	-0.00940
H	-2.56215	-1.87772	-1.67869
H	-0.16065	-2.12266	-2.56637
H	1.70650	-1.07472	-2.70279
H	1.36410	-2.62513	-1.12773
O	-0.34550	-1.38773	1.44895
O	-1.15866	0.63735	1.67852
O	1.46305	0.68642	0.65893
O	2.81611	-0.65280	-0.56579
P	-2.36381	-0.64108	-0.96170
P	0.78212	-1.44656	-1.68312
Ru	-0.31323	-0.01988	-0.22497
C	0.01383	1.30974	-1.93181
C	-0.53537	1.97617	-1.00191
C	-1.06888	3.12595	-0.25492
H	0.46951	1.22662	-2.92040
H	-1.01382	4.05393	-0.86831
H	-0.48845	3.27813	0.68157
H	-2.12710	2.96018	0.04600

Vibrational Spectrum

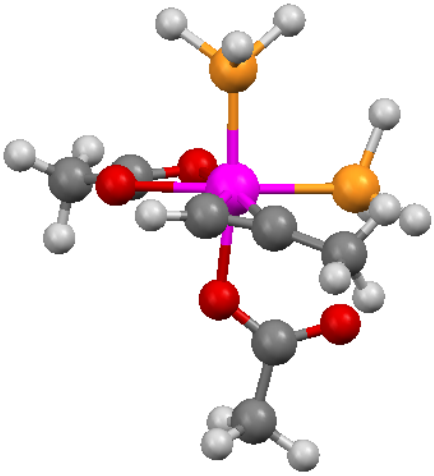
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	20.44	0.12376	YES	YES
8	a	37.81	1.24842	YES	YES
9	a	53.24	0.27657	YES	YES
10	a	69.58	0.85144	YES	YES
11	a	75.32	0.77355	YES	YES
12	a	79.90	0.42587	YES	YES
13	a	89.26	2.24158	YES	YES
14	a	92.54	0.23731	YES	YES
15	a	120.78	9.25150	YES	YES
16	a	126.68	2.46621	YES	YES
17	a	133.90	3.19738	YES	YES
18	a	147.97	1.19700	YES	YES
19	a	167.05	8.82457	YES	YES
20	a	171.18	1.12867	YES	YES
21	a	197.51	13.09449	YES	YES
22	a	221.22	9.10643	YES	YES
23	a	224.11	2.26037	YES	YES
24	a	234.22	2.39535	YES	YES
25	a	273.77	14.79114	YES	YES
26	a	295.95	6.15299	YES	YES
27	a	322.16	15.60530	YES	YES
28	a	331.91	9.90000	YES	YES
29	a	360.44	4.13944	YES	YES
30	a	372.75	16.42905	YES	YES
31	a	398.79	9.14020	YES	YES
32	a	421.42	7.28107	YES	YES
33	a	447.98	0.29152	YES	YES
34	a	484.19	2.17566	YES	YES
35	a	507.67	0.63219	YES	YES
36	a	562.40	4.25950	YES	YES
37	a	576.68	12.30543	YES	YES
38	a	590.94	5.95118	YES	YES
39	a	594.75	1.12537	YES	YES
40	a	608.03	21.89363	YES	YES
41	a	612.19	4.37166	YES	YES
42	a	654.68	5.18285	YES	YES
43	a	670.85	57.87838	YES	YES
44	a	676.26	58.24630	YES	YES
45	a	822.15	1.54180	YES	YES
46	a	927.83	13.02103	YES	YES
47	a	932.77	5.42680	YES	YES
48	a	944.58	23.68423	YES	YES
49	a	983.16	0.97002	YES	YES

50	a	993.10	2.74805	YES	YES
51	a	1000.84	95.50390	YES	YES
52	a	1008.37	38.02864	YES	YES
53	a	1021.74	5.44839	YES	YES
54	a	1022.53	7.29446	YES	YES
55	a	1024.71	6.99157	YES	YES
56	a	1037.56	165.29450	YES	YES
57	a	1084.47	65.29646	YES	YES
58	a	1090.10	15.40555	YES	YES
59	a	1096.15	23.02179	YES	YES
60	a	1143.58	12.50098	YES	YES
61	a	1318.51	32.60785	YES	YES
62	a	1328.41	0.57307	YES	YES
63	a	1349.93	4.23400	YES	YES
64	a	1373.47	317.36149	YES	YES
65	a	1398.38	30.09657	YES	YES
66	a	1401.25	13.52371	YES	YES
67	a	1406.73	19.54868	YES	YES
68	a	1409.25	31.91710	YES	YES
69	a	1409.35	10.99288	YES	YES
70	a	1420.59	19.68351	YES	YES
71	a	1466.23	282.84938	YES	YES
72	a	1539.75	73.42662	YES	YES
73	a	1631.13	236.13682	YES	YES
74	a	1934.93	17.95652	YES	YES
75	a	2203.25	197.03935	YES	YES
76	a	2283.93	121.60252	YES	YES
77	a	2306.39	110.10972	YES	YES
78	a	2320.27	90.95544	YES	YES
79	a	2403.30	53.15273	YES	YES
80	a	2427.42	15.74398	YES	YES
81	a	2935.91	21.79030	YES	YES
82	a	2958.43	11.95850	YES	YES
83	a	2960.64	2.60496	YES	YES
84	a	3019.42	5.32292	YES	YES
85	a	3028.43	1.57606	YES	YES
86	a	3042.57	7.32852	YES	YES
87	a	3046.82	2.45030	YES	YES
88	a	3076.20	9.16568	YES	YES
89	a	3077.61	2.60127	YES	YES
90	a	3235.52	7.70056	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2115829 Hartree *

Cis 2_afy



bp86_svp SCF energy = -1354.5135435110
pbe0_tzvpp SCF energy = -1354.293189987

xyz Coordinates

30

C	-2.15741	-0.01293	1.40169
C	-3.15240	-0.05851	2.53130
C	1.95365	-0.01099	1.71126
C	2.58505	0.42806	3.03190
H	3.59846	-0.00681	3.14100
H	1.94655	0.09681	3.87999
H	2.64013	1.53688	3.08034
H	-1.45000	0.59218	-3.26190
H	-3.04431	-0.03523	-1.93562
H	-1.67934	-1.50263	-2.75227
H	0.49166	-2.48996	-1.92301
H	2.40324	-1.68926	-1.36182
H	1.12970	-2.74611	0.12062
O	-1.53527	-1.07037	1.02480
O	-1.88177	1.08517	0.80422
O	0.79329	0.51192	1.47615
O	2.55357	-0.81898	0.96590
P	-1.62272	-0.22525	-2.08348
P	1.07396	-1.69888	-0.84753
Ru	-0.27715	0.09352	-0.28709
C	1.29184	1.27110	-1.40203
C	0.30041	1.97869	-1.05206
H	-0.27180	2.89877	-0.91726
C	2.63443	1.02295	-1.95710
H	3.28372	0.52187	-1.20452
H	3.10841	1.98783	-2.24742
H	2.60433	0.37595	-2.86345
H	-3.97190	0.66860	2.35512
H	-2.63958	0.22821	3.47645
H	-3.56015	-1.08274	2.65048

Vibrational Spectrum

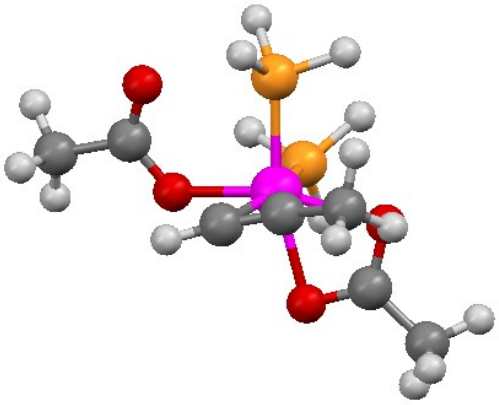
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.30	1.28458	YES	YES
8	a	45.43	0.27097	YES	YES
9	a	64.45	0.38482	YES	YES
10	a	69.23	1.00183	YES	YES
11	a	76.06	0.22128	YES	YES
12	a	78.20	0.07989	YES	YES
13	a	97.16	5.48340	YES	YES
14	a	105.56	1.40796	YES	YES
15	a	120.03	5.38067	YES	YES
16	a	148.55	5.14126	YES	YES
17	a	161.60	6.45577	YES	YES
18	a	164.53	6.74955	YES	YES
19	a	179.76	3.24027	YES	YES
20	a	202.24	13.35753	YES	YES
21	a	214.31	2.86486	YES	YES
22	a	220.27	2.25603	YES	YES
23	a	226.69	5.02892	YES	YES
24	a	234.58	0.99251	YES	YES
25	a	272.79	12.97087	YES	YES
26	a	289.13	6.33466	YES	YES
27	a	321.02	15.52067	YES	YES
28	a	326.90	9.94890	YES	YES
29	a	347.32	14.58365	YES	YES
30	a	364.01	1.05972	YES	YES
31	a	373.48	2.73032	YES	YES
32	a	386.58	3.76625	YES	YES
33	a	481.41	4.73557	YES	YES
34	a	489.74	4.90604	YES	YES
35	a	507.61	1.11312	YES	YES
36	a	558.52	3.60805	YES	YES
37	a	577.67	12.31167	YES	YES
38	a	592.60	7.47612	YES	YES
39	a	596.32	0.57846	YES	YES
40	a	610.67	4.12701	YES	YES
41	a	649.75	21.99638	YES	YES
42	a	655.13	1.06123	YES	YES
43	a	669.05	53.86982	YES	YES
44	a	676.44	63.69850	YES	YES
45	a	785.22	7.33352	YES	YES
46	a	930.93	6.05921	YES	YES
47	a	935.30	11.57859	YES	YES
48	a	942.96	30.50932	YES	YES
49	a	983.56	1.24893	YES	YES
50	a	992.58	5.56072	YES	YES

51	a	1009.95	57.06638	YES	YES
52	a	1011.81	73.55000	YES	YES
53	a	1022.29	7.64784	YES	YES
54	a	1024.86	0.69780	YES	YES
55	a	1025.85	5.48752	YES	YES
56	a	1034.77	154.07703	YES	YES
57	a	1088.54	48.19926	YES	YES
58	a	1090.26	6.42563	YES	YES
59	a	1095.45	29.59894	YES	YES
60	a	1135.67	11.96243	YES	YES
61	a	1317.03	28.66023	YES	YES
62	a	1330.00	0.76389	YES	YES
63	a	1349.72	5.02923	YES	YES
64	a	1375.14	327.69119	YES	YES
65	a	1398.12	34.95737	YES	YES
66	a	1405.61	24.62461	YES	YES
67	a	1407.83	10.65017	YES	YES
68	a	1409.35	29.68720	YES	YES
69	a	1418.45	9.15120	YES	YES
70	a	1429.08	6.95437	YES	YES
71	a	1466.78	294.55192	YES	YES
72	a	1537.00	74.59247	YES	YES
73	a	1622.28	216.39366	YES	YES
74	a	1935.33	20.39572	YES	YES
75	a	2214.44	180.82306	YES	YES
76	a	2290.77	118.00786	YES	YES
77	a	2307.82	105.34245	YES	YES
78	a	2316.82	97.49472	YES	YES
79	a	2406.74	45.69297	YES	YES
80	a	2428.07	18.05176	YES	YES
81	a	2926.54	30.31259	YES	YES
82	a	2958.92	11.80474	YES	YES
83	a	2961.34	2.47149	YES	YES
84	a	3003.37	6.04515	YES	YES
85	a	3019.17	2.15590	YES	YES
86	a	3041.48	5.54430	YES	YES
87	a	3047.32	2.31506	YES	YES
88	a	3075.77	10.02441	YES	YES
89	a	3078.19	2.50048	YES	YES
90	a	3247.09	13.48615	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2118848 Hartree *

Cis 2_pfex



bp86_svp SCF energy = -1354.5045140680

pbe0_tzvpp SCF energy = -1354.283077837

xyz Coordinates

30

C	-0.63640	0.45627	2.57906
C	-0.92948	0.69683	4.04195
H	-0.06360	1.21754	4.50895
H	-1.08467	-0.26292	4.57571
H	-1.81702	1.35271	4.15325
C	-0.19013	0.68524	-2.79606
C	-0.73992	1.58571	-3.90264
H	-0.96407	0.97598	-4.80304
H	0.04383	2.32186	-4.18976
H	-1.64231	2.14119	-3.57650
H	-2.68811	-1.13376	-1.36847
H	-3.22444	-0.60016	0.66664
H	-2.22034	-2.47238	0.28281
H	0.45122	-2.50495	-1.99269
H	2.34349	-1.46355	-1.53741
H	1.39861	-2.75448	-0.07832
O	-0.10441	-0.66158	2.20725
O	-0.87662	1.33880	1.69751
O	-0.63153	0.98379	-1.60516
O	0.62098	-0.21720	-3.06571
P	-2.08362	-1.08569	-0.06959
P	1.03952	-1.67434	-0.98431
Ru	-0.01664	-0.01424	0.13037
C	1.61996	1.37288	-0.11961
C	2.03618	0.61414	0.79826
C	2.87236	0.02170	1.85414
H	1.61103	2.20054	-0.82855
H	3.64834	0.74507	2.19287
H	3.39229	-0.89281	1.48724
H	2.25449	-0.28454	2.72523

Vibrational Spectrum

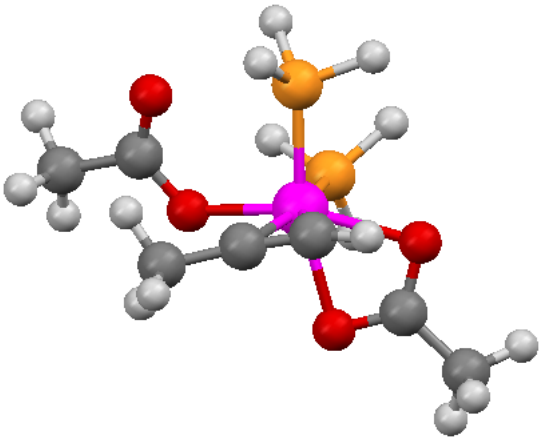
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	38.15	0.26836	YES	YES
8	a	44.78	0.91629	YES	YES
9	a	49.89	1.64632	YES	YES
10	a	58.66	0.50630	YES	YES
11	a	60.74	0.80942	YES	YES
12	a	70.54	0.45018	YES	YES
13	a	76.22	1.67088	YES	YES
14	a	88.57	0.13381	YES	YES
15	a	99.47	0.73200	YES	YES
16	a	109.97	1.38647	YES	YES
17	a	122.44	4.06046	YES	YES
18	a	147.65	2.52535	YES	YES
19	a	164.50	26.30590	YES	YES
20	a	179.62	2.88698	YES	YES
21	a	195.06	1.10411	YES	YES
22	a	203.39	1.92802	YES	YES
23	a	228.39	9.49875	YES	YES
24	a	248.67	0.84142	YES	YES
25	a	261.05	10.97851	YES	YES
26	a	285.42	16.19359	YES	YES
27	a	296.47	12.10390	YES	YES
28	a	325.80	14.72434	YES	YES
29	a	337.64	10.09309	YES	YES
30	a	343.06	2.63554	YES	YES
31	a	360.06	0.76498	YES	YES
32	a	373.52	11.03712	YES	YES
33	a	434.33	2.79345	YES	YES
34	a	474.28	1.68227	YES	YES
35	a	508.45	2.68767	YES	YES
36	a	518.21	4.92062	YES	YES
37	a	531.69	2.82605	YES	YES
38	a	592.94	5.80865	YES	YES
39	a	604.93	0.67779	YES	YES
40	a	612.78	7.84143	YES	YES
41	a	630.43	5.00851	YES	YES
42	a	656.33	25.18278	YES	YES
43	a	668.92	66.64460	YES	YES
44	a	672.11	30.54827	YES	YES
45	a	739.89	1.21800	YES	YES
46	a	924.36	12.92284	YES	YES
47	a	929.14	5.02750	YES	YES
48	a	937.92	27.15417	YES	YES
49	a	981.95	1.87690	YES	YES
50	a	988.75	3.13154	YES	YES
51	a	1002.07	38.59242	YES	YES

52	a	1007.57	164.96522	YES	YES
53	a	1021.32	8.34667	YES	YES
54	a	1024.17	19.01739	YES	YES
55	a	1027.22	4.15310	YES	YES
56	a	1030.94	65.62434	YES	YES
57	a	1078.55	89.52836	YES	YES
58	a	1085.72	13.57005	YES	YES
59	a	1108.60	9.21689	YES	YES
60	a	1127.75	11.80908	YES	YES
61	a	1312.66	125.22164	YES	YES
62	a	1327.13	2.48754	YES	YES
63	a	1342.21	208.43587	YES	YES
64	a	1348.60	11.66698	YES	YES
65	a	1394.92	56.03200	YES	YES
66	a	1402.05	18.62596	YES	YES
67	a	1410.36	35.98953	YES	YES
68	a	1412.19	22.37701	YES	YES
69	a	1419.63	7.35831	YES	YES
70	a	1420.92	15.24909	YES	YES
71	a	1443.92	222.19385	YES	YES
72	a	1553.12	95.86479	YES	YES
73	a	1655.97	210.37211	YES	YES
74	a	1964.28	11.41518	YES	YES
75	a	2227.58	163.86633	YES	YES
76	a	2314.29	117.65013	YES	YES
77	a	2353.54	49.62337	YES	YES
78	a	2363.88	100.85744	YES	YES
79	a	2380.33	25.03934	YES	YES
80	a	2384.63	31.32770	YES	YES
81	a	2932.73	29.45456	YES	YES
82	a	2957.16	12.63120	YES	YES
83	a	2959.35	3.47145	YES	YES
84	a	3007.38	5.05789	YES	YES
85	a	3035.46	0.47735	YES	YES
86	a	3041.22	6.75533	YES	YES
87	a	3044.80	3.16922	YES	YES
88	a	3072.40	7.83271	YES	YES
89	a	3078.17	2.56928	YES	YES
90	a	3272.49	13.43187	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2107862 Hartree *

Cis 2_pfey



bp86_svp SCF energy = -1354.5062397770

pbe0_tzvpp SCF energy = -1354.284902762

xyz Coordinates

30

C	0.23977	0.49874	2.73197
C	0.43458	0.78689	4.20237
H	1.45899	0.47353	4.50395
H	-0.29213	0.21423	4.81431
H	0.33769	1.87408	4.39811
C	-0.17246	0.71547	-2.63901
C	-0.20696	1.84014	-3.67471
H	-0.91755	1.57781	-4.48607
H	0.80111	1.93722	-4.13641
H	-0.47936	2.81437	-3.22102
H	-2.97102	0.90101	-0.71109
H	-2.65597	1.53876	1.34030
H	-3.21466	-0.50608	0.93182
H	-1.67008	-2.15762	-1.75353
H	0.47046	-2.67795	-1.66729
H	-0.84784	-3.10402	-0.00396
O	-0.20733	-0.65444	2.36003
O	0.53009	1.35613	1.83930
O	-0.07364	1.13697	-1.40749
O	-0.20487	-0.47336	-2.99955
P	-2.26694	0.46497	0.45974
P	-0.53135	-2.00397	-0.89740
Ru	-0.01399	-0.12786	0.25569
C	1.90098	-1.05854	0.63806
C	2.13722	-0.27476	-0.32389
C	2.84043	0.45881	-1.38338
H	2.11319	-1.75132	1.45364
H	3.94208	0.33509	-1.27662
H	2.59289	1.54124	-1.34852
H	2.53945	0.07872	-2.38485

Vibrational Spectrum

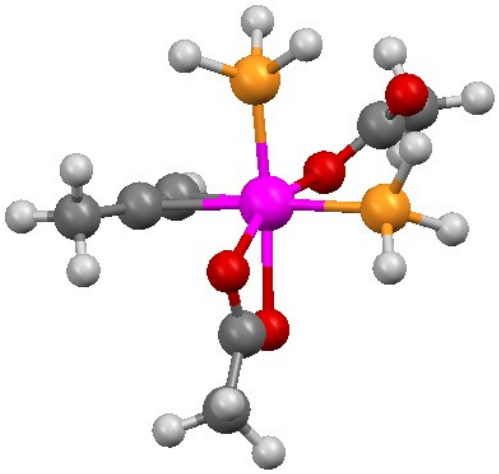
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	38.44	0.65150	YES	YES
8	a	39.08	0.37762	YES	YES
9	a	48.73	0.09060	YES	YES
10	a	57.74	2.41386	YES	YES
11	a	61.08	0.74705	YES	YES
12	a	66.15	1.26063	YES	YES
13	a	82.25	2.61326	YES	YES
14	a	92.64	1.00680	YES	YES
15	a	111.47	1.30633	YES	YES
16	a	124.05	3.29214	YES	YES
17	a	151.38	1.04887	YES	YES
18	a	158.51	21.23493	YES	YES
19	a	165.40	1.28664	YES	YES
20	a	172.44	3.48146	YES	YES
21	a	193.59	2.03596	YES	YES
22	a	209.16	1.65223	YES	YES
23	a	236.75	6.61348	YES	YES
24	a	244.98	3.42876	YES	YES
25	a	260.52	6.49626	YES	YES
26	a	284.95	12.09316	YES	YES
27	a	294.91	15.45855	YES	YES
28	a	323.99	10.27486	YES	YES
29	a	332.90	0.97611	YES	YES
30	a	341.85	14.46904	YES	YES
31	a	348.75	5.97352	YES	YES
32	a	374.32	10.67062	YES	YES
33	a	444.00	2.65390	YES	YES
34	a	473.85	2.05591	YES	YES
35	a	508.60	2.40766	YES	YES
36	a	516.09	5.01644	YES	YES
37	a	531.56	2.24124	YES	YES
38	a	592.58	5.06915	YES	YES
39	a	604.63	0.61795	YES	YES
40	a	610.69	9.16746	YES	YES
41	a	623.90	3.44841	YES	YES
42	a	633.61	24.95160	YES	YES
43	a	670.00	72.79705	YES	YES
44	a	670.74	27.10314	YES	YES
45	a	748.52	4.13477	YES	YES
46	a	927.36	10.16042	YES	YES
47	a	927.94	5.29591	YES	YES
48	a	939.13	28.77469	YES	YES
49	a	981.25	1.78076	YES	YES
50	a	988.73	3.12850	YES	YES

51	a	1003.53	78.28028	YES	YES
52	a	1007.65	138.14403	YES	YES
53	a	1021.58	8.65509	YES	YES
54	a	1025.71	10.54948	YES	YES
55	a	1028.21	27.44306	YES	YES
56	a	1032.03	41.27247	YES	YES
57	a	1074.30	94.28623	YES	YES
58	a	1085.22	15.33865	YES	YES
59	a	1108.38	9.56455	YES	YES
60	a	1124.54	11.46312	YES	YES
61	a	1310.73	130.43390	YES	YES
62	a	1326.24	2.13729	YES	YES
63	a	1340.87	196.02803	YES	YES
64	a	1350.82	4.61527	YES	YES
65	a	1396.60	50.39946	YES	YES
66	a	1398.01	23.90493	YES	YES
67	a	1409.74	44.07881	YES	YES
68	a	1412.43	16.08513	YES	YES
69	a	1417.08	1.94657	YES	YES
70	a	1422.19	20.88980	YES	YES
71	a	1444.79	241.05150	YES	YES
72	a	1553.15	96.38519	YES	YES
73	a	1655.85	200.54251	YES	YES
74	a	1959.84	15.56001	YES	YES
75	a	2245.72	163.29106	YES	YES
76	a	2313.20	117.37842	YES	YES
77	a	2356.72	48.59050	YES	YES
78	a	2365.09	104.95558	YES	YES
79	a	2380.94	28.67714	YES	YES
80	a	2381.96	27.52510	YES	YES
81	a	2938.41	21.52851	YES	YES
82	a	2956.91	11.94884	YES	YES
83	a	2960.42	3.65083	YES	YES
84	a	3018.06	3.93999	YES	YES
85	a	3036.90	0.95325	YES	YES
86	a	3041.38	6.78463	YES	YES
87	a	3046.01	3.18037	YES	YES
88	a	3073.17	7.41552	YES	YES
89	a	3078.41	2.69461	YES	YES
90	a	3255.01	12.06138	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2108832 Hartree *

Cis 2_pftx



bp86_svp SCF energy = -1354.5057069060
pbe0_tzvpp SCF energy = -1354.285381752

xyz Coordinates

30

C	-0.49599	0.88735	2.34505
C	-0.81619	1.41111	3.72661
H	0.01601	1.15981	4.42172
H	-1.74622	0.94965	4.11567
H	-0.91183	2.51646	3.70284
C	0.22447	0.81867	-2.81665
C	1.00051	1.46880	-3.96048
H	0.29787	1.98897	-4.64377
H	1.51246	0.67320	-4.54770
H	1.77002	2.17392	-3.58595
H	-2.07166	2.11105	-1.34129
H	-2.86029	1.27881	0.49729
H	-3.05151	0.15334	-1.34461
H	-1.77946	-2.16461	-1.70264
H	0.29453	-2.25056	-2.34733
H	-0.30344	-3.20563	-0.50481
O	-0.94071	-0.26497	1.97167
O	0.22070	1.55064	1.52922
O	0.86141	0.80611	-1.68110
O	-0.91049	0.33667	-3.00913
P	-2.04452	0.87342	-0.62419
P	-0.46736	-1.93147	-1.16653
Ru	-0.00481	-0.08048	0.02374
C	2.11703	-0.58333	0.19705
C	1.60111	-1.25538	1.12774
C	1.43591	-2.14862	2.28388
H	2.85644	-0.15034	-0.47552
H	2.42375	-2.54739	2.60948
H	0.77501	-3.01005	2.03985
H	0.96431	-1.61965	3.13931

Vibrational Spectrum

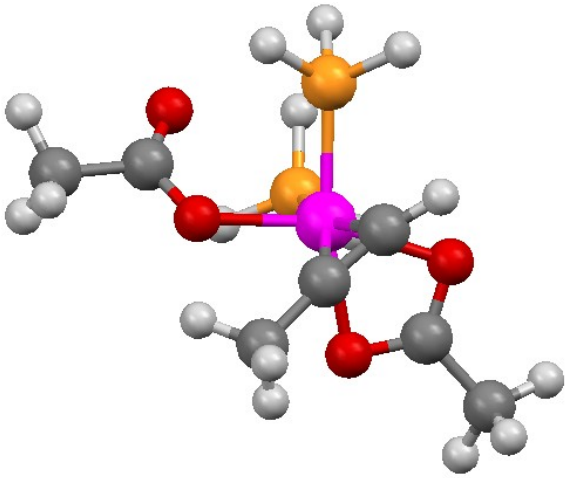
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	24.66	0.02406	YES	YES
8	a	37.44	0.25467	YES	YES
9	a	50.46	2.20084	YES	YES
10	a	54.99	0.66619	YES	YES
11	a	62.43	2.53722	YES	YES
12	a	77.86	2.79085	YES	YES
13	a	87.17	0.19452	YES	YES
14	a	101.07	0.87858	YES	YES
15	a	113.61	1.24497	YES	YES
16	a	130.06	5.69522	YES	YES
17	a	146.91	2.84999	YES	YES
18	a	161.51	10.29712	YES	YES
19	a	176.51	7.55166	YES	YES
20	a	187.39	1.63296	YES	YES
21	a	192.21	0.74926	YES	YES
22	a	202.98	0.89620	YES	YES
23	a	231.10	19.02977	YES	YES
24	a	240.69	1.46338	YES	YES
25	a	261.15	1.80896	YES	YES
26	a	277.71	11.27151	YES	YES
27	a	291.95	7.50870	YES	YES
28	a	301.21	9.81877	YES	YES
29	a	324.40	13.88929	YES	YES
30	a	332.79	5.64680	YES	YES
31	a	338.22	7.79678	YES	YES
32	a	377.85	9.56361	YES	YES
33	a	416.96	2.53946	YES	YES
34	a	475.16	4.22545	YES	YES
35	a	503.81	0.54162	YES	YES
36	a	528.14	8.69323	YES	YES
37	a	585.01	6.29394	YES	YES
38	a	598.38	4.81178	YES	YES
39	a	599.82	5.29329	YES	YES
40	a	605.57	4.60560	YES	YES
41	a	614.34	3.60317	YES	YES
42	a	669.59	91.85123	YES	YES
43	a	672.52	3.22460	YES	YES
44	a	676.99	20.35304	YES	YES
45	a	718.19	2.78679	YES	YES
46	a	922.53	14.35736	YES	YES
47	a	934.19	4.95407	YES	YES
48	a	938.71	27.89101	YES	YES
49	a	980.44	1.81755	YES	YES

50	a	989.06	3.10079	YES	YES
51	a	1001.83	53.21285	YES	YES
52	a	1013.05	122.89819	YES	YES
53	a	1021.56	24.50172	YES	YES
54	a	1024.28	4.30616	YES	YES
55	a	1027.28	11.87953	YES	YES
56	a	1056.59	118.34300	YES	YES
57	a	1072.79	13.58780	YES	YES
58	a	1077.07	12.04304	YES	YES
59	a	1106.31	13.37023	YES	YES
60	a	1112.97	9.82725	YES	YES
61	a	1316.06	61.94944	YES	YES
62	a	1327.30	1.40450	YES	YES
63	a	1351.15	239.83046	YES	YES
64	a	1356.51	10.28486	YES	YES
65	a	1395.86	44.55589	YES	YES
66	a	1403.30	22.22711	YES	YES
67	a	1408.78	28.54639	YES	YES
68	a	1410.36	18.57601	YES	YES
69	a	1413.08	18.58562	YES	YES
70	a	1420.65	19.35913	YES	YES
71	a	1447.68	227.21189	YES	YES
72	a	1549.19	93.69614	YES	YES
73	a	1631.87	180.95418	YES	YES
74	a	1977.18	12.86318	YES	YES
75	a	2289.97	106.35158	YES	YES
76	a	2303.14	127.66284	YES	YES
77	a	2313.46	106.27517	YES	YES
78	a	2352.91	48.56716	YES	YES
79	a	2377.87	67.72627	YES	YES
80	a	2398.83	23.89356	YES	YES
81	a	2937.90	28.80632	YES	YES
82	a	2955.39	10.97011	YES	YES
83	a	2959.16	3.49301	YES	YES
84	a	3015.46	4.93888	YES	YES
85	a	3034.95	2.31130	YES	YES
86	a	3040.96	7.46330	YES	YES
87	a	3044.27	2.56763	YES	YES
88	a	3074.08	6.33308	YES	YES
89	a	3077.83	2.47893	YES	YES
90	a	3280.83	18.68554	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2109434 Hartree *

Cis 2_pfty



bp86_svp SCF energy = -1354.5078189990
pbe0_tzvpp SCF energy = -1354.289088934

xyz Coordinates

30

C	1.06780	1.67152	-1.88187
C	1.81086	2.36773	-2.99668
H	2.90479	2.31369	-2.79820
H	1.51931	3.43606	-3.05389
H	1.61798	1.86057	-3.96467
C	-1.63433	-1.84118	0.98613
C	-1.75883	-3.34067	1.25216
H	-2.07616	-3.85104	0.31466
H	-2.54059	-3.52298	2.01779
H	-0.79369	-3.78308	1.57319
H	-3.27225	1.23924	-0.25006
H	-2.70199	-0.41008	-1.56764
H	-2.15425	1.62511	-2.06650
H	-2.37012	1.56566	2.13737
H	-1.02983	0.18858	3.16661
H	-0.41469	2.22735	2.79357
O	0.59435	2.34062	-0.89436
O	0.91548	0.40075	-1.87971
O	-0.44411	-1.46169	0.61261
O	-2.62316	-1.08938	1.09942
P	-2.11907	0.73205	-0.93092
P	-1.00564	1.12392	2.07217
Ru	-0.05720	0.53884	0.10817
C	1.83813	0.93777	1.19793
C	2.04883	-0.19489	0.70156
C	2.55831	-1.48318	0.23041
H	2.07131	1.86685	1.71821
H	3.55920	-1.69733	0.67007
H	2.64462	-1.47820	-0.87834
H	1.85116	-2.29402	0.50804

Vibrational Spectrum

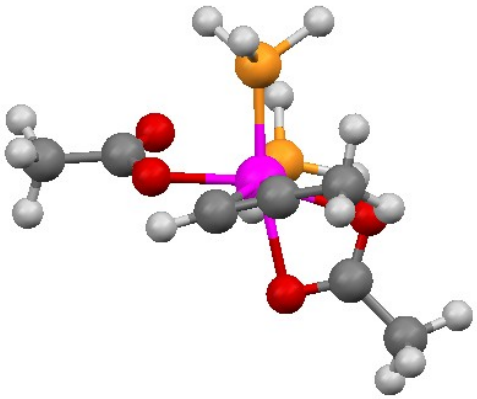
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	38.65	0.75995	YES	YES
8	a	49.75	0.40612	YES	YES
9	a	56.83	1.24618	YES	YES
10	a	65.43	0.73938	YES	YES
11	a	67.12	2.84389	YES	YES
12	a	77.88	1.51918	YES	YES
13	a	105.27	0.53380	YES	YES
14	a	106.78	0.39891	YES	YES
15	a	129.14	2.90542	YES	YES
16	a	132.13	2.43301	YES	YES
17	a	157.67	4.34548	YES	YES
18	a	164.93	11.94372	YES	YES
19	a	176.46	5.35247	YES	YES
20	a	188.77	9.76969	YES	YES
21	a	197.08	0.73400	YES	YES
22	a	212.70	6.44998	YES	YES
23	a	231.58	1.51354	YES	YES
24	a	237.38	2.50513	YES	YES
25	a	258.63	0.94029	YES	YES
26	a	272.50	1.90126	YES	YES
27	a	286.05	12.25842	YES	YES
28	a	301.75	13.04560	YES	YES
29	a	320.68	16.79302	YES	YES
30	a	334.78	7.39810	YES	YES
31	a	339.04	8.60623	YES	YES
32	a	377.68	13.22592	YES	YES
33	a	397.44	5.92514	YES	YES
34	a	478.16	3.80237	YES	YES
35	a	505.89	0.48818	YES	YES
36	a	534.47	10.85322	YES	YES
37	a	585.31	5.93762	YES	YES
38	a	593.17	4.32017	YES	YES
39	a	599.70	6.05959	YES	YES
40	a	603.92	2.70393	YES	YES
41	a	620.57	11.99595	YES	YES
42	a	624.20	16.60639	YES	YES
43	a	670.22	79.68028	YES	YES
44	a	675.11	18.30209	YES	YES
45	a	752.38	1.90086	YES	YES
46	a	923.12	10.09813	YES	YES
47	a	930.16	5.74397	YES	YES
48	a	941.02	31.85578	YES	YES
49	a	981.80	1.66849	YES	YES
50	a	989.24	4.44684	YES	YES

51	a	1002.71	59.71170	YES	YES
52	a	1014.58	113.89222	YES	YES
53	a	1021.81	29.29767	YES	YES
54	a	1025.44	6.00645	YES	YES
55	a	1025.71	10.20722	YES	YES
56	a	1049.47	105.97897	YES	YES
57	a	1071.99	33.17433	YES	YES
58	a	1076.94	29.17525	YES	YES
59	a	1109.37	9.08967	YES	YES
60	a	1116.82	6.37988	YES	YES
61	a	1314.60	84.23760	YES	YES
62	a	1328.25	1.13643	YES	YES
63	a	1339.53	21.75825	YES	YES
64	a	1351.45	209.99965	YES	YES
65	a	1391.41	12.91037	YES	YES
66	a	1398.75	32.55335	YES	YES
67	a	1409.00	21.18174	YES	YES
68	a	1410.26	31.60082	YES	YES
69	a	1418.84	4.68297	YES	YES
70	a	1421.88	20.03189	YES	YES
71	a	1456.51	272.36041	YES	YES
72	a	1539.12	80.80682	YES	YES
73	a	1635.12	185.96465	YES	YES
74	a	2004.08	13.94500	YES	YES
75	a	2292.53	126.23704	YES	YES
76	a	2297.23	133.14343	YES	YES
77	a	2321.28	104.41854	YES	YES
78	a	2358.91	47.60040	YES	YES
79	a	2378.91	73.84660	YES	YES
80	a	2394.31	17.30508	YES	YES
81	a	2940.01	23.23589	YES	YES
82	a	2954.77	11.86653	YES	YES
83	a	2959.27	3.64617	YES	YES
84	a	3024.67	2.13219	YES	YES
85	a	3040.55	7.53226	YES	YES
86	a	3042.60	0.15872	YES	YES
87	a	3044.41	2.81551	YES	YES
88	a	3072.69	7.70172	YES	YES
89	a	3077.32	2.66991	YES	YES
90	a	3269.20	15.85765	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2111744 Hartree *

Cis 2_pfpx



bp86_svp SCF energy = -1354.5059275090
pbe0_tzvpp SCF energy = -1354.285143350

xyz Coordinates

30

C	-1.34795	-0.30629	-2.07458
C	-2.13470	-0.53152	-3.34330
H	-1.52739	-1.13867	-4.05171
H	-2.37620	0.43529	-3.83044
H	-3.06305	-1.09797	-3.12373
C	-0.27415	-0.58420	2.91184
C	-0.00798	-1.52091	4.08898
H	-0.13700	-0.97242	5.04409
H	1.00481	-1.96965	4.03117
H	-0.75112	-2.34964	4.06598
H	-1.70823	2.42312	1.72667
H	-2.90442	0.60339	1.37307
H	-2.41887	1.94025	-0.24881
H	1.54496	1.94588	2.19246
H	2.92916	1.44606	0.59176
H	1.46194	3.01858	0.31267
O	-0.63786	0.76164	-1.93670
O	-1.34277	-1.16059	-1.13022
O	0.34232	-0.92287	1.81857
O	-1.05034	0.38268	3.04615
P	-1.75711	1.28523	0.86423
P	1.51400	1.65538	0.78115
Ru	0.09827	0.11719	-0.00742
C	1.63147	-1.38685	-0.42348
C	1.76672	-0.59053	-1.38734
C	2.23636	0.04942	-2.62572
H	1.77303	-2.23185	0.24796
H	2.86232	-0.65616	-3.21749
H	2.85271	0.95011	-2.40284
H	1.38004	0.38606	-3.24759

Vibrational Spectrum

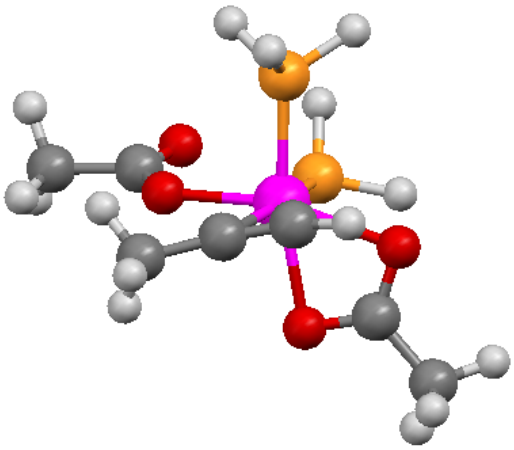
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	30.27	0.50252	YES	YES
8	a	40.35	0.28250	YES	YES
9	a	48.17	0.32229	YES	YES
10	a	57.95	1.61835	YES	YES
11	a	76.12	0.53777	YES	YES
12	a	82.25	1.10812	YES	YES
13	a	85.48	0.98899	YES	YES
14	a	102.78	0.78316	YES	YES
15	a	109.96	2.12737	YES	YES
16	a	118.36	0.66802	YES	YES
17	a	119.07	2.42912	YES	YES
18	a	152.24	1.65955	YES	YES
19	a	171.76	12.88699	YES	YES
20	a	176.37	0.51977	YES	YES
21	a	188.65	6.82143	YES	YES
22	a	204.95	8.70863	YES	YES
23	a	234.32	27.29037	YES	YES
24	a	248.05	0.25292	YES	YES
25	a	262.15	1.80905	YES	YES
26	a	286.78	15.37264	YES	YES
27	a	293.94	13.15949	YES	YES
28	a	323.01	15.53963	YES	YES
29	a	330.30	2.89170	YES	YES
30	a	339.51	9.10611	YES	YES
31	a	377.09	4.37356	YES	YES
32	a	392.81	4.94356	YES	YES
33	a	416.48	4.68220	YES	YES
34	a	477.09	4.09076	YES	YES
35	a	512.42	2.87497	YES	YES
36	a	549.39	6.94471	YES	YES
37	a	590.34	7.47035	YES	YES
38	a	595.02	2.75956	YES	YES
39	a	602.71	2.68038	YES	YES
40	a	607.57	3.08766	YES	YES
41	a	621.99	6.98791	YES	YES
42	a	670.30	89.90214	YES	YES
43	a	672.38	0.95826	YES	YES
44	a	674.54	23.51687	YES	YES
45	a	719.01	3.59296	YES	YES
46	a	920.65	12.08082	YES	YES
47	a	937.28	6.87598	YES	YES
48	a	939.84	24.11440	YES	YES
49	a	983.42	1.62893	YES	YES
50	a	992.53	2.36309	YES	YES
51	a	1003.03	42.27001	YES	YES

52	a	1007.68	140.19959	YES	YES
53	a	1020.17	8.58477	YES	YES
54	a	1023.59	6.34694	YES	YES
55	a	1028.04	8.13015	YES	YES
56	a	1045.09	135.88235	YES	YES
57	a	1073.55	45.98640	YES	YES
58	a	1091.36	10.63082	YES	YES
59	a	1098.76	7.95323	YES	YES
60	a	1135.65	12.22730	YES	YES
61	a	1317.24	46.38625	YES	YES
62	a	1330.13	1.66311	YES	YES
63	a	1347.43	4.66497	YES	YES
64	a	1356.22	275.08284	YES	YES
65	a	1396.99	41.69347	YES	YES
66	a	1402.77	14.07475	YES	YES
67	a	1408.49	22.91441	YES	YES
68	a	1411.26	33.15115	YES	YES
69	a	1419.51	8.41286	YES	YES
70	a	1420.00	18.47194	YES	YES
71	a	1452.85	242.41890	YES	YES
72	a	1546.97	87.08112	YES	YES
73	a	1641.77	225.27761	YES	YES
74	a	1982.12	11.76108	YES	YES
75	a	2260.67	153.05644	YES	YES
76	a	2302.93	87.20640	YES	YES
77	a	2308.42	70.36472	YES	YES
78	a	2318.65	94.69863	YES	YES
79	a	2392.79	69.32432	YES	YES
80	a	2409.99	18.88954	YES	YES
81	a	2934.74	30.27351	YES	YES
82	a	2957.04	11.06762	YES	YES
83	a	2958.60	2.96702	YES	YES
84	a	3008.78	6.18197	YES	YES
85	a	3039.91	0.37715	YES	YES
86	a	3043.12	7.38583	YES	YES
87	a	3044.16	2.53898	YES	YES
88	a	3075.41	7.06713	YES	YES
89	a	3076.97	2.18868	YES	YES
90	a	3289.63	19.81673	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2112274 Hartree *

Cis 2_pfpy



bp86_svp SCF energy = -1354.5071354430
pbe0_tzvpp SCF energy = -1354.286068825

xyz Coordinates

30

C	-0.46369	0.75585	2.51843
C	-0.74434	1.28078	3.90566
H	0.21598	1.38994	4.45770
H	-1.39006	0.57580	4.46779
H	-1.21909	2.28178	3.84885
C	-0.38169	0.84540	-2.55225
C	0.11920	1.56136	-3.80571
H	-0.57719	2.38939	-4.05774
H	0.10508	0.85163	-4.66235
H	1.14629	1.95697	-3.67655
H	-2.91515	-1.09590	-1.06401
H	-2.92757	1.02222	-0.45014
H	-2.87728	-0.55570	1.02027
H	0.02409	-2.40548	-2.13559
H	1.60265	-2.87470	-0.71092
H	-0.46184	-3.35297	-0.25198
O	-0.50426	-0.51120	2.28615
O	-0.15856	1.53628	1.55821
O	0.52059	0.67865	-1.63207
O	-1.57078	0.47403	-2.49133
P	-2.20858	-0.19023	-0.21434
P	0.31074	-2.23365	-0.73217
Ru	0.11097	-0.22403	0.22871
C	1.98689	-0.62163	1.27245
C	2.34417	0.15699	0.34900
C	3.14314	1.02477	-0.52254
H	2.06210	-1.20973	2.18738
H	4.20181	1.05138	-0.17748
H	2.73809	2.05987	-0.52107
H	3.11320	0.67192	-1.57527

Vibrational Spectrum

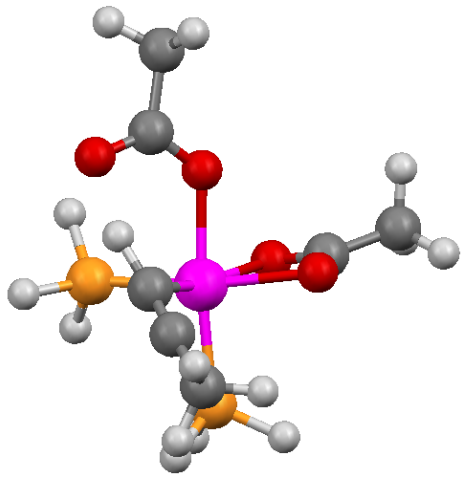
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.32	1.35070	YES	YES
8	a	23.59	0.42230	YES	YES
9	a	35.47	1.04160	YES	YES
10	a	47.80	0.36176	YES	YES
11	a	59.67	0.90306	YES	YES
12	a	84.87	1.25843	YES	YES
13	a	86.72	2.68851	YES	YES
14	a	106.16	0.90710	YES	YES
15	a	114.47	0.59983	YES	YES
16	a	120.72	2.12553	YES	YES
17	a	130.81	0.32842	YES	YES
18	a	160.90	0.29289	YES	YES
19	a	176.32	10.91191	YES	YES
20	a	183.06	8.08325	YES	YES
21	a	198.22	4.93337	YES	YES
22	a	211.19	10.23004	YES	YES
23	a	231.24	15.67573	YES	YES
24	a	251.87	2.31709	YES	YES
25	a	264.17	0.43906	YES	YES
26	a	289.19	12.18835	YES	YES
27	a	296.12	22.89260	YES	YES
28	a	318.36	9.78959	YES	YES
29	a	336.56	4.97513	YES	YES
30	a	341.01	10.06666	YES	YES
31	a	376.46	6.50293	YES	YES
32	a	392.95	5.61158	YES	YES
33	a	431.43	3.07430	YES	YES
34	a	476.11	4.58664	YES	YES
35	a	509.60	4.41989	YES	YES
36	a	548.15	6.76631	YES	YES
37	a	586.23	6.54616	YES	YES
38	a	593.36	4.31350	YES	YES
39	a	602.90	3.52079	YES	YES
40	a	607.33	2.02311	YES	YES
41	a	618.78	7.78472	YES	YES
42	a	637.92	24.08350	YES	YES
43	a	671.95	67.65986	YES	YES
44	a	675.30	25.08395	YES	YES
45	a	750.53	2.13621	YES	YES
46	a	927.16	10.79046	YES	YES
47	a	934.95	3.33982	YES	YES
48	a	940.34	30.58788	YES	YES
49	a	981.66	1.32351	YES	YES
50	a	990.16	1.37332	YES	YES
51	a	1000.17	50.77660	YES	YES

52	a	1007.93	146.79355	YES	YES
53	a	1020.35	6.38636	YES	YES
54	a	1025.41	11.05539	YES	YES
55	a	1026.91	1.03368	YES	YES
56	a	1041.82	130.86449	YES	YES
57	a	1072.73	41.80303	YES	YES
58	a	1090.01	15.44295	YES	YES
59	a	1098.62	9.69718	YES	YES
60	a	1133.91	11.16249	YES	YES
61	a	1318.35	43.22728	YES	YES
62	a	1327.20	1.26531	YES	YES
63	a	1348.86	160.05849	YES	YES
64	a	1356.01	91.56606	YES	YES
65	a	1396.16	53.94909	YES	YES
66	a	1397.60	5.45341	YES	YES
67	a	1405.75	12.07288	YES	YES
68	a	1410.17	32.73531	YES	YES
69	a	1415.13	23.71349	YES	YES
70	a	1420.43	20.37206	YES	YES
71	a	1453.59	260.55837	YES	YES
72	a	1544.71	87.12889	YES	YES
73	a	1640.11	230.34522	YES	YES
74	a	1977.27	16.65004	YES	YES
75	a	2263.08	149.09363	YES	YES
76	a	2303.89	64.54190	YES	YES
77	a	2308.37	70.11323	YES	YES
78	a	2311.77	133.74902	YES	YES
79	a	2389.41	73.57202	YES	YES
80	a	2405.74	20.56970	YES	YES
81	a	2942.42	25.42181	YES	YES
82	a	2958.29	13.07160	YES	YES
83	a	2959.75	3.00248	YES	YES
84	a	3027.03	4.75862	YES	YES
85	a	3040.21	1.13263	YES	YES
86	a	3041.07	5.23488	YES	YES
87	a	3045.70	2.54039	YES	YES
88	a	3074.23	8.57828	YES	YES
89	a	3078.16	2.36635	YES	YES
90	a	3264.66	14.94675	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2111248 Hartree *

Cis TS_{24}_afx



bp86_svp SCF energy = -1354.4857342570
pbe0_tzvpp SCF energy = -1354.264383580

xyz Coordinates

30

C	-0.75326	-0.63302	2.30330
C	-0.96527	-0.57700	3.79475
H	-0.04263	-0.18195	4.27536
H	-1.16254	-1.59019	4.20071
H	-1.80095	0.11069	4.03885
C	2.78473	0.28657	0.11053
C	3.99463	0.63428	0.97373
H	4.93091	0.45576	0.40667
H	3.99191	0.05572	1.91981
H	3.95180	1.71651	1.23176
H	-2.62625	-1.06086	-2.14422
H	-3.28250	-1.01571	-0.08519
H	-2.42181	-2.81114	-0.91222
H	0.43231	-3.54013	-1.54580
H	1.39501	-2.02071	-2.74195
H	2.28993	-2.66391	-0.86953
O	-0.30536	-1.70499	1.74977
O	-0.98118	0.37873	1.55774
O	1.72360	-0.05257	0.75833
O	2.88480	0.37655	-1.14335
P	-2.11127	-1.40130	-0.83753
P	1.01181	-2.23007	-1.36656
Ru	-0.09259	-0.70436	-0.12970
C	0.24580	0.82495	-1.69311
C	-0.70272	1.54544	-2.06485
C	-1.83677	2.38473	-2.41088
H	1.39436	0.64917	-1.64852
H	-2.47779	1.95292	-3.21256
H	-1.46820	3.37454	-2.76844
H	-2.46669	2.58530	-1.51377

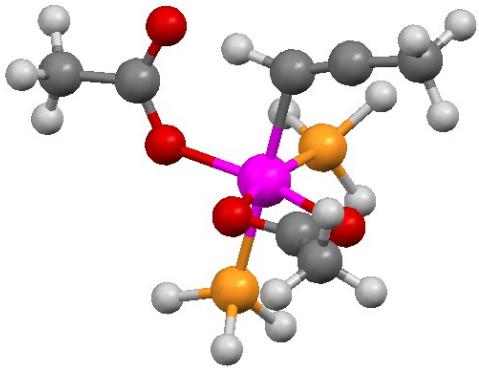
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-141.53	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	27.21	1.44405	YES	YES
9	a	34.81	1.83048	YES	YES
10	a	49.64	1.27630	YES	YES
11	a	55.24	0.51230	YES	YES
12	a	60.72	0.79715	YES	YES
13	a	73.08	2.66177	YES	YES
14	a	77.03	0.23216	YES	YES
15	a	78.33	0.44344	YES	YES
16	a	94.92	0.53291	YES	YES
17	a	102.89	7.56015	YES	YES
18	a	130.88	3.00974	YES	YES
19	a	142.59	5.22670	YES	YES
20	a	153.53	0.06674	YES	YES
21	a	161.51	0.27941	YES	YES
22	a	171.15	1.74368	YES	YES
23	a	188.58	3.34241	YES	YES
24	a	207.02	0.16801	YES	YES
25	a	241.61	12.86495	YES	YES
26	a	270.45	26.97500	YES	YES
27	a	285.70	15.29272	YES	YES
28	a	287.70	6.84324	YES	YES
29	a	325.74	11.44472	YES	YES
30	a	329.85	22.06283	YES	YES
31	a	366.50	15.15870	YES	YES
32	a	376.91	6.89031	YES	YES
33	a	391.43	1.10882	YES	YES
34	a	478.95	7.72772	YES	YES
35	a	504.33	5.87497	YES	YES
36	a	564.88	2.23873	YES	YES
37	a	579.12	4.70822	YES	YES
38	a	590.74	8.52861	YES	YES
39	a	597.92	4.65035	YES	YES
40	a	599.18	2.23462	YES	YES
41	a	612.79	4.34394	YES	YES
42	a	665.00	59.21057	YES	YES
43	a	674.09	73.62223	YES	YES
44	a	895.06	130.40563	YES	YES
45	a	932.74	34.53748	YES	YES
46	a	938.67	38.00216	YES	YES

47	a	945.18	54.13184	YES	YES
48	a	981.51	1.66783	YES	YES
49	a	993.31	16.72259	YES	YES
50	a	994.43	8.44783	YES	YES
51	a	1011.87	54.54149	YES	YES
52	a	1021.80	8.71057	YES	YES
53	a	1025.53	2.29970	YES	YES
54	a	1029.31	40.06780	YES	YES
55	a	1037.23	249.72794	YES	YES
56	a	1061.44	136.58138	YES	YES
57	a	1086.26	10.25196	YES	YES
58	a	1095.54	15.01248	YES	YES
59	a	1099.60	9.60056	YES	YES
60	a	1103.92	14.85789	YES	YES
61	a	1321.85	16.03109	YES	YES
62	a	1327.16	0.82157	YES	YES
63	a	1342.27	5.63855	YES	YES
64	a	1380.45	255.44681	YES	YES
65	a	1397.39	19.49394	YES	YES
66	a	1398.02	29.58845	YES	YES
67	a	1406.62	27.20067	YES	YES
68	a	1408.59	38.39111	YES	YES
69	a	1410.26	19.82479	YES	YES
70	a	1423.11	41.45380	YES	YES
71	a	1458.12	281.64960	YES	YES
72	a	1533.83	96.31702	YES	YES
73	a	1554.90	189.25669	YES	YES
74	a	1964.61	224.31437	YES	YES
75	a	2278.70	39.91551	YES	YES
76	a	2288.76	90.72098	YES	YES
77	a	2294.67	118.17831	YES	YES
78	a	2297.45	78.39753	YES	YES
79	a	2305.60	198.04042	YES	YES
80	a	2339.19	17.42738	YES	YES
81	a	2369.16	1139.68565	YES	YES
82	a	2924.34	13.22793	YES	YES
83	a	2957.55	9.82970	YES	YES
84	a	2961.22	2.92859	YES	YES
85	a	3003.80	3.74967	YES	YES
86	a	3009.44	4.89237	YES	YES
87	a	3044.10	7.42218	YES	YES
88	a	3047.66	2.83903	YES	YES
89	a	3076.64	2.82772	YES	YES
90	a	3077.28	7.08182	YES	YES

* zero point VIBRATIONAL energy : 0.2057761 Hartree *

Cis TS_{24}_pf



bp86_svp SCF energy = -1354.4865999160
pbe0_tzvpp SCF energy = -1354.264968561

xyz Coordinates

30

C	0.09552	-1.52387	-1.84176
C	0.56846	-2.23021	-3.08992
H	1.52640	-1.77668	-3.42919
H	-0.17783	-2.12972	-3.90403
H	0.76450	-3.30079	-2.87407
C	0.94540	0.19534	2.83958
C	1.16401	-0.24363	4.28536
H	0.25336	-0.70927	4.71227
H	1.48133	0.62546	4.89863
H	1.99102	-0.98816	4.31133
H	-2.26106	-2.92074	0.02060
H	-3.62837	-1.31095	0.48804
H	-2.36651	-2.13982	2.05341
H	-1.95604	2.11625	2.01240
H	-1.59473	2.82202	-0.00676
H	-3.29277	1.54739	0.41545
O	-0.77211	-0.57887	-1.91246
O	0.56732	-1.82794	-0.69382
O	-0.06518	-0.36005	2.25254
O	1.75048	1.01477	2.33250
P	-2.24303	-1.65108	0.70321
P	-1.87153	1.58176	0.67075
Ru	-0.59073	-0.20391	0.22152
C	1.10721	1.19240	-0.28995
C	1.22685	1.64456	-1.44191
C	1.27497	2.08237	-2.82788
H	0.49664	1.52456	-3.39929
H	2.25962	1.86247	-3.30043
H	1.06695	3.17045	-2.94074
H	1.45344	1.13244	0.83633

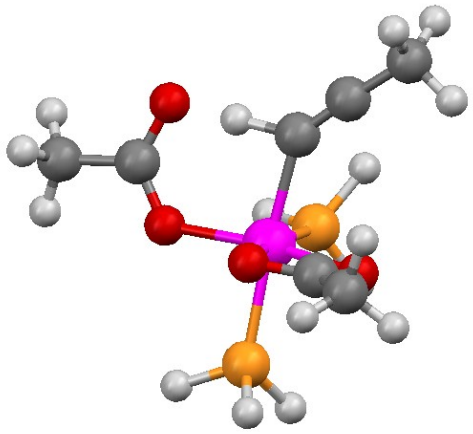
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-68.51	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	28.41	0.81563	YES	YES
9	a	53.77	3.10513	YES	YES
10	a	57.03	0.14848	YES	YES
11	a	61.58	0.24794	YES	YES
12	a	63.77	0.03858	YES	YES
13	a	71.87	1.25103	YES	YES
14	a	80.31	0.61794	YES	YES
15	a	84.41	0.91202	YES	YES
16	a	102.90	1.47300	YES	YES
17	a	109.53	0.76201	YES	YES
18	a	110.15	2.15931	YES	YES
19	a	132.97	1.07803	YES	YES
20	a	141.23	3.57944	YES	YES
21	a	168.79	1.64694	YES	YES
22	a	177.87	3.47229	YES	YES
23	a	186.71	1.09651	YES	YES
24	a	190.03	8.97408	YES	YES
25	a	247.95	16.73983	YES	YES
26	a	262.50	16.77881	YES	YES
27	a	282.82	13.49867	YES	YES
28	a	298.94	15.04165	YES	YES
29	a	321.19	37.67109	YES	YES
30	a	339.56	2.73994	YES	YES
31	a	363.16	8.19747	YES	YES
32	a	382.76	7.29179	YES	YES
33	a	396.14	2.14190	YES	YES
34	a	475.28	5.14664	YES	YES
35	a	522.11	11.59583	YES	YES
36	a	555.92	2.59179	YES	YES
37	a	569.20	5.09814	YES	YES
38	a	584.79	4.35354	YES	YES
39	a	591.40	5.87766	YES	YES
40	a	595.17	0.86949	YES	YES
41	a	605.70	4.37393	YES	YES
42	a	666.18	35.97985	YES	YES
43	a	670.44	77.13791	YES	YES
44	a	906.61	76.11244	YES	YES
45	a	935.76	26.88879	YES	YES
46	a	939.84	35.78176	YES	YES

47	a	948.27	13.55499	YES	YES
48	a	982.06	1.73380	YES	YES
49	a	989.47	18.79996	YES	YES
50	a	993.81	2.15154	YES	YES
51	a	1020.25	78.96529	YES	YES
52	a	1021.91	128.57258	YES	YES
53	a	1024.57	64.39114	YES	YES
54	a	1036.90	0.98291	YES	YES
55	a	1048.34	185.47243	YES	YES
56	a	1082.28	109.25781	YES	YES
57	a	1085.92	32.93858	YES	YES
58	a	1088.28	13.49293	YES	YES
59	a	1090.08	4.41159	YES	YES
60	a	1098.64	15.46966	YES	YES
61	a	1320.80	22.92600	YES	YES
62	a	1325.64	0.72152	YES	YES
63	a	1341.37	11.19538	YES	YES
64	a	1366.03	210.75131	YES	YES
65	a	1397.15	44.02797	YES	YES
66	a	1402.70	6.21159	YES	YES
67	a	1410.54	28.82277	YES	YES
68	a	1411.45	26.01407	YES	YES
69	a	1412.37	6.83494	YES	YES
70	a	1421.64	29.40493	YES	YES
71	a	1455.99	235.03729	YES	YES
72	a	1533.56	396.13052	YES	YES
73	a	1545.61	89.95263	YES	YES
74	a	1918.91	696.29029	YES	YES
75	a	2270.45	268.13706	YES	YES
76	a	2275.43	929.21356	YES	YES
77	a	2294.63	83.86219	YES	YES
78	a	2307.13	96.51098	YES	YES
79	a	2316.22	228.56322	YES	YES
80	a	2317.62	37.15407	YES	YES
81	a	2326.21	66.84772	YES	YES
82	a	2924.87	19.19823	YES	YES
83	a	2958.58	11.99777	YES	YES
84	a	2959.75	3.78652	YES	YES
85	a	3005.82	4.93557	YES	YES
86	a	3010.03	5.27741	YES	YES
87	a	3043.57	6.13205	YES	YES
88	a	3045.10	2.88768	YES	YES
89	a	3076.69	7.60901	YES	YES
90	a	3076.71	2.87155	YES	YES

* zero point VIBRATIONAL energy : 0.2067816 Hartree *

Cis TS_{34}_pfs



bp86_svp SCF energy = -1354.4882443120
pbe0_tzvpp SCF energy = -1354.264589950

xyz Coordinates

30

C	0.06596	-1.47053	-1.97266
C	0.46497	-2.16329	-3.25420
H	1.34660	-1.65094	-3.69910
H	-0.36462	-2.12375	-3.99001
H	0.74841	-3.21553	-3.04730
C	0.83716	0.05738	2.78323
C	1.05856	-0.35659	4.23053
H	0.15402	-0.85353	4.63538
H	1.32835	0.52293	4.85079
H	1.90693	-1.07524	4.27750
H	-2.29264	-2.93065	-0.32301
H	-3.66382	-1.36017	0.24279
H	-2.45711	-2.33182	1.76113
H	-2.01467	1.88360	2.10307
H	-1.45614	2.83782	0.23801
H	-3.23125	1.59934	0.34432
O	-0.76375	-0.49170	-1.98819
O	0.54781	-1.83842	-0.84659
O	-0.12396	-0.54278	2.17903
O	1.60160	0.92310	2.26340
P	-2.28690	-1.72456	0.46545
P	-1.83645	1.53265	0.70986
Ru	-0.58234	-0.24461	0.15593
C	1.01821	1.10292	-0.33244
C	1.48366	1.73833	-1.30165
C	1.97866	2.43610	-2.48027
H	1.33556	2.18211	-3.35632
H	3.02086	2.14211	-2.74414
H	1.95031	3.54423	-2.36651
H	1.31069	1.00789	0.89313

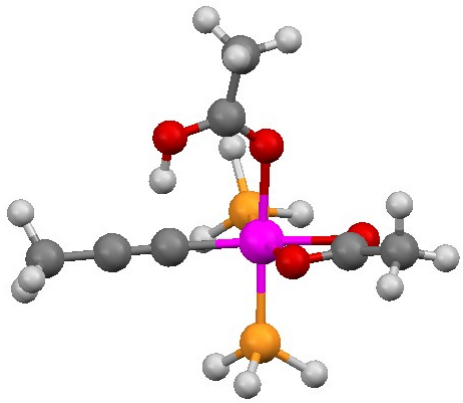
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-64.52	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	29.81	0.32952	YES	YES
9	a	43.76	0.93915	YES	YES
10	a	44.63	0.86456	YES	YES
11	a	59.39	1.30496	YES	YES
12	a	65.66	0.28161	YES	YES
13	a	69.57	1.76586	YES	YES
14	a	74.20	0.70933	YES	YES
15	a	79.57	4.35727	YES	YES
16	a	88.18	1.24223	YES	YES
17	a	101.97	0.77729	YES	YES
18	a	103.95	0.53006	YES	YES
19	a	129.88	5.86528	YES	YES
20	a	157.07	21.18262	YES	YES
21	a	170.42	22.56489	YES	YES
22	a	180.48	13.28840	YES	YES
23	a	190.99	0.79015	YES	YES
24	a	211.19	3.20156	YES	YES
25	a	249.81	66.30916	YES	YES
26	a	263.24	17.86005	YES	YES
27	a	292.36	5.51304	YES	YES
28	a	302.65	16.34932	YES	YES
29	a	330.48	34.70587	YES	YES
30	a	342.01	13.14902	YES	YES
31	a	375.44	3.64810	YES	YES
32	a	385.70	6.22129	YES	YES
33	a	438.47	14.21024	YES	YES
34	a	478.82	3.65197	YES	YES
35	a	522.87	81.68434	YES	YES
36	a	537.79	8.82565	YES	YES
37	a	553.53	8.45548	YES	YES
38	a	587.60	2.75045	YES	YES
39	a	592.84	4.98051	YES	YES
40	a	597.61	0.44467	YES	YES
41	a	606.42	6.14637	YES	YES
42	a	669.10	101.50579	YES	YES
43	a	671.91	95.34058	YES	YES
44	a	852.13	559.58859	YES	YES
45	a	922.58	15.71936	YES	YES

46	a	940.48	31.65853	YES	YES
47	a	980.01	14.42616	YES	YES
48	a	981.87	4.57791	YES	YES
49	a	989.49	30.77790	YES	YES
50	a	997.18	5.40831	YES	YES
51	a	1017.96	220.95943	YES	YES
52	a	1023.78	13.85315	YES	YES
53	a	1024.94	20.56744	YES	YES
54	a	1037.56	12.89490	YES	YES
55	a	1048.94	171.63469	YES	YES
56	a	1087.85	3.36170	YES	YES
57	a	1090.70	2.78498	YES	YES
58	a	1091.61	1.42122	YES	YES
59	a	1098.68	26.67348	YES	YES
60	a	1115.87	280.98975	YES	YES
61	a	1197.37	1003.08708	YES	YES
62	a	1326.73	2.75466	YES	YES
63	a	1328.19	3.39164	YES	YES
64	a	1351.64	11.52676	YES	YES
65	a	1391.11	142.23698	YES	YES
66	a	1399.38	36.08039	YES	YES
67	a	1401.80	2.11437	YES	YES
68	a	1410.28	32.55519	YES	YES
69	a	1413.32	7.05122	YES	YES
70	a	1415.20	4.54394	YES	YES
71	a	1428.88	63.19484	YES	YES
72	a	1457.03	257.67515	YES	YES
73	a	1544.26	59.65892	YES	YES
74	a	1696.23	638.22905	YES	YES
75	a	2082.72	99.97388	YES	YES
76	a	2265.42	123.86308	YES	YES
77	a	2300.83	85.14204	YES	YES
78	a	2316.02	124.92959	YES	YES
79	a	2318.45	180.84258	YES	YES
80	a	2323.39	42.84158	YES	YES
81	a	2333.93	64.99438	YES	YES
82	a	2916.26	38.19320	YES	YES
83	a	2960.82	4.66015	YES	YES
84	a	2961.44	9.23959	YES	YES
85	a	2990.29	9.70039	YES	YES
86	a	2998.79	4.76459	YES	YES
87	a	3046.47	2.92026	YES	YES
88	a	3047.35	4.42483	YES	YES
89	a	3074.92	2.96898	YES	YES
90	a	3078.10	5.08841	YES	YES

* zero point VIBRATIONAL energy : 0.2049132 Hartree *

Cis 4_af



bp86_svp SCF energy = -1354.5135977000
pbe0_tzvpp SCF energy = -1354.300621020

XYZ coordinates

	x	y	z
C	-2.48288	-0.19887	0.71027
C	-3.81261	-0.70017	1.22984
H	-3.85175	-1.80790	1.12878
H	-4.64718	-0.26611	0.64286
H	-3.92633	-0.45667	2.30667
C	0.46228	-2.61456	-0.25433
C	0.14186	-4.05826	-0.56021
H	-0.09969	-4.58957	0.38633
H	1.03159	-4.55966	-0.99819
H	-0.71653	-4.12342	-1.25552
H	-0.38463	2.69753	1.96760
H	-1.27027	3.43394	0.12961
H	0.88872	3.39997	0.35373
H	-0.00788	1.58095	-3.19486
H	1.90007	1.87057	-2.21343
H	1.34662	-0.08653	-2.94735
O	-2.36920	0.25154	-0.47728
O	-1.44125	-0.25061	1.46214
O	-0.23971	-1.69305	-0.72520
O	1.50321	-2.44135	0.52196
P	-0.23358	2.52110	0.54769
P	0.77599	0.96960	-2.14739
Ru	-0.16579	0.41151	-0.18984
C	1.67153	0.33644	0.56805
C	2.81278	0.31696	1.07062
C	4.13532	0.26049	1.69902
H	4.76433	-0.56093	1.28196
H	4.07207	0.09719	2.80070
H	4.70216	1.20822	1.54328
H	1.68885	-1.41767	0.66903

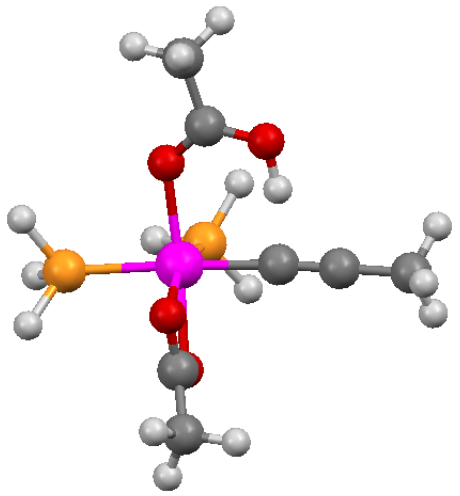
Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	29.20	0.14035	YES	YES
8	a	33.18	1.02861	YES	YES
9	a	43.65	0.68861	YES	YES
10	a	46.20	1.02699	YES	YES
11	a	50.63	0.29060	YES	YES
12	a	61.78	0.61209	YES	YES
13	a	65.65	0.06182	YES	YES
14	a	71.66	0.22305	YES	YES
15	a	78.43	1.35139	YES	YES
16	a	82.46	2.65463	YES	YES
17	a	118.55	0.59677	YES	YES
18	a	118.69	11.12076	YES	YES
19	a	129.01	4.32013	YES	YES
20	a	149.32	0.82719	YES	YES
21	a	161.77	0.75453	YES	YES
22	a	184.48	0.35295	YES	YES
23	a	201.33	1.17673	YES	YES
24	a	216.21	0.46576	YES	YES
25	a	239.29	3.19410	YES	YES
26	a	271.66	18.22590	YES	YES
27	a	275.38	3.03647	YES	YES
28	a	296.42	23.92694	YES	YES
29	a	364.14	11.55123	YES	YES
30	a	374.20	15.19723	YES	YES
31	a	383.99	8.86478	YES	YES
32	a	426.41	2.40594	YES	YES
33	a	444.40	6.61928	YES	YES
34	a	472.48	1.34464	YES	YES
35	a	485.21	20.99014	YES	YES
36	a	574.45	5.22833	YES	YES
37	a	587.68	1.15070	YES	YES
38	a	591.44	3.44906	YES	YES

39	a	602.19	1.65522	YES	YES
40	a	604.08	4.87077	YES	YES
41	a	617.64	7.08619	YES	YES
42	a	644.05	7.96132	YES	YES
43	a	672.28	76.85576	YES	YES
44	a	902.21	8.73544	YES	YES
45	a	917.18	36.83993	YES	YES
46	a	936.10	34.09400	YES	YES
47	a	982.40	3.16598	YES	YES
48	a	986.12	13.17912	YES	YES
49	a	998.74	4.68288	YES	YES
50	a	1015.30	4.06495	YES	YES
51	a	1020.49	0.70309	YES	YES
52	a	1026.08	3.93541	YES	YES
53	a	1029.28	5.46256	YES	YES
54	a	1033.96	261.08184	YES	YES
55	a	1062.10	154.27727	YES	YES
56	a	1088.78	6.09971	YES	YES
57	a	1093.07	13.94629	YES	YES
58	a	1099.45	6.27532	YES	YES
59	a	1104.77	5.92366	YES	YES
60	a	1267.46	68.17341	YES	YES
61	a	1325.15	2.37063	YES	YES
62	a	1331.54	2.47513	YES	YES
63	a	1365.38	26.58945	YES	YES
64	a	1399.50	33.17846	YES	YES
65	a	1405.62	32.08648	YES	YES
66	a	1410.31	43.76889	YES	YES
67	a	1414.06	8.82439	YES	YES
68	a	1414.81	8.34722	YES	YES
69	a	1418.69	6.65336	YES	YES
70	a	1433.53	136.13798	YES	YES
71	a	1447.59	325.74491	YES	YES
72	a	1551.94	87.07438	YES	YES
73	a	1648.35	345.45601	YES	YES
74	a	2104.38	103.02129	YES	YES
75	a	2297.87	51.57743	YES	YES
76	a	2305.16	163.27579	YES	YES
77	a	2307.71	25.64236	YES	YES
78	a	2310.38	163.17781	YES	YES
79	a	2336.80	66.68193	YES	YES
80	a	2337.79	54.76054	YES	YES
81	a	2459.67	1408.65884	YES	YES
82	a	2907.01	96.47022	YES	YES
83	a	2958.75	5.81084	YES	YES
84	a	2966.95	2.57307	YES	YES
85	a	2977.11	12.39493	YES	YES
86	a	2980.41	10.53302	YES	YES
87	a	3043.49	4.54592	YES	YES
88	a	3046.34	0.94253	YES	YES
89	a	3076.15	4.01296	YES	YES
90	a	3096.70	1.48847	YES	YES

zero point VIBRATIONAL energy : 0.2105305 Hartree

Cis 4_pf



bp86_svp SCF energy = -1354.4980697700
pbe0_tzvpp SCF energy = -1354.282924480

xyz Coordinates

30

C	-2.16760	-0.93947	0.99978
C	-3.25214	-1.77106	1.63789
H	-2.92511	-2.83461	1.66434
H	-4.18862	-1.71370	1.04591
H	-3.42981	-1.43895	2.68130
C	2.51716	0.76386	0.95322
C	3.57367	1.63976	1.58112
H	4.57396	1.38935	1.16779
H	3.61204	1.43991	2.67500
H	3.34144	2.70835	1.41057
H	-0.83153	3.41408	0.74447
H	-2.70602	2.35515	0.66132
H	-1.80359	3.08749	-1.14191
H	-0.24139	-0.50354	-3.25695
H	-0.17877	1.65604	-3.12375
H	1.61443	0.50378	-2.78670
O	-2.15020	-0.76279	-0.27413
O	-1.22882	-0.41936	1.69178
O	1.47253	1.27526	0.48300
O	2.78211	-0.51689	0.96656
P	-1.41711	2.31533	0.01487
P	0.23654	0.50661	-2.35136
Ru	-0.28932	0.26670	-0.18766
C	0.59944	-1.54996	-0.34113
C	1.06999	-2.69547	-0.47183
C	1.62308	-4.04516	-0.60137
H	1.04966	-4.64530	-1.34592
H	1.59111	-4.60562	0.36192
H	2.68482	-4.03407	-0.94198
H	1.99579	-1.05933	0.51125

Vibrational Spectrum

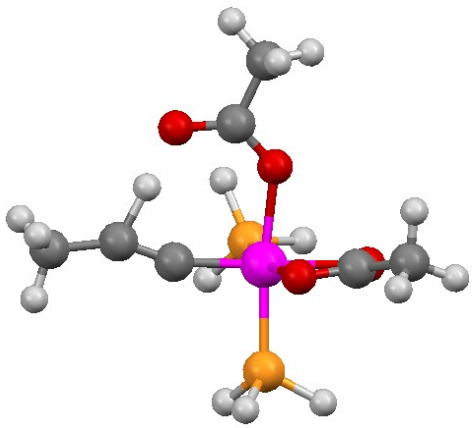
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	30.09	0.09810	YES	YES
8	a	35.39	0.49651	YES	YES
9	a	49.20	0.50530	YES	YES
10	a	53.35	1.21481	YES	YES
11	a	54.49	0.91834	YES	YES
12	a	61.38	0.21414	YES	YES
13	a	67.03	0.46791	YES	YES
14	a	68.94	0.90731	YES	YES
15	a	76.41	1.65230	YES	YES
16	a	85.96	3.23169	YES	YES
17	a	101.95	4.69806	YES	YES
18	a	108.98	1.63718	YES	YES
19	a	120.50	3.56762	YES	YES
20	a	162.25	0.36150	YES	YES
21	a	177.48	1.34831	YES	YES
22	a	186.42	1.62099	YES	YES
23	a	200.91	0.46761	YES	YES
24	a	220.24	1.56031	YES	YES
25	a	245.65	0.86625	YES	YES
26	a	282.05	17.77525	YES	YES
27	a	297.11	17.00601	YES	YES
28	a	299.00	14.28841	YES	YES
29	a	322.43	13.40860	YES	YES
30	a	339.07	3.86083	YES	YES
31	a	380.75	9.98486	YES	YES
32	a	406.21	1.41886	YES	YES
33	a	411.53	6.88310	YES	YES
34	a	483.57	5.56749	YES	YES
35	a	485.34	12.55053	YES	YES
36	a	517.32	4.56456	YES	YES
37	a	527.41	8.37012	YES	YES
38	a	586.75	0.19891	YES	YES
39	a	592.02	5.70747	YES	YES
40	a	595.10	1.95894	YES	YES
41	a	609.27	7.62452	YES	YES
42	a	648.64	7.54816	YES	YES
43	a	674.26	63.31715	YES	YES
44	a	902.61	11.02536	YES	YES
45	a	913.05	32.94522	YES	YES
46	a	941.77	27.50351	YES	YES
47	a	980.13	1.95008	YES	YES
48	a	981.64	1.63069	YES	YES

49	a	999.69	1.14042	YES	YES
50	a	1013.58	9.46547	YES	YES
51	a	1021.87	61.39247	YES	YES
52	a	1022.62	124.16885	YES	YES
53	a	1024.31	56.87103	YES	YES
54	a	1026.51	25.62394	YES	YES
55	a	1055.58	186.74299	YES	YES
56	a	1093.42	2.40554	YES	YES
57	a	1096.36	11.28236	YES	YES
58	a	1097.57	3.22535	YES	YES
59	a	1098.96	10.78416	YES	YES
60	a	1248.68	56.74031	YES	YES
61	a	1326.87	1.42816	YES	YES
62	a	1332.09	2.52584	YES	YES
63	a	1363.69	23.83520	YES	YES
64	a	1399.41	36.62930	YES	YES
65	a	1405.61	34.09124	YES	YES
66	a	1408.61	29.82226	YES	YES
67	a	1411.95	32.28742	YES	YES
68	a	1413.62	3.41133	YES	YES
69	a	1417.60	8.16385	YES	YES
70	a	1429.38	127.04552	YES	YES
71	a	1458.60	273.38561	YES	YES
72	a	1544.02	63.53686	YES	YES
73	a	1631.81	269.48297	YES	YES
74	a	2110.09	55.56241	YES	YES
75	a	2284.99	103.34149	YES	YES
76	a	2286.99	117.24785	YES	YES
77	a	2305.19	208.02719	YES	YES
78	a	2307.64	58.39677	YES	YES
79	a	2314.45	65.82680	YES	YES
80	a	2337.32	48.53687	YES	YES
81	a	2351.70	1398.58235	YES	YES
82	a	2912.16	85.58884	YES	YES
83	a	2959.51	4.02950	YES	YES
84	a	2964.25	5.67727	YES	YES
85	a	2984.81	10.47209	YES	YES
86	a	2986.90	9.24914	YES	YES
87	a	3043.65	1.43867	YES	YES
88	a	3045.18	3.17972	YES	YES
89	a	3075.70	3.33871	YES	YES
90	a	3094.09	1.99102	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2095703 Hartree

Cis TS_{45}_af



bp86_svp SCF energy = -1354.5027943630
pbe0_tzvpp SCF energy = -1354.279073699

xyz Coordinates

30

C	-2.69352	0.01916	0.33634
C	-3.99997	-0.61249	0.75859
H	-3.91837	-1.71642	0.64338
H	-4.82831	-0.25996	0.11064
H	-4.21567	-0.39377	1.82434
C	0.65986	-2.18277	-0.36189
C	0.28302	-3.63067	-0.66168
H	-0.29519	-4.03414	0.19989
H	1.19640	-4.24839	-0.77961
H	-0.35720	-3.69824	-1.56461
H	-1.03283	3.34845	1.41087
H	-2.04675	3.53317	-0.49802
H	0.05784	4.02586	-0.33328
H	-0.03184	1.34104	-3.53892
H	1.59485	2.30972	-2.48579
H	1.63622	0.16698	-2.79522
O	-2.49684	0.36882	-0.87657
O	-1.75189	0.18179	1.19432
O	-0.20817	-1.30983	-0.72561
O	1.76383	-1.97874	0.22418
P	-0.83823	2.96327	0.03866
P	0.72260	1.17429	-2.32283
Ru	-0.36422	0.77946	-0.39019
C	1.30728	0.87386	0.51098
C	2.39625	0.51816	1.07720
C	3.59969	0.74123	1.91700
H	3.56825	0.12208	2.84189
H	3.68301	1.80693	2.22379
H	4.53394	0.46762	1.37601
H	2.07677	-0.67611	0.64682

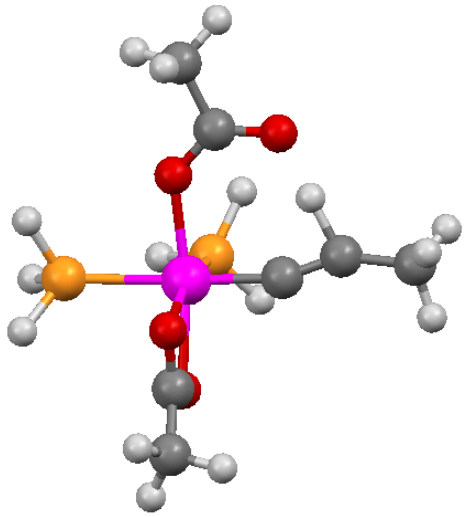
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-395.57	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	34.37	0.42071	YES	YES
9	a	46.92	0.05053	YES	YES
10	a	51.40	0.14091	YES	YES
11	a	58.22	0.81713	YES	YES
12	a	62.30	1.05215	YES	YES
13	a	72.17	4.65376	YES	YES
14	a	74.98	0.32982	YES	YES
15	a	77.89	0.31475	YES	YES
16	a	80.02	1.46807	YES	YES
17	a	98.81	7.58969	YES	YES
18	a	107.32	1.24250	YES	YES
19	a	121.80	6.09344	YES	YES
20	a	138.00	4.34923	YES	YES
21	a	163.79	0.91654	YES	YES
22	a	174.42	2.45139	YES	YES
23	a	193.35	0.58742	YES	YES
24	a	209.63	0.12837	YES	YES
25	a	249.68	62.20200	YES	YES
26	a	258.65	90.46534	YES	YES
27	a	275.44	16.51921	YES	YES
28	a	301.52	18.70259	YES	YES
29	a	354.88	6.39158	YES	YES
30	a	368.26	22.59270	YES	YES
31	a	375.25	11.37358	YES	YES
32	a	444.06	1.92281	YES	YES
33	a	453.32	104.60832	YES	YES
34	a	478.42	3.73246	YES	YES
35	a	547.44	70.41594	YES	YES
36	a	570.17	23.56551	YES	YES
37	a	575.13	52.46993	YES	YES
38	a	586.12	1.33872	YES	YES
39	a	586.81	17.58052	YES	YES
40	a	591.81	23.96409	YES	YES
41	a	602.37	3.83013	YES	YES
42	a	626.94	17.98837	YES	YES
43	a	675.71	78.41122	YES	YES
44	a	689.46	47.85139	YES	YES
45	a	923.51	18.41794	YES	YES
46	a	929.51	10.13903	YES	YES
47	a	937.33	31.42642	YES	YES
48	a	982.86	2.38422	YES	YES
49	a	987.18	108.91422	YES	YES
50	a	999.61	26.10015	YES	YES

51	a	1000.39	11.64392	YES	YES
52	a	1021.85	13.54171	YES	YES
53	a	1026.60	41.88610	YES	YES
54	a	1030.35	247.54410	YES	YES
55	a	1034.57	14.29295	YES	YES
56	a	1056.05	156.74288	YES	YES
57	a	1092.50	4.67280	YES	YES
58	a	1093.86	3.97465	YES	YES
59	a	1100.24	7.10196	YES	YES
60	a	1103.93	5.17956	YES	YES
61	a	1322.15	10.65260	YES	YES
62	a	1325.17	0.41388	YES	YES
63	a	1330.64	97.23513	YES	YES
64	a	1362.52	2.03514	YES	YES
65	a	1395.88	261.20616	YES	YES
66	a	1399.45	42.05473	YES	YES
67	a	1405.94	17.36952	YES	YES
68	a	1409.75	51.01248	YES	YES
69	a	1415.88	8.06530	YES	YES
70	a	1424.72	52.78704	YES	YES
71	a	1429.46	82.80081	YES	YES
72	a	1453.68	339.56286	YES	YES
73	a	1544.85	78.27262	YES	YES
74	a	1698.99	812.60706	YES	YES
75	a	1960.14	202.41037	YES	YES
76	a	2318.12	88.36029	YES	YES
77	a	2324.97	83.73155	YES	YES
78	a	2330.35	110.85189	YES	YES
79	a	2333.05	74.10266	YES	YES
80	a	2337.87	57.48225	YES	YES
81	a	2340.90	55.88599	YES	YES
82	a	2930.47	75.53213	YES	YES
83	a	2959.17	6.31200	YES	YES
84	a	2960.93	3.81614	YES	YES
85	a	3000.94	9.19154	YES	YES
86	a	3020.86	8.79701	YES	YES
87	a	3045.79	6.58326	YES	YES
88	a	3047.02	4.07513	YES	YES
89	a	3077.40	3.57880	YES	YES
90	a	3078.93	6.70252	YES	YES

* zero point VIBRATIONAL energy : 0.2064818 Hartree *

Cis TS_{45}_pf



bp86_svp SCF energy = -1354.4854376840
pbe0_tzvpp SCF energy = -1354.259630170

xyz Coordinates

30

C	-2.59461	-0.71581	0.72113
C	-3.76026	-1.48304	1.29639
H	-3.51472	-2.56875	1.30229
H	-4.66807	-1.33899	0.67553
H	-3.94962	-1.17001	2.34358
C	2.26665	1.01087	0.76627
C	3.10157	2.01732	1.55435
H	2.86749	3.05807	1.25035
H	4.18178	1.80563	1.42166
H	2.85874	1.91520	2.63610
H	-1.99172	3.48912	-1.06697
H	-1.04104	3.51791	0.86685
H	-2.99380	2.62034	0.62035
H	-0.25744	-0.07603	-3.47996
H	-0.44059	2.05512	-3.15770
H	1.44090	1.06416	-2.76761
O	-2.53210	-0.48515	-0.54326
O	-1.63708	-0.30829	1.45916
O	1.09227	1.42442	0.44533
O	2.78619	-0.11711	0.52531
P	-1.69353	2.57242	0.00458
P	0.04195	0.88978	-2.45666
Ru	-0.59882	0.44132	-0.35564
C	0.33118	-1.23197	-0.52387
C	1.24541	-2.12185	-0.46801
C	1.77990	-3.49818	-0.61603
H	1.01720	-4.17725	-1.05603
H	2.08725	-3.91906	0.36806
H	2.67902	-3.51840	-1.27233
H	1.97084	-1.15222	0.00342

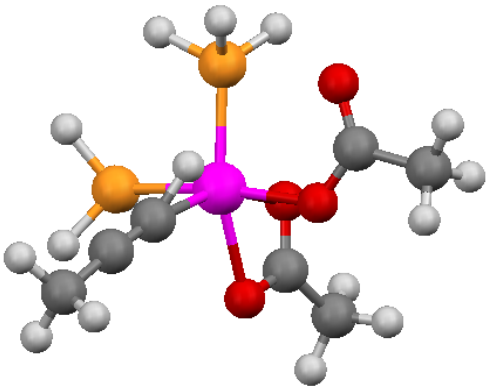
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-395.58	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	28.96	0.22375	YES	YES
9	a	36.28	0.41086	YES	YES
10	a	42.74	0.13236	YES	YES
11	a	52.75	0.55897	YES	YES
12	a	65.67	1.79846	YES	YES
13	a	67.08	0.31672	YES	YES
14	a	69.08	2.80254	YES	YES
15	a	78.04	1.42856	YES	YES
16	a	86.85	0.62218	YES	YES
17	a	89.92	0.70666	YES	YES
18	a	103.51	10.15289	YES	YES
19	a	111.03	2.43863	YES	YES
20	a	143.44	1.54055	YES	YES
21	a	159.73	3.34170	YES	YES
22	a	173.26	0.82683	YES	YES
23	a	188.32	5.23527	YES	YES
24	a	210.09	0.95221	YES	YES
25	a	235.38	14.49543	YES	YES
26	a	250.03	16.52110	YES	YES
27	a	290.36	32.69960	YES	YES
28	a	297.57	64.52895	YES	YES
29	a	314.46	37.60134	YES	YES
30	a	364.36	13.76906	YES	YES
31	a	376.79	12.18431	YES	YES
32	a	410.96	0.74505	YES	YES
33	a	439.10	80.28851	YES	YES
34	a	455.81	91.48336	YES	YES
35	a	478.05	15.00289	YES	YES
36	a	503.94	4.90646	YES	YES
37	a	571.33	85.65119	YES	YES
38	a	575.50	21.81672	YES	YES
39	a	583.78	0.46724	YES	YES
40	a	595.78	9.81932	YES	YES
41	a	599.96	2.76267	YES	YES
42	a	614.40	1.06868	YES	YES
43	a	673.21	77.35122	YES	YES
44	a	694.33	58.64862	YES	YES
45	a	912.95	21.62724	YES	YES
46	a	928.55	5.29712	YES	YES
47	a	940.58	29.60758	YES	YES
48	a	981.50	5.64428	YES	YES

49	a	984.25	58.00193	YES	YES
50	a	994.67	30.54011	YES	YES
51	a	999.65	1.42381	YES	YES
52	a	1010.51	247.95113	YES	YES
53	a	1019.63	14.33674	YES	YES
54	a	1026.49	15.98631	YES	YES
55	a	1032.77	1.72317	YES	YES
56	a	1054.79	177.96903	YES	YES
57	a	1093.31	9.41384	YES	YES
58	a	1094.90	8.99226	YES	YES
59	a	1100.91	7.07553	YES	YES
60	a	1102.61	9.25791	YES	YES
61	a	1321.51	9.55433	YES	YES
62	a	1327.48	9.37863	YES	YES
63	a	1332.21	85.25333	YES	YES
64	a	1361.18	2.70793	YES	YES
65	a	1389.81	311.92695	YES	YES
66	a	1398.47	38.79934	YES	YES
67	a	1406.07	15.11021	YES	YES
68	a	1409.61	31.62862	YES	YES
69	a	1416.15	7.64060	YES	YES
70	a	1422.51	35.43622	YES	YES
71	a	1427.34	63.44520	YES	YES
72	a	1455.77	281.90010	YES	YES
73	a	1545.73	68.91211	YES	YES
74	a	1707.34	755.52878	YES	YES
75	a	1958.55	150.82005	YES	YES
76	a	2296.47	96.42561	YES	YES
77	a	2307.39	80.38700	YES	YES
78	a	2324.63	154.60546	YES	YES
79	a	2336.83	83.09743	YES	YES
80	a	2340.59	58.90703	YES	YES
81	a	2367.14	33.53824	YES	YES
82	a	2932.87	68.45269	YES	YES
83	a	2958.24	8.13474	YES	YES
84	a	2959.51	3.37018	YES	YES
85	a	3004.76	8.11908	YES	YES
86	a	3024.48	7.76559	YES	YES
87	a	3044.51	6.74447	YES	YES
88	a	3045.14	2.83768	YES	YES
89	a	3077.34	2.87955	YES	YES
90	a	3077.75	6.83779	YES	YES

* zero point VIBRATIONAL energy : 0.2055126 Hartree *

Cis 3_afx



bp86_svp SCF energy = -1354.4893539830
pbe0_tzvpp SCF energy = -1354.268470165

xyz Coordinates

30

C	-2.23961	-0.76453	-0.73656
C	-3.41334	-1.35786	-1.47051
H	-3.03290	-1.97196	-2.31703
H	-4.06074	-0.55873	-1.88588
H	-3.99366	-2.02149	-0.79760
C	1.45933	-0.54027	-2.24531
C	1.82511	-1.52993	-3.34923
H	2.77579	-1.22811	-3.83328
H	1.02308	-1.52111	-4.12135
H	1.89936	-2.56317	-2.95239
H	-1.43853	0.58221	3.11618
H	-2.51067	1.75792	1.63559
H	-0.64412	2.48901	2.45307
H	0.73843	3.22013	0.40974
H	2.43088	2.27376	-0.51253
H	0.59056	2.70675	-1.68613
O	-1.76381	0.38231	-1.09022
O	-1.66680	-1.37657	0.22179
O	0.66048	-1.01929	-1.34166
O	1.90021	0.62734	-2.27913
P	-1.17568	1.27650	1.88525
P	1.01449	2.09224	-0.46913
Ru	-0.09637	0.18694	0.19654
C	1.07984	-0.64451	1.70791
C	1.53271	-1.25281	2.69199
C	1.99698	-2.02347	3.83904
H	1.14235	-2.34539	4.47934
H	2.68721	-1.43381	4.48578
H	2.53536	-2.94664	3.52325
H	1.57783	-0.01756	0.82577

Vibrational Spectrum

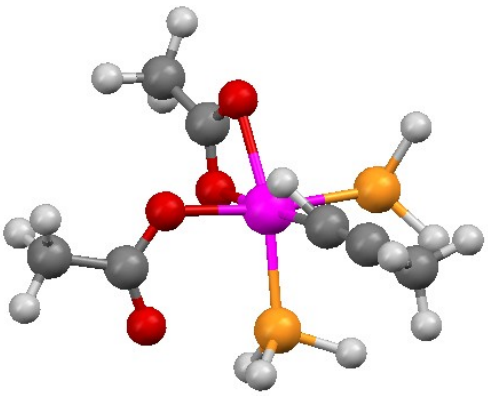
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.84	0.13960	YES	YES
8	a	29.55	0.12119	YES	YES
9	a	29.93	0.49585	YES	YES
10	a	38.15	0.73625	YES	YES
11	a	55.78	1.99099	YES	YES
12	a	63.96	0.87802	YES	YES
13	a	67.79	0.20766	YES	YES
14	a	72.10	0.19974	YES	YES
15	a	87.30	0.20359	YES	YES
16	a	99.65	6.91576	YES	YES
17	a	112.37	9.49931	YES	YES
18	a	151.08	6.05469	YES	YES
19	a	165.26	2.73640	YES	YES
20	a	183.48	1.32983	YES	YES
21	a	193.49	14.73439	YES	YES
22	a	199.79	1.70989	YES	YES
23	a	213.38	3.31499	YES	YES
24	a	231.94	1.38968	YES	YES
25	a	274.33	21.13292	YES	YES
26	a	285.74	18.16383	YES	YES
27	a	303.53	11.43941	YES	YES
28	a	337.54	13.31358	YES	YES
29	a	354.96	20.07020	YES	YES
30	a	363.28	15.27579	YES	YES
31	a	387.16	0.44166	YES	YES
32	a	401.70	3.98122	YES	YES
33	a	422.91	3.84617	YES	YES
34	a	427.85	39.36578	YES	YES
35	a	484.51	4.32136	YES	YES
36	a	509.68	0.21209	YES	YES
37	a	559.60	1.27303	YES	YES
38	a	571.44	12.48355	YES	YES
39	a	585.72	7.52626	YES	YES
40	a	595.17	2.06869	YES	YES
41	a	606.60	5.98340	YES	YES
42	a	648.44	12.20018	YES	YES
43	a	675.11	52.25363	YES	YES
44	a	681.16	70.32187	YES	YES
45	a	933.56	3.78101	YES	YES
46	a	941.85	29.64560	YES	YES
47	a	961.48	97.06532	YES	YES
48	a	982.35	1.08463	YES	YES
49	a	992.03	1.38095	YES	YES
50	a	1002.36	103.02759	YES	YES
51	a	1005.42	24.01639	YES	YES

52	a	1018.78	2.37379	YES	YES
53	a	1022.62	6.60995	YES	YES
54	a	1025.74	6.18166	YES	YES
55	a	1029.26	159.87978	YES	YES
56	a	1081.28	93.75935	YES	YES
57	a	1093.58	3.04952	YES	YES
58	a	1096.30	11.18405	YES	YES
59	a	1133.29	11.66868	YES	YES
60	a	1208.32	329.23172	YES	YES
61	a	1316.96	40.98679	YES	YES
62	a	1328.53	0.99464	YES	YES
63	a	1360.36	43.85934	YES	YES
64	a	1364.68	284.20838	YES	YES
65	a	1396.66	42.05549	YES	YES
66	a	1406.81	2.81333	YES	YES
67	a	1407.16	26.20625	YES	YES
68	a	1408.62	35.75425	YES	YES
69	a	1411.56	8.72567	YES	YES
70	a	1421.07	25.16575	YES	YES
71	a	1457.52	274.07688	YES	YES
72	a	1542.66	79.91300	YES	YES
73	a	1636.49	246.74445	YES	YES
74	a	2041.83	83.88285	YES	YES
75	a	2214.25	194.44611	YES	YES
76	a	2322.74	109.10849	YES	YES
77	a	2324.76	117.01330	YES	YES
78	a	2329.37	48.46437	YES	YES
79	a	2348.95	60.29704	YES	YES
80	a	2390.96	62.82450	YES	YES
81	a	2412.42	18.77943	YES	YES
82	a	2916.72	57.59255	YES	YES
83	a	2957.48	10.92897	YES	YES
84	a	2962.58	1.76024	YES	YES
85	a	2989.90	5.69546	YES	YES
86	a	2997.96	4.78012	YES	YES
87	a	3043.68	7.78498	YES	YES
88	a	3049.23	2.44166	YES	YES
89	a	3077.27	7.40492	YES	YES
90	a	3079.35	2.10188	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2094206 Hartree

Cis 3_afy



bp86_svp SCF energy = -1354.4890982660
pbe0_tzvpp SCF energy = -1354.266529307

xyz Coordinates

30

C	-1.43841	0.32692	2.14888
C	-1.94581	0.49923	3.55695
H	-1.12930	0.92058	4.18490
H	-2.24465	-0.47809	3.98802
H	-2.79626	1.21118	3.57568
C	2.32414	0.17650	1.33376
C	3.26721	0.86020	2.32236
H	4.28028	0.41516	2.25503
H	2.88357	0.70161	3.35512
H	3.30945	1.95460	2.14425
H	-3.19089	0.28890	-1.50890
H	-3.09333	-1.55244	-0.37018
H	-2.15627	-1.43052	-2.32537
H	0.39184	-2.30679	-2.05453
H	2.29108	-1.47027	-1.49576
H	1.18638	-2.83675	-0.11094
O	-0.87559	-0.77405	1.78824
O	-1.52449	1.26690	1.28868
O	1.28017	0.88505	1.02012
O	2.57395	-0.97120	0.91735
P	-2.20898	-0.67949	-1.09899
P	1.00817	-1.66378	-0.90498
Ru	-0.29647	0.04333	-0.08471
C	0.17154	0.81333	-1.99541
C	0.40519	1.05728	-3.19463
C	0.68797	1.31175	-4.60177
H	1.23582	0.46168	-5.07146
H	1.33043	2.21489	-4.72555
H	-0.24076	1.48148	-5.19377
H	0.11872	1.51159	-1.04358

Vibrational Spectrum

mode symmetry wave number IR intensity selection rules

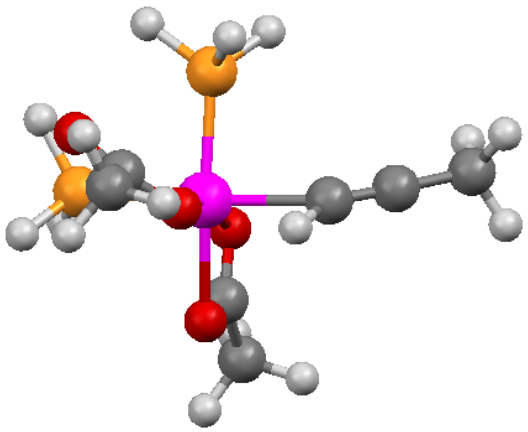
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.80	0.09500	YES	YES
8	a	27.31	0.46913	YES	YES
9	a	44.53	0.59835	YES	YES
10	a	53.67	1.17637	YES	YES
11	a	54.86	0.53770	YES	YES
12	a	71.80	0.52730	YES	YES
13	a	76.95	0.37279	YES	YES
14	a	79.67	0.66197	YES	YES
15	a	97.60	4.59579	YES	YES
16	a	108.70	1.99412	YES	YES
17	a	115.47	6.48175	YES	YES
18	a	152.32	9.87557	YES	YES
19	a	159.03	3.84708	YES	YES
20	a	183.93	6.52780	YES	YES
21	a	191.25	1.56218	YES	YES
22	a	204.03	8.56064	YES	YES
23	a	209.19	2.97754	YES	YES
24	a	232.63	0.51691	YES	YES
25	a	271.41	30.52687	YES	YES
26	a	279.45	22.13817	YES	YES
27	a	293.49	5.36578	YES	YES
28	a	334.51	16.83758	YES	YES
29	a	343.82	1.70602	YES	YES
30	a	371.93	13.08367	YES	YES
31	a	378.35	2.17973	YES	YES
32	a	400.57	0.51896	YES	YES
33	a	418.87	22.30991	YES	YES
34	a	434.91	14.24273	YES	YES
35	a	488.67	1.98821	YES	YES
36	a	508.89	0.44596	YES	YES
37	a	554.39	2.99760	YES	YES
38	a	575.32	10.13124	YES	YES
39	a	589.90	2.13232	YES	YES
40	a	596.18	2.46883	YES	YES
41	a	607.55	6.72925	YES	YES
42	a	646.16	11.28370	YES	YES
43	a	672.40	43.44316	YES	YES
44	a	679.47	75.50489	YES	YES
45	a	931.55	4.38778	YES	YES
46	a	940.51	21.75127	YES	YES
47	a	960.37	60.39094	YES	YES
48	a	982.14	0.74578	YES	YES
49	a	991.55	1.69777	YES	YES
50	a	1000.08	88.82053	YES	YES
51	a	1004.68	15.35665	YES	YES
52	a	1015.74	13.88327	YES	YES

53	a	1022.11	5.59184	YES	YES
54	a	1026.41	4.55446	YES	YES
55	a	1030.67	181.10694	YES	YES
56	a	1076.37	73.42197	YES	YES
57	a	1094.73	3.71159	YES	YES
58	a	1100.14	6.00768	YES	YES
59	a	1140.16	7.17616	YES	YES
60	a	1203.50	365.88775	YES	YES
61	a	1315.80	58.95352	YES	YES
62	a	1327.90	1.29942	YES	YES
63	a	1358.16	250.58721	YES	YES
64	a	1360.62	56.71507	YES	YES
65	a	1397.01	39.69224	YES	YES
66	a	1407.37	20.59562	YES	YES
67	a	1407.55	30.53891	YES	YES
68	a	1407.85	17.39722	YES	YES
69	a	1408.77	10.44699	YES	YES
70	a	1420.77	20.72049	YES	YES
71	a	1460.01	314.87467	YES	YES
72	a	1535.95	78.14741	YES	YES
73	a	1643.38	227.07541	YES	YES
74	a	2041.10	47.67929	YES	YES
75	a	2228.94	164.71608	YES	YES
76	a	2328.97	144.80420	YES	YES
77	a	2337.45	31.32037	YES	YES
78	a	2339.39	48.27762	YES	YES
79	a	2380.09	110.78640	YES	YES
80	a	2405.31	46.27384	YES	YES
81	a	2429.48	21.18588	YES	YES
82	a	2915.33	55.44161	YES	YES
83	a	2958.38	11.81476	YES	YES
84	a	2961.69	2.02564	YES	YES
85	a	2988.58	3.58233	YES	YES
86	a	2995.38	6.32519	YES	YES
87	a	3043.93	8.07599	YES	YES
88	a	3048.21	2.39025	YES	YES
89	a	3076.57	8.01858	YES	YES
90	a	3078.16	2.47306	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2097163 Hartree

Cis 3_pftx



bp86_svp SCF energy = -1354.4850478560
pbe0_tzvpp SCF energy = -1354.263821880

xyz Coordinates

30

C	-1.68297	-0.38683	-1.97606
C	-2.56295	-0.64263	-3.17564
H	-1.97561	-1.18278	-3.95163
H	-2.91939	0.31351	-3.60981
H	-3.42166	-1.28618	-2.89365
C	0.47373	-0.80033	2.75346
C	0.95121	-1.81636	3.78783
H	0.07770	-2.41284	4.13519
H	1.36887	-1.28832	4.66974
H	1.69971	-2.51592	3.36322
H	-2.48149	0.10874	2.12273
H	-2.89191	1.32117	0.36492
H	-1.61055	2.12054	1.92814
H	0.85231	2.71954	1.46624
H	2.50138	1.31036	1.40505
H	1.98779	2.44777	-0.36507
O	-1.06668	0.72877	-1.84099
O	-1.50791	-1.28958	-1.08432
O	0.59737	-1.19532	1.51763
O	-0.01813	0.28963	3.10799
P	-1.76871	0.91323	1.17784
P	1.32930	1.64719	0.63540
Ru	-0.06471	0.01417	-0.05140
C	1.51748	-0.55909	-1.46036
C	2.24286	-0.41782	-2.45831
C	3.04028	-0.15589	-3.64751
H	2.78574	0.84109	-4.07837
H	2.85544	-0.91413	-4.44260
H	4.13172	-0.15279	-3.42450
H	1.28149	-1.30508	-0.64202

Vibrational Spectrum

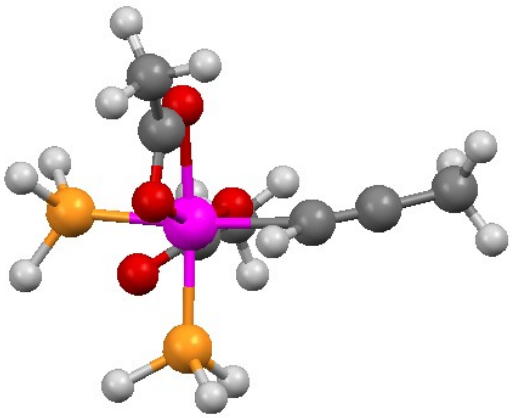
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	28.35	0.51890	YES	YES
8	a	38.76	0.34413	YES	YES
9	a	40.83	0.85527	YES	YES
10	a	48.19	0.52069	YES	YES
11	a	52.94	0.79451	YES	YES
12	a	65.42	0.51648	YES	YES
13	a	70.51	2.25346	YES	YES
14	a	72.75	6.27694	YES	YES
15	a	97.36	3.98090	YES	YES
16	a	111.88	5.86282	YES	YES
17	a	138.75	4.22022	YES	YES
18	a	158.31	4.92021	YES	YES
19	a	171.14	2.67675	YES	YES
20	a	173.79	8.46381	YES	YES
21	a	182.12	0.26247	YES	YES
22	a	192.57	2.79191	YES	YES
23	a	201.43	2.36402	YES	YES
24	a	214.66	6.27673	YES	YES
25	a	255.56	2.58420	YES	YES
26	a	269.13	2.58469	YES	YES
27	a	293.35	5.87125	YES	YES
28	a	306.37	11.94007	YES	YES
29	a	326.74	23.61699	YES	YES
30	a	336.01	38.25212	YES	YES
31	a	355.29	17.30159	YES	YES
32	a	381.65	8.23539	YES	YES
33	a	394.64	11.90685	YES	YES
34	a	454.05	32.84867	YES	YES
35	a	476.89	4.29920	YES	YES
36	a	507.12	2.24255	YES	YES
37	a	565.27	17.75080	YES	YES
38	a	589.53	8.41528	YES	YES
39	a	596.27	2.67115	YES	YES
40	a	602.02	2.99518	YES	YES
41	a	608.41	5.10023	YES	YES
42	a	616.28	3.26277	YES	YES
43	a	671.73	104.17404	YES	YES
44	a	674.64	11.39671	YES	YES
45	a	916.11	304.56036	YES	YES
46	a	936.63	79.18061	YES	YES
47	a	941.64	28.10274	YES	YES
48	a	955.77	15.58257	YES	YES
49	a	981.06	1.66433	YES	YES
50	a	988.76	6.57603	YES	YES

51	a	1004.12	10.57826	YES	YES
52	a	1016.14	145.54548	YES	YES
53	a	1020.75	1.83826	YES	YES
54	a	1022.18	40.34322	YES	YES
55	a	1026.03	18.90287	YES	YES
56	a	1051.90	107.51151	YES	YES
57	a	1066.18	25.56164	YES	YES
58	a	1081.01	7.24528	YES	YES
59	a	1105.01	11.00719	YES	YES
60	a	1113.44	6.61969	YES	YES
61	a	1315.23	88.06442	YES	YES
62	a	1326.65	0.95982	YES	YES
63	a	1348.84	228.92775	YES	YES
64	a	1355.54	12.65611	YES	YES
65	a	1399.06	37.35892	YES	YES
66	a	1402.12	4.11030	YES	YES
67	a	1409.52	25.49698	YES	YES
68	a	1409.81	31.85831	YES	YES
69	a	1409.93	7.02790	YES	YES
70	a	1420.74	18.64268	YES	YES
71	a	1456.69	268.37819	YES	YES
72	a	1541.57	86.12907	YES	YES
73	a	1633.94	174.16860	YES	YES
74	a	2057.42	5.45546	YES	YES
75	a	2296.39	144.05498	YES	YES
76	a	2307.40	80.45481	YES	YES
77	a	2322.77	102.10919	YES	YES
78	a	2344.04	52.54155	YES	YES
79	a	2382.88	85.88742	YES	YES
80	a	2398.92	20.81205	YES	YES
81	a	2816.43	172.37345	YES	YES
82	a	2920.53	42.49607	YES	YES
83	a	2956.43	12.89965	YES	YES
84	a	2959.70	3.79480	YES	YES
85	a	2995.32	4.47590	YES	YES
86	a	3005.38	3.05266	YES	YES
87	a	3041.68	6.86859	YES	YES
88	a	3045.06	2.83626	YES	YES
89	a	3073.25	6.99542	YES	YES
90	a	3077.44	2.87738	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2095872 Hartree

Cis 3_pfty



bp86_svp SCF energy = -1354.4808423120
pbe0_tzvpp SCF energy = -1354.260986334

xyz Coordinates

30

C	-0.65599	-0.54166	-2.85975
C	-0.66370	-0.99429	-4.29970
H	0.35157	-0.85043	-4.73336
H	-1.38504	-0.39867	-4.89468
H	-0.90496	-2.07553	-4.36173
C	-0.50332	-0.54949	2.37075
C	0.15637	-1.21487	3.57649
H	-0.52182	-1.99638	3.98201
H	0.29367	-0.45772	4.37969
H	1.13709	-1.66229	3.31955
H	-2.73315	-1.72981	0.67244
H	-3.31054	-0.80143	-1.20397
H	-3.58938	0.29831	0.65142
H	-2.30604	2.50967	1.10081
H	-0.29862	2.48988	1.93858
H	-0.67704	3.48209	0.05472
O	-1.03047	0.64996	-2.54813
O	-0.24221	-1.30913	-1.92748
O	0.22787	-0.52678	1.29679
O	-1.65755	-0.07768	2.46632
P	-2.57791	-0.47649	0.00007
P	-0.96143	2.21617	0.68902
Ru	-0.50011	0.33312	-0.46080
C	1.64615	0.84867	-0.72328
C	2.84507	0.70304	-0.44984
C	4.21907	0.44258	-0.04956
H	4.24174	-0.34438	0.74006
H	4.71334	1.34962	0.36705
H	4.83366	0.07367	-0.90227
H	0.91301	1.35415	-1.41620

Vibrational Spectrum

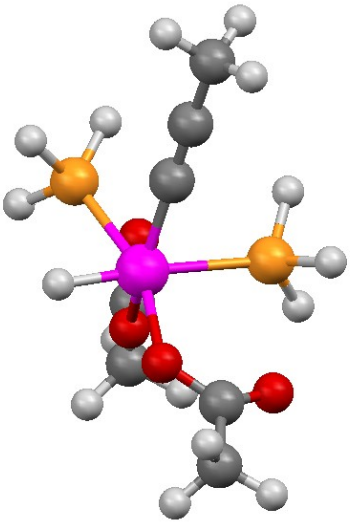
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.31	0.24376	YES	YES
8	a	22.17	0.53818	YES	YES
9	a	33.97	2.14973	YES	YES
10	a	48.12	1.05292	YES	YES
11	a	54.23	3.62898	YES	YES
12	a	56.80	0.16195	YES	YES
13	a	63.60	2.24168	YES	YES
14	a	75.45	5.91584	YES	YES
15	a	108.70	2.23565	YES	YES
16	a	124.21	10.17065	YES	YES
17	a	137.55	6.30500	YES	YES
18	a	141.45	1.99558	YES	YES
19	a	169.17	9.79554	YES	YES
20	a	175.62	10.52380	YES	YES
21	a	187.85	0.26126	YES	YES
22	a	199.42	3.72678	YES	YES
23	a	207.71	1.28607	YES	YES
24	a	212.56	1.05064	YES	YES
25	a	242.46	4.21531	YES	YES
26	a	272.40	1.29935	YES	YES
27	a	294.92	12.19352	YES	YES
28	a	314.85	11.37727	YES	YES
29	a	323.12	16.78077	YES	YES
30	a	336.87	37.28980	YES	YES
31	a	352.41	9.60806	YES	YES
32	a	378.90	13.17163	YES	YES
33	a	391.53	14.62358	YES	YES
34	a	468.48	19.58736	YES	YES
35	a	490.66	23.38264	YES	YES
36	a	503.43	1.88912	YES	YES
37	a	579.77	3.99403	YES	YES
38	a	593.12	7.54344	YES	YES
39	a	595.91	3.29510	YES	YES
40	a	604.29	14.90130	YES	YES
41	a	610.09	5.43869	YES	YES
42	a	618.75	1.07967	YES	YES
43	a	672.39	88.39215	YES	YES
44	a	678.05	22.15929	YES	YES
45	a	861.49	452.66685	YES	YES
46	a	931.97	5.11046	YES	YES
47	a	941.16	31.90005	YES	YES
48	a	952.24	1.82389	YES	YES
49	a	982.57	1.51540	YES	YES
50	a	988.03	2.40207	YES	YES
51	a	1002.81	6.31378	YES	YES

52	a	1018.21	91.66556	YES	YES
53	a	1022.78	23.20239	YES	YES
54	a	1023.14	57.79100	YES	YES
55	a	1026.44	19.73481	YES	YES
56	a	1054.91	112.35281	YES	YES
57	a	1067.69	43.13803	YES	YES
58	a	1078.61	22.83499	YES	YES
59	a	1106.97	14.28436	YES	YES
60	a	1112.36	4.73366	YES	YES
61	a	1318.18	48.72047	YES	YES
62	a	1326.89	1.50566	YES	YES
63	a	1351.33	223.05005	YES	YES
64	a	1354.12	7.08306	YES	YES
65	a	1395.78	43.43153	YES	YES
66	a	1401.27	9.63085	YES	YES
67	a	1409.66	33.28784	YES	YES
68	a	1409.91	6.28189	YES	YES
69	a	1414.91	31.92487	YES	YES
70	a	1419.62	18.98755	YES	YES
71	a	1453.55	261.85010	YES	YES
72	a	1540.90	92.36082	YES	YES
73	a	1622.20	187.86930	YES	YES
74	a	2066.83	1.07889	YES	YES
75	a	2287.79	155.64960	YES	YES
76	a	2298.05	98.07641	YES	YES
77	a	2315.31	112.18251	YES	YES
78	a	2350.63	55.69760	YES	YES
79	a	2383.46	79.58876	YES	YES
80	a	2395.34	19.47247	YES	YES
81	a	2831.46	185.86886	YES	YES
82	a	2924.84	33.50798	YES	YES
83	a	2957.42	13.77671	YES	YES
84	a	2958.70	3.35586	YES	YES
85	a	3003.13	4.75663	YES	YES
86	a	3008.46	3.09332	YES	YES
87	a	3038.43	5.69297	YES	YES
88	a	3044.04	2.65827	YES	YES
89	a	3074.16	7.89465	YES	YES
90	a	3079.59	2.70995	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2095154 Hartree *

Cis 4h _afy



bp86_svp SCF energy = -1354.4350438160
pbe0_tzvpp SCF energy = -1354.201310806

xyz Coordinates
30

C	2.55837	-0.29758	-0.95149
C	3.40349	-0.37665	-2.21824
H	3.38994	0.58820	-2.76692
H	2.97988	-1.14986	-2.89664
H	4.44201	-0.65750	-1.95228
C	-1.92178	0.15922	-2.22048
C	-2.94100	0.83446	-3.12763
H	-3.40025	0.09154	-3.80943
H	-2.43916	1.62957	-3.72142
H	-3.72611	1.33331	-2.51951
H	2.73074	1.53657	1.35443
H	2.07776	-0.17710	2.59361
H	1.12405	1.76539	2.80562
H	0.17835	-2.74572	0.87736
H	-1.66456	-2.57512	-0.21056
H	0.24894	-2.58850	-1.27811
O	1.41670	0.32099	-1.14250
O	2.91582	-0.78318	0.12833
O	-1.42074	0.98937	-1.31268
O	-1.60783	-1.02554	-2.34490
P	1.54152	0.86203	1.77231
P	-0.38603	-1.93583	-0.17544
Ru	-0.13372	0.52952	0.18188
C	-0.89848	-0.03804	1.85847
C	-1.46844	-0.35595	2.92332
C	-2.21767	-0.68220	4.12897
H	-1.75737	-1.55768	4.64512
H	-3.26947	-0.96847	3.89566
H	-2.24209	0.15838	4.86046
H	0.06447	2.14676	0.28734

Vibrational Spectrum

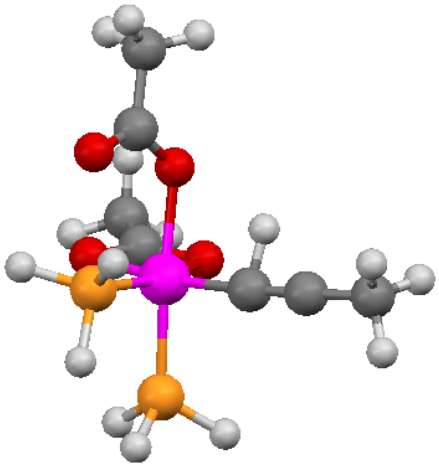
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	24.83	0.46860	YES	YES
8	a	31.88	0.65429	YES	YES
9	a	33.48	0.45393	YES	YES
10	a	36.25	0.47514	YES	YES
11	a	45.86	0.96421	YES	YES
12	a	53.64	0.99567	YES	YES
13	a	62.17	3.00774	YES	YES
14	a	88.56	0.87734	YES	YES
15	a	96.66	0.37108	YES	YES
16	a	100.07	4.43077	YES	YES
17	a	139.10	4.19279	YES	YES
18	a	143.18	13.88602	YES	YES
19	a	160.89	1.50827	YES	YES
20	a	164.94	2.81613	YES	YES
21	a	171.50	2.68977	YES	YES
22	a	197.78	0.49825	YES	YES
23	a	209.48	5.61085	YES	YES
24	a	216.97	4.40013	YES	YES
25	a	232.18	7.89831	YES	YES
26	a	276.48	10.35470	YES	YES
27	a	284.19	22.44361	YES	YES
28	a	313.94	0.31826	YES	YES
29	a	346.34	3.17277	YES	YES
30	a	357.27	0.84582	YES	YES
31	a	384.89	1.38024	YES	YES
32	a	390.85	10.09618	YES	YES
33	a	416.39	5.19658	YES	YES
34	a	432.12	6.38028	YES	YES
35	a	509.54	2.77453	YES	YES
36	a	523.18	4.86353	YES	YES
37	a	533.57	5.87096	YES	YES
38	a	583.55	5.74222	YES	YES
39	a	588.59	2.33146	YES	YES
40	a	597.13	3.88183	YES	YES
41	a	629.89	32.17969	YES	YES
42	a	639.92	3.24165	YES	YES
43	a	655.07	62.51312	YES	YES
44	a	663.29	69.25374	YES	YES

45	a	840.69	8.14418	YES	YES
46	a	915.21	7.29671	YES	YES
47	a	927.13	20.47164	YES	YES
48	a	980.05	60.28010	YES	YES
49	a	982.06	5.60124	YES	YES
50	a	992.16	106.12203	YES	YES
51	a	993.81	36.52252	YES	YES
52	a	1009.99	34.71989	YES	YES
53	a	1017.04	10.61971	YES	YES
54	a	1019.13	19.88271	YES	YES
55	a	1024.56	5.68949	YES	YES
56	a	1027.67	58.74128	YES	YES
57	a	1076.95	26.02583	YES	YES
58	a	1077.67	16.00428	YES	YES
59	a	1116.71	5.27223	YES	YES
60	a	1119.86	9.67282	YES	YES
61	a	1250.09	656.25625	YES	YES
62	a	1296.96	292.76665	YES	YES
63	a	1329.48	80.56926	YES	YES
64	a	1336.72	101.65733	YES	YES
65	a	1353.09	5.18316	YES	YES
66	a	1396.62	11.52129	YES	YES
67	a	1405.32	19.78638	YES	YES
68	a	1406.87	24.74856	YES	YES
69	a	1414.10	16.43198	YES	YES
70	a	1414.54	12.43023	YES	YES
71	a	1415.28	10.25777	YES	YES
72	a	1671.76	168.19308	YES	YES
73	a	1678.18	158.44309	YES	YES
74	a	1929.99	259.07754	YES	YES
75	a	2067.44	118.69269	YES	YES
76	a	2314.33	94.04001	YES	YES
77	a	2368.23	73.70071	YES	YES
78	a	2392.13	61.89715	YES	YES
79	a	2393.58	35.39361	YES	YES
80	a	2414.03	14.13587	YES	YES
81	a	2417.29	19.63266	YES	YES
82	a	2915.08	32.81472	YES	YES
83	a	2961.01	4.22129	YES	YES
84	a	2962.21	4.99503	YES	YES
85	a	2990.42	11.53079	YES	YES
86	a	2995.66	5.91637	YES	YES
87	a	3043.27	2.85003	YES	YES
88	a	3048.03	2.87441	YES	YES
89	a	3080.50	8.35291	YES	YES
90	a	3081.46	3.35064	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2077688 Hartree*

Cis TS_{35}_afx



bp86_svp SCF energy = -1354.4746713360
pbe0_tzvpp SCF energy = -1354.253055077

xyz Coordinates

30

C	-1.68559	-0.69255	-1.97914
C	-2.10632	-1.17971	-3.34509
H	-1.21214	-1.21079	-4.00697
H	-2.84429	-0.48522	-3.79651
H	-2.52318	-2.20565	-3.28145
C	1.84598	1.04747	-1.20379
C	2.95043	0.78032	-2.22753
H	3.79059	1.48865	-2.07844
H	2.53760	0.94206	-3.24864
H	3.30852	-0.26864	-2.17383
H	-3.00608	0.98045	2.33888
H	-3.02800	-1.15120	1.97787
H	-3.88785	0.20004	0.52451
H	-1.15005	2.70982	2.01895
H	0.96991	2.60819	1.69955
H	-0.36789	3.40287	0.12848
O	-1.67594	0.56142	-1.70959
O	-1.30119	-1.51723	-1.07941
O	1.07188	0.02045	-0.98139
O	1.72884	2.17098	-0.68582
P	-2.66847	0.05791	1.28091
P	-0.22316	2.26860	0.98662
Ru	-0.68781	0.17797	0.18909
C	0.27079	-0.62586	1.71358
C	0.92541	-1.19053	2.64947
C	1.67777	-1.88766	3.68157
H	1.85556	-2.95998	3.43565
H	1.07526	-1.86698	4.62106
H	2.65348	-1.40153	3.91222
H	1.20973	-0.91356	1.06889

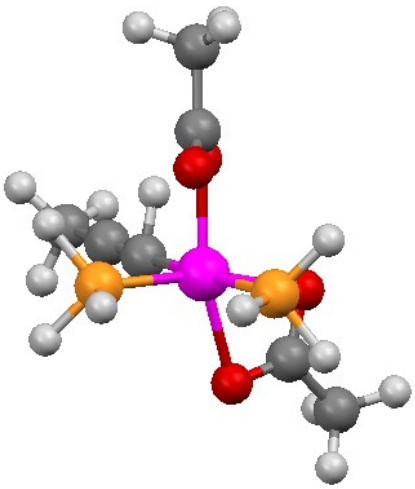
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-737.84	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	29.92	1.16185	YES	YES
9	a	42.29	1.24004	YES	YES
10	a	47.46	2.04906	YES	YES
11	a	59.26	1.47882	YES	YES
12	a	63.77	0.65811	YES	YES
13	a	75.98	0.20647	YES	YES
14	a	79.00	0.64358	YES	YES
15	a	83.17	1.07588	YES	YES
16	a	84.80	1.10236	YES	YES
17	a	100.68	6.87626	YES	YES
18	a	112.24	7.64655	YES	YES
19	a	145.10	0.83435	YES	YES
20	a	156.90	8.72445	YES	YES
21	a	166.29	0.44579	YES	YES
22	a	192.92	1.81969	YES	YES
23	a	196.05	13.25230	YES	YES
24	a	208.65	1.97457	YES	YES
25	a	240.22	5.86897	YES	YES
26	a	266.21	19.35820	YES	YES
27	a	277.78	12.45348	YES	YES
28	a	304.96	26.84828	YES	YES
29	a	329.19	28.19828	YES	YES
30	a	352.23	5.07600	YES	YES
31	a	366.17	14.98723	YES	YES
32	a	370.39	11.78841	YES	YES
33	a	386.59	12.48689	YES	YES
34	a	431.74	1.88322	YES	YES
35	a	443.42	59.20774	YES	YES
36	a	479.57	1.08359	YES	YES
37	a	503.49	0.75151	YES	YES
38	a	566.17	2.22501	YES	YES
39	a	583.52	13.90744	YES	YES
40	a	592.04	3.46476	YES	YES
41	a	595.66	4.91891	YES	YES
42	a	605.05	4.82725	YES	YES
43	a	638.85	12.82351	YES	YES
44	a	666.69	37.59224	YES	YES
45	a	674.91	72.75872	YES	YES
46	a	925.75	3.84394	YES	YES
47	a	938.10	24.03410	YES	YES
48	a	948.41	83.58311	YES	YES
49	a	983.36	1.57608	YES	YES

50	a	989.97	6.84235	YES	YES
51	a	995.80	40.71194	YES	YES
52	a	1020.21	109.58796	YES	YES
53	a	1021.03	23.96728	YES	YES
54	a	1022.76	0.85228	YES	YES
55	a	1026.66	11.78822	YES	YES
56	a	1043.07	167.29015	YES	YES
57	a	1081.07	75.12699	YES	YES
58	a	1095.86	4.77747	YES	YES
59	a	1099.01	7.63166	YES	YES
60	a	1128.24	11.56845	YES	YES
61	a	1309.82	125.76586	YES	YES
62	a	1326.61	1.55303	YES	YES
63	a	1343.83	4.32000	YES	YES
64	a	1347.34	266.34013	YES	YES
65	a	1386.51	10.59300	YES	YES
66	a	1399.16	30.03002	YES	YES
67	a	1408.84	16.57653	YES	YES
68	a	1409.51	44.27032	YES	YES
69	a	1418.35	16.79621	YES	YES
70	a	1419.57	16.49857	YES	YES
71	a	1457.63	316.22671	YES	YES
72	a	1540.86	72.62400	YES	YES
73	a	1655.49	238.83467	YES	YES
74	a	1970.64	124.44469	YES	YES
75	a	2216.78	196.90427	YES	YES
76	a	2300.44	98.89750	YES	YES
77	a	2315.77	100.29126	YES	YES
78	a	2319.04	110.87005	YES	YES
79	a	2378.30	76.80921	YES	YES
80	a	2399.71	24.02558	YES	YES
81	a	2567.39	49.19380	YES	YES
82	a	2915.69	32.57279	YES	YES
83	a	2956.44	12.53015	YES	YES
84	a	2960.44	3.98708	YES	YES
85	a	2993.27	9.95249	YES	YES
86	a	3000.85	2.79279	YES	YES
87	a	3041.37	8.64622	YES	YES
88	a	3046.39	3.67877	YES	YES
89	a	3072.60	9.70788	YES	YES
90	a	3076.11	3.58508	YES	YES

* zero point VIBRATIONAL energy : 0.2070224 Hartree *

Cis TS_{35}_pftx



bp86_svp SCF energy = -1354.4642054970

pbe0_tzvpp SCF energy = -1354.244432293

xyz Coordinates

30

C	-1.94165	0.55287	2.06868
C	-2.69496	1.08125	3.26767
H	-2.02732	1.74720	3.85921
H	-3.02068	0.24722	3.92197
H	-3.56831	1.68182	2.93971
C	-0.25837	-0.19853	-2.83944
C	0.16415	0.52969	-4.11567
H	-0.49790	0.23234	-4.95480
H	1.20151	0.22546	-4.38239
H	0.14957	1.63087	-3.98345
H	-3.21645	-0.81803	-1.80657
H	-3.55902	-1.53643	0.20213
H	-2.43994	-2.75719	-1.18865
H	0.09249	-3.36658	-0.78643
H	1.77603	-2.08613	-1.26330
H	1.45531	-2.72606	0.77367
O	-1.33188	-0.57382	2.12888
O	-1.87260	1.22843	0.98520
O	-0.05776	0.48376	-1.74559
O	-0.72583	-1.35182	-2.88858
P	-2.46503	-1.39914	-0.73298
P	0.69457	-2.15097	-0.31011
Ru	-0.55197	-0.33230	0.12246
C	1.05456	0.61712	0.85680
C	2.07171	1.25666	1.27593
C	3.22030	2.00368	1.77316
H	3.48101	1.60092	2.78038
H	3.00159	3.08801	1.90186
H	4.12140	1.88885	1.12928
H	1.25170	1.39053	-0.02433

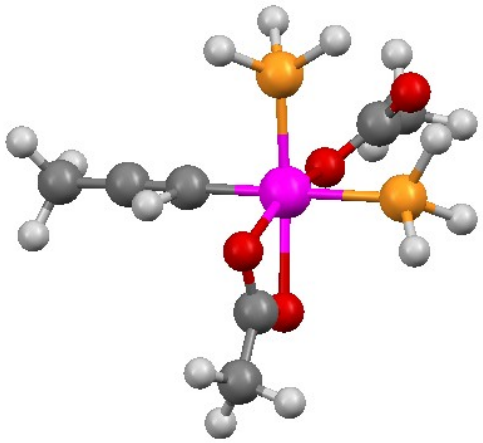
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-799.32	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	12.89	0.29269	YES	YES
9	a	31.61	2.87658	YES	YES
10	a	42.69	0.73695	YES	YES
11	a	46.61	2.29409	YES	YES
12	a	57.99	0.77860	YES	YES
13	a	66.82	1.23438	YES	YES
14	a	74.81	4.39678	YES	YES
15	a	77.03	1.89906	YES	YES
16	a	99.91	2.97728	YES	YES
17	a	124.73	8.39244	YES	YES
18	a	135.00	4.36161	YES	YES
19	a	159.24	7.21343	YES	YES
20	a	166.56	0.93774	YES	YES
21	a	185.85	1.80745	YES	YES
22	a	192.78	0.10290	YES	YES
23	a	193.92	0.76897	YES	YES
24	a	215.37	8.76709	YES	YES
25	a	232.25	2.77553	YES	YES
26	a	258.79	1.46899	YES	YES
27	a	267.82	4.02865	YES	YES
28	a	276.52	33.47664	YES	YES
29	a	296.91	14.69525	YES	YES
30	a	304.29	13.95559	YES	YES
31	a	323.21	32.61439	YES	YES
32	a	343.71	28.93520	YES	YES
33	a	376.15	9.16699	YES	YES
34	a	418.17	5.13967	YES	YES
35	a	435.57	39.61662	YES	YES
36	a	476.66	4.34469	YES	YES
37	a	504.89	1.14755	YES	YES
38	a	533.20	23.64230	YES	YES
39	a	559.39	6.69841	YES	YES
40	a	596.68	4.51851	YES	YES
41	a	598.46	2.52352	YES	YES
42	a	601.95	5.31587	YES	YES
43	a	617.94	5.67832	YES	YES
44	a	670.55	92.17116	YES	YES
45	a	673.16	10.76881	YES	YES
46	a	927.79	13.31102	YES	YES
47	a	940.29	28.72354	YES	YES
48	a	942.09	80.97792	YES	YES
49	a	981.59	1.32692	YES	YES

50	a	987.76	4.22593	YES	YES
51	a	993.47	12.01113	YES	YES
52	a	1013.87	172.76796	YES	YES
53	a	1019.42	31.14855	YES	YES
54	a	1025.04	2.58240	YES	YES
55	a	1025.44	12.31294	YES	YES
56	a	1055.02	146.39064	YES	YES
57	a	1075.40	14.58630	YES	YES
58	a	1080.38	15.14885	YES	YES
59	a	1107.83	16.19258	YES	YES
60	a	1112.10	1.49246	YES	YES
61	a	1311.55	97.53316	YES	YES
62	a	1327.05	1.71163	YES	YES
63	a	1344.57	10.93268	YES	YES
64	a	1345.60	216.44011	YES	YES
65	a	1390.42	11.36543	YES	YES
66	a	1400.01	34.00574	YES	YES
67	a	1409.81	22.08737	YES	YES
68	a	1410.93	30.21338	YES	YES
69	a	1416.94	13.87862	YES	YES
70	a	1421.70	14.87139	YES	YES
71	a	1454.72	266.03961	YES	YES
72	a	1548.62	94.02638	YES	YES
73	a	1642.37	178.07522	YES	YES
74	a	1978.83	139.22105	YES	YES
75	a	2293.67	44.79229	YES	YES
76	a	2295.71	197.76421	YES	YES
77	a	2304.24	144.35755	YES	YES
78	a	2343.36	62.38427	YES	YES
79	a	2371.68	91.35081	YES	YES
80	a	2385.48	24.97791	YES	YES
81	a	2528.62	15.36158	YES	YES
82	a	2923.75	28.02133	YES	YES
83	a	2953.99	14.23109	YES	YES
84	a	2958.16	5.67375	YES	YES
85	a	3003.08	6.97908	YES	YES
86	a	3012.48	1.93712	YES	YES
87	a	3039.30	9.14167	YES	YES
88	a	3043.35	3.44472	YES	YES
89	a	3071.81	7.59374	YES	YES
90	a	3077.03	3.41625	YES	YES

* zero point VIBRATIONAL energy : 0.2064099 Hartree *

Cis TS_{35}_pfty



bp86_svp SCF energy = -1354.4615796230
pbe0_tzvpp SCF energy = -1354.241843401

xyz Coordinates

30

C	-1.76610	0.41293	2.09504
C	-2.65008	0.83132	3.24881
H	-2.65805	1.93670	3.34712
H	-2.31051	0.36010	4.19339
H	-3.69575	0.50547	3.05050
C	0.04034	-0.24982	-2.79358
C	0.36909	0.51084	-4.07755
H	-0.48716	0.42693	-4.78218
H	1.24246	0.03136	-4.57231
H	0.59233	1.57871	-3.88446
H	-2.85174	-0.93216	-1.90573
H	-3.28596	-1.63910	0.08658
H	-2.07766	-2.85481	-1.22972
H	0.46750	-3.38155	-0.79182
H	2.10372	-2.02627	-1.25654
H	1.79944	-2.69387	0.77294
O	-1.06386	-0.66181	2.17272
O	-1.71964	1.09772	1.02033
O	0.14894	0.45642	-1.70695
O	-0.29979	-1.45069	-2.84259
P	-2.14527	-1.49266	-0.79151
P	1.01970	-2.14467	-0.31396
Ru	-0.29699	-0.38420	0.15005
C	1.28056	0.63771	0.84757
C	2.28742	1.32957	1.20902
C	3.41850	2.14912	1.61997
H	3.83065	2.63346	0.70302
H	4.24292	1.55620	2.07706
H	3.12599	2.96724	2.31650
H	1.28584	0.46038	2.01797

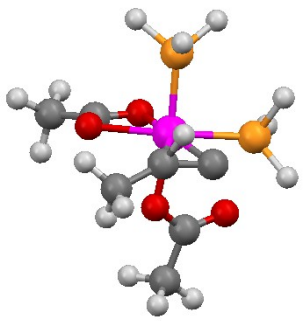
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-787.66	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	33.58	0.69509	YES	YES
9	a	34.82	0.73181	YES	YES
10	a	38.14	0.97990	YES	YES
11	a	44.71	1.54261	YES	YES
12	a	55.43	3.28813	YES	YES
13	a	68.20	0.86347	YES	YES
14	a	76.30	3.41603	YES	YES
15	a	80.29	2.27452	YES	YES
16	a	108.09	2.62729	YES	YES
17	a	124.74	6.65155	YES	YES
18	a	132.76	3.20487	YES	YES
19	a	161.15	12.76958	YES	YES
20	a	167.82	1.01325	YES	YES
21	a	182.25	1.58855	YES	YES
22	a	192.88	1.58687	YES	YES
23	a	218.50	2.53295	YES	YES
24	a	228.77	1.56343	YES	YES
25	a	234.01	4.60100	YES	YES
26	a	264.86	1.09252	YES	YES
27	a	274.26	0.79842	YES	YES
28	a	293.28	16.82647	YES	YES
29	a	299.16	24.04896	YES	YES
30	a	305.12	15.29468	YES	YES
31	a	322.14	39.53369	YES	YES
32	a	342.65	22.07272	YES	YES
33	a	373.10	9.20066	YES	YES
34	a	413.83	18.56561	YES	YES
35	a	434.85	47.73737	YES	YES
36	a	470.48	3.36808	YES	YES
37	a	502.44	0.51171	YES	YES
38	a	536.64	10.02780	YES	YES
39	a	552.45	14.48457	YES	YES
40	a	595.64	4.32451	YES	YES
41	a	600.20	1.06231	YES	YES
42	a	613.14	5.28927	YES	YES
43	a	623.39	7.47881	YES	YES
44	a	668.00	82.72618	YES	YES
45	a	676.83	19.31774	YES	YES
46	a	929.68	6.85547	YES	YES
47	a	938.19	52.99960	YES	YES
48	a	938.84	58.44431	YES	YES
49	a	980.81	1.71827	YES	YES
50	a	986.59	2.55447	YES	YES
51	a	990.31	9.40036	YES	YES

52	a	1013.27	174.13480	YES	YES
53	a	1021.91	18.09907	YES	YES
54	a	1024.76	15.40516	YES	YES
55	a	1025.78	10.34695	YES	YES
56	a	1052.67	132.09943	YES	YES
57	a	1074.16	19.06453	YES	YES
58	a	1077.47	28.90377	YES	YES
59	a	1107.39	13.85747	YES	YES
60	a	1112.91	3.51807	YES	YES
61	a	1316.49	61.64141	YES	YES
62	a	1326.32	1.20779	YES	YES
63	a	1342.37	11.18100	YES	YES
64	a	1349.23	223.49251	YES	YES
65	a	1388.04	11.16699	YES	YES
66	a	1397.48	50.57084	YES	YES
67	a	1410.37	34.85434	YES	YES
68	a	1415.62	9.74326	YES	YES
69	a	1416.10	38.71584	YES	YES
70	a	1419.16	11.93940	YES	YES
71	a	1449.26	244.36691	YES	YES
72	a	1548.83	101.69738	YES	YES
73	a	1629.29	199.08161	YES	YES
74	a	1970.48	136.72894	YES	YES
75	a	2281.59	119.29150	YES	YES
76	a	2286.86	164.29523	YES	YES
77	a	2309.35	121.98778	YES	YES
78	a	2352.38	56.63094	YES	YES
79	a	2371.97	92.45485	YES	YES
80	a	2385.92	25.39209	YES	YES
81	a	2568.11	5.18737	YES	YES
82	a	2922.73	26.30884	YES	YES
83	a	2954.36	16.69571	YES	YES
84	a	2958.45	5.18734	YES	YES
85	a	3002.15	10.74437	YES	YES
86	a	3011.78	1.93717	YES	YES
87	a	3033.72	6.43823	YES	YES
88	a	3043.13	3.18432	YES	YES
89	a	3073.67	9.14909	YES	YES
90	a	3076.00	3.76560	YES	YES

* zero point VIBRATIONAL energy : 0.2064052 Hartree *

Cis TS_{25}_afxd



bp86_svp SCF energy = -1354.4424397410
pbe0_tzvpp SCF energy = -1354.223851892

xyz Coordinates

30

C	-0.82782	2.09903	0.52743
C	-0.77510	3.57936	0.80526
C	2.19302	-0.21397	1.05321
C	3.60045	0.37364	0.95714
H	4.06482	0.10340	-0.01606
H	4.22981	0.00194	1.78978
H	3.54920	1.48368	0.99678
H	-3.41071	-1.48349	-1.10832
H	-3.74689	0.41690	-0.12471
H	-3.60328	-1.40201	1.03958
H	-1.47804	-3.01023	1.66265
H	0.67862	-3.07979	1.58540
H	-0.37187	-1.74204	3.03435
O	-0.81955	1.25099	1.48967
O	-0.85184	1.64905	-0.67137
O	1.41110	0.12427	0.06758
O	1.87475	-0.94187	2.01138
P	-2.87301	-0.72172	-0.00115
P	-0.35028	-2.09956	1.64852
Ru	-0.63053	-0.39172	0.11439
C	-0.22682	-1.16170	-1.82279
C	-0.13212	-2.25073	-1.04870
H	-1.12030	-1.95505	-2.08651
C	0.29216	-0.32919	-2.94863
H	-0.45359	0.42457	-3.27451
H	0.59222	-0.96447	-3.81146
H	1.18002	0.21369	-2.56117
H	-1.30926	4.14278	0.01286
H	0.28779	3.90918	0.80473
H	-1.20621	3.80476	1.80195

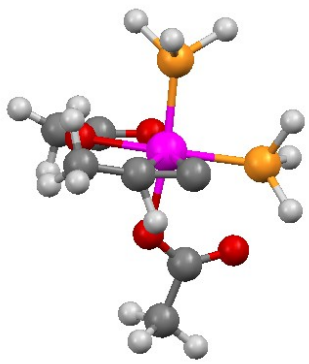
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-634.49	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	28.58	1.34956	YES	YES
9	a	44.48	0.70037	YES	YES
10	a	70.14	1.66610	YES	YES
11	a	74.61	0.03480	YES	YES
12	a	76.17	1.42600	YES	YES
13	a	83.46	0.44738	YES	YES
14	a	86.00	0.93977	YES	YES
15	a	94.58	0.93636	YES	YES
16	a	113.50	8.57777	YES	YES
17	a	132.13	10.22730	YES	YES
18	a	142.46	0.75578	YES	YES
19	a	161.19	11.80284	YES	YES
20	a	168.09	1.83445	YES	YES
21	a	188.11	4.32161	YES	YES
22	a	196.89	11.45649	YES	YES
23	a	211.25	1.03494	YES	YES
24	a	224.48	3.79223	YES	YES
25	a	228.99	0.67573	YES	YES
26	a	274.99	17.01969	YES	YES
27	a	298.07	7.87897	YES	YES
28	a	319.99	13.32688	YES	YES
29	a	351.24	7.58488	YES	YES
30	a	362.21	7.31597	YES	YES
31	a	393.25	20.37664	YES	YES
32	a	406.48	1.45986	YES	YES
33	a	421.03	3.43274	YES	YES
34	a	481.49	2.70457	YES	YES
35	a	507.93	0.36873	YES	YES
36	a	544.33	9.20716	YES	YES
37	a	555.57	6.05585	YES	YES
38	a	571.49	11.16219	YES	YES
39	a	593.14	4.35107	YES	YES
40	a	594.77	2.03177	YES	YES
41	a	608.04	9.44608	YES	YES
42	a	641.43	13.56740	YES	YES
43	a	668.21	41.10711	YES	YES
44	a	677.27	67.73985	YES	YES
45	a	858.28	3.47519	YES	YES
46	a	896.63	5.81657	YES	YES
47	a	928.76	4.18875	YES	YES
48	a	942.37	28.25272	YES	YES
49	a	983.52	0.92678	YES	YES
50	a	990.69	6.23801	YES	YES
51	a	1007.33	120.50443	YES	YES
52	a	1020.99	3.55134	YES	YES
53	a	1026.07	3.02685	YES	YES

54	a	1030.15	106.63499	YES	YES
55	a	1040.55	71.65980	YES	YES
56	a	1063.94	32.44237	YES	YES
57	a	1075.83	50.79376	YES	YES
58	a	1089.80	19.50724	YES	YES
59	a	1093.67	5.42675	YES	YES
60	a	1124.73	9.56333	YES	YES
61	a	1311.93	66.60997	YES	YES
62	a	1328.97	0.71533	YES	YES
63	a	1336.04	7.61642	YES	YES
64	a	1358.96	298.08416	YES	YES
65	a	1398.18	28.08972	YES	YES
66	a	1406.03	20.90910	YES	YES
67	a	1407.45	15.19994	YES	YES
68	a	1408.96	35.16334	YES	YES
69	a	1417.04	16.94880	YES	YES
70	a	1418.24	2.66712	YES	YES
71	a	1465.25	295.74779	YES	YES
72	a	1537.71	70.93979	YES	YES
73	a	1646.53	197.80922	YES	YES
74	a	1665.43	42.76641	YES	YES
75	a	2238.46	10.04092	YES	YES
76	a	2259.53	126.11029	YES	YES
77	a	2272.56	132.54990	YES	YES
78	a	2314.59	103.36586	YES	YES
79	a	2326.24	84.88627	YES	YES
80	a	2390.14	54.52705	YES	YES
81	a	2444.09	15.33934	YES	YES
82	a	2954.72	18.51237	YES	YES
83	a	2958.06	11.50822	YES	YES
84	a	2961.52	2.05402	YES	YES
85	a	3039.35	6.31172	YES	YES
86	a	3047.37	4.27477	YES	YES
87	a	3047.75	2.26267	YES	YES
88	a	3067.31	2.66989	YES	YES
89	a	3077.63	8.84992	YES	YES
90	a	3078.25	2.57683	YES	YES

* zero point VIBRATIONAL energy : 0.2069695 Hartree *

Cis TS_{25}_afxu



bp86_svp SCF energy = -1354.4447292810
pbe0_tzvpp SCF energy = -1354.226070239

xyz Coordinates

30

C	-1.10638	1.97633	0.43444
C	-1.27541	3.45265	0.68776
C	2.23858	0.15093	0.94507
C	3.53042	0.95457	0.80320
H	3.96421	0.82424	-0.21138
H	4.26249	0.64517	1.57521
H	3.30693	2.03754	0.92567
H	-3.22577	-1.97596	-1.02506
H	-3.73775	-0.08598	-0.10471
H	-3.30667	-1.81727	1.11800
H	-0.93135	-3.18745	1.60890
H	1.20548	-2.88626	1.51397
H	-0.04414	-1.74839	2.97154
O	-0.95669	1.15685	1.40951
O	-1.07690	1.50682	-0.75684
O	1.40588	0.31277	-0.04904
O	2.04097	-0.56576	1.94058
P	-2.72311	-1.10339	0.00984
P	0.02304	-2.09871	1.58456
Ru	-0.53730	-0.46305	0.05036
C	-0.10449	-1.19805	-1.88706
C	0.04667	-2.28924	-1.13194
H	1.08598	-1.43224	-1.72105
C	-0.47352	-0.55599	-3.18400
H	-0.07610	0.47834	-3.23955
H	-1.58104	-0.49252	-3.24596
H	-0.10073	-1.15150	-4.04706
H	-1.88466	3.91736	-0.11437
H	-0.27383	3.93761	0.68347
H	-1.73917	3.62721	1.68003

Vibrational Spectrum

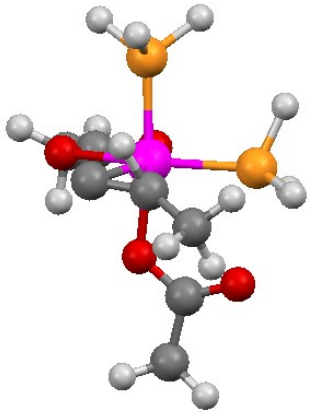
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1	a	-627.07	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	25.62	0.51833	YES	YES
9	a	41.96	1.12943	YES	YES
10	a	48.82	0.38346	YES	YES
11	a	71.36	0.84800	YES	YES
12	a	72.76	1.35235	YES	YES
13	a	77.04	0.92517	YES	YES
14	a	79.25	0.16335	YES	YES
15	a	84.43	0.56409	YES	YES
16	a	113.42	7.52186	YES	YES
17	a	122.09	5.46530	YES	YES
18	a	138.63	7.74570	YES	YES
19	a	159.80	3.37038	YES	YES
20	a	162.40	9.12595	YES	YES
21	a	178.77	1.71482	YES	YES
22	a	193.70	9.31887	YES	YES
23	a	209.47	8.46599	YES	YES
24	a	219.80	2.29735	YES	YES
25	a	233.00	0.67257	YES	YES
26	a	276.58	15.77438	YES	YES
27	a	297.54	6.21886	YES	YES
28	a	320.20	13.39408	YES	YES
29	a	354.62	15.63223	YES	YES
30	a	355.80	2.82823	YES	YES
31	a	404.52	2.14408	YES	YES
32	a	420.73	1.95588	YES	YES
33	a	432.51	18.93778	YES	YES
34	a	481.54	2.66270	YES	YES
35	a	509.68	0.55456	YES	YES
36	a	539.10	17.70731	YES	YES
37	a	562.16	2.96930	YES	YES
38	a	570.87	9.60870	YES	YES
39	a	595.93	1.40726	YES	YES
40	a	596.76	3.83396	YES	YES
41	a	612.27	12.39299	YES	YES
42	a	650.53	12.93650	YES	YES
43	a	669.90	42.41132	YES	YES
44	a	677.01	66.08847	YES	YES
45	a	829.88	4.54513	YES	YES
46	a	900.15	7.35317	YES	YES
47	a	926.77	3.70272	YES	YES
48	a	942.18	27.99297	YES	YES
49	a	983.23	1.13924	YES	YES
50	a	989.59	8.72545	YES	YES
51	a	1014.76	123.26671	YES	YES
52	a	1021.56	3.81289	YES	YES

53	a	1026.59	6.59298	YES	YES
54	a	1029.24	58.39585	YES	YES
55	a	1045.25	147.70159	YES	YES
56	a	1061.95	8.46385	YES	YES
57	a	1082.12	60.46549	YES	YES
58	a	1091.28	5.37898	YES	YES
59	a	1100.42	15.05900	YES	YES
60	a	1125.21	9.53380	YES	YES
61	a	1308.42	115.44165	YES	YES
62	a	1329.67	0.71891	YES	YES
63	a	1346.06	5.88529	YES	YES
64	a	1350.36	279.94089	YES	YES
65	a	1398.21	27.83837	YES	YES
66	a	1403.20	11.24227	YES	YES
67	a	1406.20	20.46027	YES	YES
68	a	1409.16	32.91768	YES	YES
69	a	1417.53	14.62434	YES	YES
70	a	1419.70	7.43842	YES	YES
71	a	1464.25	294.65327	YES	YES
72	a	1537.91	70.66354	YES	YES
73	a	1653.44	198.53529	YES	YES
74	a	1678.98	32.25807	YES	YES
75	a	2239.70	6.52445	YES	YES
76	a	2271.73	131.91144	YES	YES
77	a	2297.42	89.56100	YES	YES
78	a	2316.90	125.59530	YES	YES
79	a	2320.34	72.77591	YES	YES
80	a	2385.89	58.51604	YES	YES
81	a	2445.45	17.37736	YES	YES
82	a	2951.94	16.24160	YES	YES
83	a	2957.67	10.62386	YES	YES
84	a	2961.93	2.15579	YES	YES
85	a	3039.20	6.27726	YES	YES
86	a	3040.52	5.70211	YES	YES
87	a	3048.03	2.44888	YES	YES
88	a	3061.55	0.68394	YES	YES
89	a	3077.61	8.73282	YES	YES
90	a	3078.08	2.71013	YES	YES

* zero point VIBRATIONAL energy : 0.2079727 Hartree *

Cis TS_{25}_afyd



bp86_svp SCF energy = -1354.4367678440
pbe0_tzvpp SCF energy = -1354.217729715

xyz Coordinates

30

C	0.83613	1.48354	2.08495
C	1.57257	1.78987	3.36336
C	1.07208	-2.00939	-0.06890
C	2.31169	-2.87360	0.15271
H	3.20019	-2.41807	-0.33264
H	2.14228	-3.89893	-0.23232
H	2.52540	-2.93103	1.24332
H	-1.41239	3.62326	0.57310
H	-3.09320	2.25096	0.47160
H	-2.16640	2.96479	-1.34965
H	-3.24909	-0.35633	0.23112
H	-2.34186	-1.82336	-1.05096
H	-1.93899	-1.81396	1.13094
O	-0.17467	0.68280	2.09152
O	1.19917	1.97420	0.96848
O	1.26850	-0.74114	0.09650
O	-0.02216	-2.54187	-0.36724
P	-1.76994	2.39328	-0.08305
P	-1.93850	-0.94393	-0.00181
Ru	-0.28901	0.67210	-0.04794
C	-0.28431	0.33014	-2.21528
C	0.58441	1.29747	-1.90249
H	-0.57257	1.46496	-2.65831
C	-0.63188	-0.80678	-3.11906
H	-0.29358	-1.74516	-2.62822
H	-0.12405	-0.69642	-4.10228
H	-1.72646	-0.89080	-3.28692
H	1.98412	2.81975	3.33407
H	2.42622	1.08303	3.46469
H	0.90629	1.66060	4.24071

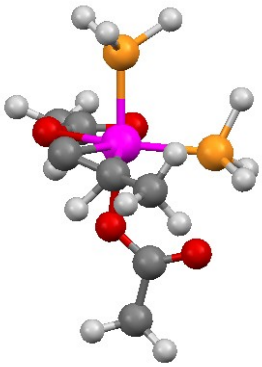
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-652.11	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	30.18	1.10092	YES	YES
9	a	49.15	1.22401	YES	YES
10	a	74.44	0.57198	YES	YES
11	a	75.43	0.81265	YES	YES
12	a	81.84	1.44202	YES	YES
13	a	83.95	0.64809	YES	YES
14	a	102.90	5.35203	YES	YES
15	a	112.48	7.74626	YES	YES
16	a	131.79	1.10766	YES	YES
17	a	147.93	2.11813	YES	YES
18	a	155.72	2.42809	YES	YES
19	a	160.19	7.40198	YES	YES
20	a	178.21	9.29625	YES	YES
21	a	197.77	4.63255	YES	YES
22	a	201.42	6.95260	YES	YES
23	a	225.57	6.45020	YES	YES
24	a	226.20	3.88359	YES	YES
25	a	234.25	1.67321	YES	YES
26	a	277.62	17.47198	YES	YES
27	a	283.98	6.91191	YES	YES
28	a	324.09	14.10948	YES	YES
29	a	354.04	29.09189	YES	YES
30	a	360.45	3.41412	YES	YES
31	a	367.02	0.28404	YES	YES
32	a	370.89	10.06803	YES	YES
33	a	436.49	4.18167	YES	YES
34	a	474.52	0.37279	YES	YES
35	a	504.99	1.24232	YES	YES
36	a	520.56	3.49663	YES	YES
37	a	559.09	5.25069	YES	YES
38	a	576.59	9.06406	YES	YES
39	a	582.90	9.23556	YES	YES
40	a	597.37	2.07300	YES	YES
41	a	607.83	1.45494	YES	YES
42	a	642.04	12.36788	YES	YES
43	a	670.44	43.30641	YES	YES
44	a	677.28	68.76987	YES	YES
45	a	876.32	3.31711	YES	YES
46	a	907.08	9.15092	YES	YES
47	a	932.37	4.88730	YES	YES
48	a	941.45	31.40868	YES	YES
49	a	983.04	1.33345	YES	YES
50	a	993.07	3.56351	YES	YES
51	a	1006.47	98.10600	YES	YES

52	a	1023.11	6.83698	YES	YES
53	a	1027.34	11.10151	YES	YES
54	a	1030.20	116.29389	YES	YES
55	a	1039.00	56.99385	YES	YES
56	a	1062.81	22.27634	YES	YES
57	a	1084.05	58.40146	YES	YES
58	a	1092.88	15.42944	YES	YES
59	a	1095.34	10.85257	YES	YES
60	a	1130.45	12.76547	YES	YES
61	a	1319.16	26.39870	YES	YES
62	a	1330.16	1.36862	YES	YES
63	a	1343.99	8.13256	YES	YES
64	a	1375.23	306.29483	YES	YES
65	a	1397.10	48.14407	YES	YES
66	a	1405.97	22.10850	YES	YES
67	a	1409.39	29.31497	YES	YES
68	a	1414.34	11.23988	YES	YES
69	a	1419.58	21.95459	YES	YES
70	a	1431.66	7.41441	YES	YES
71	a	1459.48	282.13606	YES	YES
72	a	1545.70	106.72946	YES	YES
73	a	1619.24	223.64080	YES	YES
74	a	1663.79	21.03495	YES	YES
75	a	2175.59	5.51997	YES	YES
76	a	2223.95	171.61095	YES	YES
77	a	2290.46	108.57191	YES	YES
78	a	2317.12	97.76968	YES	YES
79	a	2337.27	70.14021	YES	YES
80	a	2396.38	59.67213	YES	YES
81	a	2414.58	18.44609	YES	YES
82	a	2947.57	24.20651	YES	YES
83	a	2958.97	9.90821	YES	YES
84	a	2961.13	2.07379	YES	YES
85	a	3037.34	5.79117	YES	YES
86	a	3043.24	5.85633	YES	YES
87	a	3045.36	4.55451	YES	YES
88	a	3047.69	2.41458	YES	YES
89	a	3076.69	2.50493	YES	YES
90	a	3077.14	8.48965	YES	YES

* zero point VIBRATIONAL energy : 0.2074115 Hartree *

Cis TS_{25}_afyu



bp86_svp SCF energy = -1354.4390624710
pbe0_tzvpp SCF energy = -1354.220919770

xyz Coordinates

30

C	0.77483	1.52079	2.09521
C	1.49064	1.84088	3.38217
C	0.96384	-2.02282	-0.00693
C	2.18732	-2.91124	0.20941
H	3.08587	-2.47450	-0.27443
H	1.99569	-3.93299	-0.17521
H	2.39930	-2.97573	1.30013
H	-1.39832	3.64380	0.57772
H	-3.11119	2.32157	0.39534
H	-2.11647	3.06197	-1.37826
H	-3.32125	-0.25168	0.18849
H	-2.42153	-1.78090	-1.02143
H	-2.07428	-1.71233	1.16964
O	-0.26238	0.75459	2.10112
O	1.18159	1.96363	0.97392
O	1.20044	-0.75131	0.11585
O	-0.14952	-2.53335	-0.25468
P	-1.77103	2.44339	-0.12356
P	-2.02061	-0.87984	0.01010
Ru	-0.32446	0.68289	-0.04159
C	-0.24693	0.29007	-2.18644
C	0.44210	1.39961	-1.92031
H	1.00530	0.16468	-2.20324
C	-0.98386	-0.53323	-3.18893
H	-0.55180	-0.39516	-4.20525
H	-2.04522	-0.20103	-3.22011
H	-0.96405	-1.61125	-2.92399
H	2.00114	2.82251	3.30596
H	2.26364	1.06225	3.56813
H	0.78256	1.83473	4.23624

Vibrational Spectrum

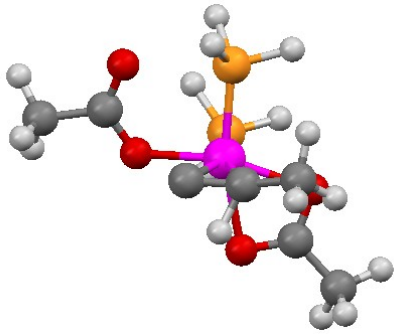
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1	a	-645.07	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	34.90	0.72045	YES	YES
9	a	49.25	0.91991	YES	YES
10	a	59.21	2.85181	YES	YES
11	a	68.04	0.26364	YES	YES
12	a	73.00	0.87802	YES	YES
13	a	75.46	1.02792	YES	YES
14	a	96.45	3.54014	YES	YES
15	a	97.33	1.08184	YES	YES
16	a	111.82	8.20493	YES	YES
17	a	144.32	1.59975	YES	YES
18	a	153.60	3.83294	YES	YES
19	a	158.07	4.06510	YES	YES
20	a	169.87	9.81403	YES	YES
21	a	199.46	11.33201	YES	YES
22	a	210.70	1.58444	YES	YES
23	a	218.86	8.31082	YES	YES
24	a	226.14	4.25269	YES	YES
25	a	246.05	1.39890	YES	YES
26	a	275.20	14.57635	YES	YES
27	a	286.45	9.76229	YES	YES
28	a	324.39	13.53382	YES	YES
29	a	351.25	4.08418	YES	YES
30	a	366.70	12.62075	YES	YES
31	a	371.75	23.87606	YES	YES
32	a	376.77	2.92757	YES	YES
33	a	421.22	4.35689	YES	YES
34	a	474.43	0.82077	YES	YES
35	a	508.46	0.36812	YES	YES
36	a	520.49	10.25231	YES	YES
37	a	559.25	2.88450	YES	YES
38	a	575.09	8.74874	YES	YES
39	a	583.74	7.78910	YES	YES
40	a	595.33	2.30139	YES	YES
41	a	607.18	2.08380	YES	YES
42	a	641.15	11.84005	YES	YES
43	a	671.89	46.53616	YES	YES
44	a	676.91	66.47280	YES	YES
45	a	839.01	10.17439	YES	YES
46	a	908.22	8.80566	YES	YES
47	a	930.68	3.76984	YES	YES
48	a	941.41	31.83927	YES	YES
49	a	982.08	1.43784	YES	YES
50	a	992.43	3.62421	YES	YES
51	a	1005.10	98.32496	YES	YES
52	a	1022.40	7.15685	YES	YES

53	a	1026.56	4.23563	YES	YES
54	a	1031.35	111.39346	YES	YES
55	a	1040.44	96.36330	YES	YES
56	a	1046.51	6.89088	YES	YES
57	a	1082.63	66.62499	YES	YES
58	a	1092.22	8.68894	YES	YES
59	a	1100.14	9.88103	YES	YES
60	a	1129.48	13.96232	YES	YES
61	a	1317.04	50.21808	YES	YES
62	a	1329.18	1.45508	YES	YES
63	a	1344.61	6.25518	YES	YES
64	a	1364.68	305.31961	YES	YES
65	a	1397.37	40.57267	YES	YES
66	a	1406.07	16.18330	YES	YES
67	a	1406.94	15.79486	YES	YES
68	a	1409.53	33.66107	YES	YES
69	a	1419.26	18.10051	YES	YES
70	a	1432.00	8.29428	YES	YES
71	a	1457.58	281.33331	YES	YES
72	a	1545.54	105.54756	YES	YES
73	a	1628.40	213.10576	YES	YES
74	a	1682.62	20.01125	YES	YES
75	a	2174.31	5.32386	YES	YES
76	a	2221.79	172.83222	YES	YES
77	a	2314.11	111.72910	YES	YES
78	a	2320.18	74.62512	YES	YES
79	a	2335.78	69.68981	YES	YES
80	a	2395.23	59.57710	YES	YES
81	a	2413.27	19.77661	YES	YES
82	a	2944.73	16.56184	YES	YES
83	a	2958.31	9.69752	YES	YES
84	a	2961.73	2.18389	YES	YES
85	a	3027.80	6.89456	YES	YES
86	a	3042.52	6.24555	YES	YES
87	a	3048.15	2.57612	YES	YES
88	a	3048.17	1.02189	YES	YES
89	a	3076.40	8.23903	YES	YES
90	a	3077.67	2.54638	YES	YES

* zero point VIBRATIONAL energy : 0.2075102 Hartree *

Cis TS_{25}_pfex



bp86_svp SCF energy = -1354.4252059900
pbe0_tzvpp SCF energy = -1354.205704813

xyz Coordinates

30

C	-0.70970	0.30994	2.46769
C	-1.02435	0.54960	3.92633
H	-0.20901	1.15026	4.38822
H	-1.10393	-0.41106	4.47402
H	-1.96322	1.13261	4.02521
C	-0.36310	0.53837	-2.90753
C	-0.83546	1.49706	-3.99712
H	-0.89485	0.96908	-4.97085
H	-0.08551	2.31403	-4.09104
H	-1.81053	1.95942	-3.74074
H	-2.53350	-1.68065	-1.55792
H	-3.36295	-0.31658	-0.08446
H	-2.59746	-2.25014	0.54159
H	0.23646	-2.67787	-2.07266
H	2.16133	-1.64126	-1.79677
H	1.31951	-2.86365	-0.22625
O	-0.16534	-0.79527	2.09467
O	-0.95117	1.19834	1.58435
O	-0.79960	0.84286	-1.71750
O	0.38940	-0.41334	-3.18427
P	-2.19776	-1.13576	-0.27377
P	0.89941	-1.81260	-1.14355
Ru	-0.11604	-0.13599	0.00651
C	1.60364	1.21821	-0.44202
C	1.87594	0.55737	0.67738
C	2.80504	-0.10020	1.64114
H	1.55968	1.73191	0.88244
H	3.67973	0.55122	1.86008
H	3.17667	-1.04075	1.18064
H	2.28719	-0.37092	2.58381

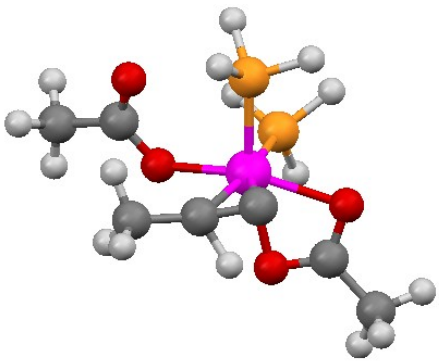
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-550.74	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	33.97	0.74411	YES	YES
9	a	42.26	0.49406	YES	YES
10	a	50.28	0.35147	YES	YES
11	a	64.91	3.12325	YES	YES
12	a	71.09	0.62305	YES	YES
13	a	79.34	0.99138	YES	YES
14	a	81.39	3.73364	YES	YES
15	a	87.91	0.94341	YES	YES
16	a	113.69	1.37812	YES	YES
17	a	124.56	3.04762	YES	YES
18	a	138.68	1.01557	YES	YES
19	a	158.46	4.52370	YES	YES
20	a	161.82	16.93324	YES	YES
21	a	175.44	12.13940	YES	YES
22	a	192.49	0.92962	YES	YES
23	a	206.08	2.43143	YES	YES
24	a	226.68	5.92660	YES	YES
25	a	251.00	4.66633	YES	YES
26	a	262.59	8.52622	YES	YES
27	a	291.12	18.79568	YES	YES
28	a	295.48	24.96298	YES	YES
29	a	322.95	23.47363	YES	YES
30	a	348.51	4.46687	YES	YES
31	a	365.90	9.89483	YES	YES
32	a	373.17	5.15906	YES	YES
33	a	391.27	3.66905	YES	YES
34	a	470.78	1.55596	YES	YES
35	a	492.57	4.58623	YES	YES
36	a	509.99	3.67802	YES	YES
37	a	525.49	1.41124	YES	YES
38	a	547.98	6.61555	YES	YES
39	a	590.22	7.32701	YES	YES
40	a	604.40	0.89953	YES	YES
41	a	612.74	7.86677	YES	YES
42	a	633.32	3.38979	YES	YES
43	a	668.34	84.08793	YES	YES
44	a	672.94	26.91785	YES	YES
45	a	782.04	10.64486	YES	YES
46	a	890.19	10.70547	YES	YES
47	a	932.07	4.96166	YES	YES
48	a	938.97	27.13893	YES	YES
49	a	981.45	1.59607	YES	YES
50	a	990.98	4.02986	YES	YES
51	a	1006.95	180.82927	YES	YES
52	a	1019.89	45.85869	YES	YES
53	a	1021.53	29.75451	YES	YES

54	a	1027.54	13.38538	YES	YES
55	a	1032.89	40.66223	YES	YES
56	a	1051.75	5.94552	YES	YES
57	a	1082.62	100.26795	YES	YES
58	a	1092.89	2.47204	YES	YES
59	a	1101.02	4.62481	YES	YES
60	a	1131.17	9.31823	YES	YES
61	a	1313.16	116.82187	YES	YES
62	a	1328.47	1.21490	YES	YES
63	a	1343.11	8.16302	YES	YES
64	a	1346.15	223.79795	YES	YES
65	a	1396.43	42.27839	YES	YES
66	a	1402.87	15.17930	YES	YES
67	a	1409.99	21.95821	YES	YES
68	a	1410.83	34.12615	YES	YES
69	a	1419.01	18.59142	YES	YES
70	a	1421.88	4.73282	YES	YES
71	a	1449.85	249.87747	YES	YES
72	a	1542.29	94.20286	YES	YES
73	a	1647.91	207.68389	YES	YES
74	a	1706.47	24.41142	YES	YES
75	a	2214.18	181.14834	YES	YES
76	a	2252.72	9.83734	YES	YES
77	a	2348.97	119.76819	YES	YES
78	a	2361.22	23.91328	YES	YES
79	a	2365.05	69.53346	YES	YES
80	a	2372.40	41.81201	YES	YES
81	a	2383.57	23.11252	YES	YES
82	a	2954.26	19.10604	YES	YES
83	a	2959.37	11.16491	YES	YES
84	a	2959.63	2.99056	YES	YES
85	a	3040.63	4.08014	YES	YES
86	a	3044.46	2.73291	YES	YES
87	a	3045.74	7.87675	YES	YES
88	a	3061.02	1.81980	YES	YES
89	a	3073.75	8.38151	YES	YES
90	a	3079.24	2.29454	YES	YES

* zero point VIBRATIONAL energy : 0.2049910 Hartree *

Cis TS_{25}_pfey



bp86_svp SCF energy = -1354.4304500110

pbe0_tzvpp SCF energy = -1354.210524730

xyz Coordinates

30

C	-0.33971	0.26877	2.84719
C	-0.47737	0.68119	4.29290
H	0.53071	0.92687	4.69586
H	-0.88779	-0.15378	4.89767
H	-1.11850	1.58171	4.38393
C	-0.22420	0.22176	-2.54090
C	-0.84290	1.08841	-3.63833
H	-1.54051	0.46600	-4.24036
H	-0.04384	1.43396	-4.32866
H	-1.38876	1.96030	-3.22608
H	-2.84510	-1.26745	-0.82390
H	-3.10141	-0.50601	1.19663
H	-2.39448	-2.53019	0.89098
H	0.06658	-2.98817	-1.66327
H	2.10926	-2.26080	-1.31914
H	1.04974	-3.34334	0.22554
O	-0.07035	-0.94567	2.54130
O	-0.45051	1.12794	1.90178
O	-0.52320	0.60701	-1.33052
O	0.49385	-0.74903	-2.83861
P	-2.11828	-1.20515	0.41181
P	0.82023	-2.24893	-0.69384
Ru	0.06646	-0.39966	0.40227
C	2.17919	-0.19113	1.01108
C	1.94575	0.71821	0.06951
C	2.34988	1.53488	-1.10763
H	1.97611	1.24482	1.17003
H	3.35313	1.98847	-0.94784
H	1.60772	2.33178	-1.31669
H	2.39122	0.86309	-1.99094

Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-564.57	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	26.11	0.80504	YES	YES
9	a	44.14	1.61250	YES	YES
10	a	58.61	0.26376	YES	YES
11	a	71.06	3.40105	YES	YES
12	a	74.92	0.32427	YES	YES
13	a	77.89	0.82484	YES	YES
14	a	83.18	4.05826	YES	YES
15	a	101.52	1.77840	YES	YES
16	a	112.62	0.87341	YES	YES
17	a	124.19	2.53837	YES	YES
18	a	149.42	3.96978	YES	YES
19	a	158.85	27.21875	YES	YES
20	a	174.80	1.49704	YES	YES
21	a	194.09	2.44465	YES	YES
22	a	195.40	0.35636	YES	YES
23	a	208.52	0.96592	YES	YES
24	a	234.76	10.09564	YES	YES
25	a	243.26	5.68393	YES	YES
26	a	260.80	7.39007	YES	YES
27	a	293.79	15.48848	YES	YES
28	a	299.04	24.27750	YES	YES
29	a	313.98	21.46154	YES	YES
30	a	336.55	0.35836	YES	YES
31	a	355.50	12.87900	YES	YES
32	a	363.76	6.12422	YES	YES
33	a	403.89	4.83716	YES	YES
34	a	470.11	2.12443	YES	YES
35	a	487.10	2.81073	YES	YES
36	a	506.80	2.30712	YES	YES
37	a	529.90	4.95076	YES	YES
38	a	545.29	4.52881	YES	YES
39	a	592.30	5.34545	YES	YES
40	a	605.30	4.04671	YES	YES
41	a	609.31	3.77641	YES	YES
42	a	624.18	4.90858	YES	YES
43	a	668.48	95.74612	YES	YES
44	a	670.96	13.17298	YES	YES
45	a	789.82	3.52713	YES	YES
46	a	896.14	11.10233	YES	YES
47	a	926.95	4.23263	YES	YES
48	a	939.70	30.15518	YES	YES
49	a	983.84	1.49799	YES	YES
50	a	989.02	2.27174	YES	YES
51	a	1009.21	192.14258	YES	YES
52	a	1021.04	18.18539	YES	YES
53	a	1026.93	5.61587	YES	YES

54	a	1028.61	56.13879	YES	YES
55	a	1042.16	56.34744	YES	YES
56	a	1066.10	9.47152	YES	YES
57	a	1072.49	64.67920	YES	YES
58	a	1088.99	5.01927	YES	YES
59	a	1103.15	6.22259	YES	YES
60	a	1124.76	11.67000	YES	YES
61	a	1311.99	144.22979	YES	YES
62	a	1328.54	1.40219	YES	YES
63	a	1340.04	169.61497	YES	YES
64	a	1346.59	4.03306	YES	YES
65	a	1398.60	35.03116	YES	YES
66	a	1405.54	16.40808	YES	YES
67	a	1409.12	44.36596	YES	YES
68	a	1415.97	25.98634	YES	YES
69	a	1421.06	9.18831	YES	YES
70	a	1426.83	11.83706	YES	YES
71	a	1454.81	291.70349	YES	YES
72	a	1533.88	80.12970	YES	YES
73	a	1650.45	205.92995	YES	YES
74	a	1702.97	27.95544	YES	YES
75	a	2277.69	122.24212	YES	YES
76	a	2287.44	19.61819	YES	YES
77	a	2336.37	101.53160	YES	YES
78	a	2360.25	37.68404	YES	YES
79	a	2364.70	107.59399	YES	YES
80	a	2375.65	24.83262	YES	YES
81	a	2377.72	23.94826	YES	YES
82	a	2955.18	17.45430	YES	YES
83	a	2959.26	3.17977	YES	YES
84	a	2959.60	12.35160	YES	YES
85	a	3041.53	5.26916	YES	YES
86	a	3043.28	2.17298	YES	YES
87	a	3045.03	2.81475	YES	YES
88	a	3064.15	2.29146	YES	YES
89	a	3074.41	7.82588	YES	YES
90	a	3076.06	2.71028	YES	YES

* zero point VIBRATIONAL energy : 0.2059839 Hartree *

Cis TS_{25}_pftx

bp86_svp SCF energy = -1354.4304500110
pbe0_tzvpp SCF energy = -1354.210524730

xyz Coordinates

30

C	-0.33971	0.26877	2.84719
C	-0.47737	0.68119	4.29290
H	0.53071	0.92687	4.69586
H	-0.88779	-0.15378	4.89767
H	-1.11850	1.58171	4.38393
C	-0.22420	0.22176	-2.54090
C	-0.84290	1.08841	-3.63833
H	-1.54051	0.46600	-4.24036
H	-0.04384	1.43396	-4.32866
H	-1.38876	1.96030	-3.22608
H	-2.84510	-1.26745	-0.82390
H	-3.10141	-0.50601	1.19663
H	-2.39448	-2.53019	0.89098
H	0.06658	-2.98817	-1.66327
H	2.10926	-2.26080	-1.31914
H	1.04974	-3.34334	0.22554
O	-0.07035	-0.94567	2.54130
O	-0.45051	1.12794	1.90178
O	-0.52320	0.60701	-1.33052
O	0.49385	-0.74903	-2.83861
P	-2.11828	-1.20515	0.41181
P	0.82023	-2.24893	-0.69384
Ru	0.06646	-0.39966	0.40227
C	2.17919	-0.19113	1.01108
C	1.94575	0.71821	0.06951
C	2.34988	1.53488	-1.10763
H	1.97611	1.24482	1.17003
H	3.35313	1.98847	-0.94784
H	1.60772	2.33178	-1.31669
H	2.39122	0.86309	-1.99094

Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-564.57	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	26.11	0.80504	YES	YES
9	a	44.14	1.61250	YES	YES
10	a	58.61	0.26376	YES	YES
11	a	71.06	3.40105	YES	YES
12	a	74.92	0.32427	YES	YES
13	a	77.89	0.82484	YES	YES
14	a	83.18	4.05826	YES	YES
15	a	101.52	1.77840	YES	YES
16	a	112.62	0.87341	YES	YES
17	a	124.19	2.53837	YES	YES
18	a	149.42	3.96978	YES	YES
19	a	158.85	27.21875	YES	YES
20	a	174.80	1.49704	YES	YES
21	a	194.09	2.44465	YES	YES
22	a	195.40	0.35636	YES	YES
23	a	208.52	0.96592	YES	YES
24	a	234.76	10.09564	YES	YES
25	a	243.26	5.68393	YES	YES
26	a	260.80	7.39007	YES	YES
27	a	293.79	15.48848	YES	YES
28	a	299.04	24.27750	YES	YES
29	a	313.98	21.46154	YES	YES
30	a	336.55	0.35836	YES	YES
31	a	355.50	12.87900	YES	YES
32	a	363.76	6.12422	YES	YES
33	a	403.89	4.83716	YES	YES
34	a	470.11	2.12443	YES	YES
35	a	487.10	2.81073	YES	YES
36	a	506.80	2.30712	YES	YES
37	a	529.90	4.95076	YES	YES
38	a	545.29	4.52881	YES	YES
39	a	592.30	5.34545	YES	YES
40	a	605.30	4.04671	YES	YES
41	a	609.31	3.77641	YES	YES
42	a	624.18	4.90858	YES	YES
43	a	668.48	95.74612	YES	YES
44	a	670.96	13.17298	YES	YES
45	a	789.82	3.52713	YES	YES
46	a	896.14	11.10233	YES	YES
47	a	926.95	4.23263	YES	YES
48	a	939.70	30.15518	YES	YES
49	a	983.84	1.49799	YES	YES
50	a	989.02	2.27174	YES	YES
51	a	1009.21	192.14258	YES	YES
52	a	1021.04	18.18539	YES	YES
53	a	1026.93	5.61587	YES	YES
54	a	1028.61	56.13879	YES	YES
55	a	1042.16	56.34744	YES	YES
56	a	1066.10	9.47152	YES	YES
57	a	1072.49	64.67920	YES	YES
58	a	1088.99	5.01927	YES	YES
59	a	1103.15	6.22259	YES	YES
60	a	1124.76	11.67000	YES	YES
61	a	1311.99	144.22979	YES	YES
62	a	1328.54	1.40219	YES	YES
63	a	1340.04	169.61497	YES	YES
64	a	1346.59	4.03306	YES	YES

65	a	1398.60	35.03116	YES	YES
66	a	1405.54	16.40808	YES	YES
67	a	1409.12	44.36596	YES	YES
68	a	1415.97	25.98634	YES	YES
69	a	1421.06	9.18831	YES	YES
70	a	1426.83	11.83706	YES	YES
71	a	1454.81	291.70349	YES	YES
72	a	1533.88	80.12970	YES	YES
73	a	1650.45	205.92995	YES	YES
74	a	1702.97	27.95544	YES	YES
75	a	2277.69	122.24212	YES	YES
76	a	2287.44	19.61819	YES	YES
77	a	2336.37	101.53160	YES	YES
78	a	2360.25	37.68404	YES	YES
79	a	2364.70	107.59399	YES	YES
80	a	2375.65	24.83262	YES	YES
81	a	2377.72	23.94826	YES	YES
82	a	2955.18	17.45430	YES	YES
83	a	2959.26	3.17977	YES	YES
84	a	2959.60	12.35160	YES	YES
85	a	3041.53	5.26916	YES	YES
86	a	3043.28	2.17298	YES	YES
87	a	3045.03	2.81475	YES	YES
88	a	3064.15	2.29146	YES	YES
89	a	3074.41	7.82588	YES	YES
90	a	3076.06	2.71028	YES	YES

* zero point VIBRATIONAL energy : 0.2059839 Hartree *

Cis TS_{25}_pfty

bp86_svp SCF energy = -1354.4309687560
pbe0_tzvpp SCF energy = -1354.212275522

xyz Coordinates

30

C	-0.02727	-0.64423	-2.77194
C	0.02832	-1.23085	-4.16111
H	1.08719	-1.25842	-4.50319
H	-0.54255	-0.59886	-4.87157
H	-0.36234	-2.26900	-4.16150
C	-1.01071	-0.16501	2.32255
C	-1.01111	-0.96652	3.62238
H	-1.24171	-0.29539	4.47550
H	-0.04898	-1.49040	3.79110
H	-1.82123	-1.72830	3.57302
H	-3.10078	1.53196	-0.16211
H	-3.07888	-0.63332	0.16466
H	-2.84067	0.17315	-1.83236
H	0.41538	2.61479	1.89272
H	0.79078	3.45503	-0.06621
H	-1.24916	3.16862	0.61683
O	-0.14891	0.61728	-2.59992
O	0.08342	-1.39095	-1.73299
O	-0.09125	-0.52184	1.47091
O	-1.86461	0.72296	2.12607
P	-2.32090	0.38049	-0.50266
P	-0.02158	2.42685	0.53157
Ru	0.01617	0.37423	-0.42643
C	2.17969	-0.04079	-0.00574
C	2.12433	0.83751	-0.99647
C	2.76942	-0.62945	1.22698
H	2.41214	-0.58390	-1.07707
H	2.30204	-1.60416	1.47086
H	2.56287	0.05815	2.07286
H	3.87031	-0.74809	1.11837

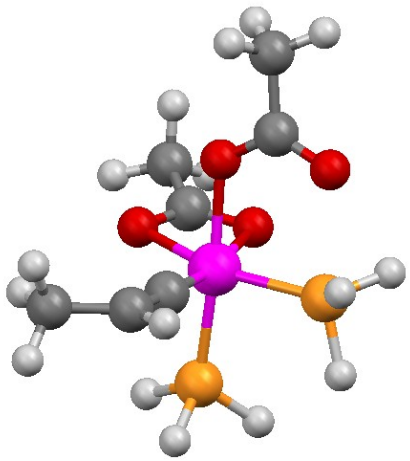
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-560.62	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	25.68	0.03157	YES	YES
9	a	36.55	3.97484	YES	YES
10	a	53.78	1.89680	YES	YES
11	a	64.16	2.14346	YES	YES
12	a	66.32	2.19424	YES	YES
13	a	81.89	4.11656	YES	YES
14	a	99.41	1.66369	YES	YES
15	a	108.68	0.96847	YES	YES
16	a	131.32	3.72731	YES	YES
17	a	141.21	0.48253	YES	YES
18	a	165.22	8.68149	YES	YES
19	a	171.14	4.28363	YES	YES
20	a	180.56	11.87009	YES	YES
21	a	189.05	0.09699	YES	YES
22	a	195.42	1.48054	YES	YES
23	a	206.98	0.98990	YES	YES
24	a	226.62	12.16652	YES	YES
25	a	240.45	8.79106	YES	YES
26	a	265.97	0.16001	YES	YES
27	a	283.80	1.60360	YES	YES
28	a	292.50	23.70140	YES	YES
29	a	303.79	17.03178	YES	YES
30	a	314.99	22.45052	YES	YES
31	a	347.46	3.55849	YES	YES
32	a	368.64	11.81720	YES	YES
33	a	395.78	4.80350	YES	YES
34	a	474.08	3.82785	YES	YES
35	a	492.54	3.50043	YES	YES
36	a	503.39	0.81838	YES	YES
37	a	540.12	11.20506	YES	YES
38	a	583.99	7.36557	YES	YES
39	a	588.68	4.58093	YES	YES
40	a	598.22	4.03557	YES	YES
41	a	608.00	3.13714	YES	YES
42	a	618.11	3.59287	YES	YES
43	a	670.51	93.20381	YES	YES
44	a	677.04	10.73153	YES	YES
45	a	785.77	4.57406	YES	YES
46	a	893.17	10.20671	YES	YES
47	a	931.84	5.76604	YES	YES
48	a	941.31	31.37677	YES	YES
49	a	982.83	1.68239	YES	YES
50	a	988.86	2.32527	YES	YES
51	a	1011.96	155.18195	YES	YES
52	a	1020.68	31.78744	YES	YES
53	a	1023.06	19.33386	YES	YES
54	a	1027.07	14.79959	YES	YES
55	a	1052.46	118.73817	YES	YES
56	a	1060.76	4.50643	YES	YES
57	a	1070.61	14.29115	YES	YES
58	a	1078.13	11.64345	YES	YES
59	a	1108.46	8.49386	YES	YES
60	a	1113.70	5.74690	YES	YES
61	a	1317.43	74.10646	YES	YES
62	a	1328.45	1.09470	YES	YES
63	a	1345.09	86.02319	YES	YES
64	a	1351.11	131.36464	YES	YES

65	a	1398.38	34.69860	YES	YES
66	a	1401.09	11.96536	YES	YES
67	a	1409.63	44.86905	YES	YES
68	a	1409.73	4.25397	YES	YES
69	a	1413.46	23.07903	YES	YES
70	a	1420.91	18.54447	YES	YES
71	a	1457.62	288.82350	YES	YES
72	a	1536.80	79.17747	YES	YES
73	a	1632.57	187.63053	YES	YES
74	a	1720.78	31.11974	YES	YES
75	a	2275.89	9.48333	YES	YES
76	a	2306.71	92.73013	YES	YES
77	a	2317.62	119.78891	YES	YES
78	a	2328.34	88.49806	YES	YES
79	a	2349.28	50.20858	YES	YES
80	a	2380.83	67.83874	YES	YES
81	a	2396.17	20.80270	YES	YES
82	a	2958.10	11.66021	YES	YES
83	a	2960.08	3.11208	YES	YES
84	a	2960.27	17.13251	YES	YES
85	a	3042.78	6.19378	YES	YES
86	a	3046.14	2.53683	YES	YES
87	a	3050.82	4.01718	YES	YES
88	a	3075.17	8.35408	YES	YES
89	a	3075.36	0.65881	YES	YES
90	a	3078.55	2.40797	YES	YES

* zero point VIBRATIONAL energy : 0.2067612 Hartree *

Cis 5_afm



bp86_svp SCF energy = -1354.5255940740
pbe0_tzvpp SCF energy = -1354.301851776

xyz Coordinates

30

C	2.47560	-0.54650	-0.34807
C	3.79544	-1.07787	-0.85266
H	3.63147	-1.56769	-1.83855
H	4.20569	-1.83749	-0.15610
H	4.51698	-0.24802	-0.99642
C	-0.95150	-0.24148	-2.46869
C	-1.10321	-1.06441	-3.74523
H	-1.53357	-0.44428	-4.55635
H	-1.77562	-1.92859	-3.54928
H	-0.12077	-1.47739	-4.05738
H	1.17308	2.34103	2.42434
H	1.85578	0.36551	2.99361
H	-0.18620	0.97886	3.42297
H	-1.20491	2.94804	0.85543
H	-0.61211	2.90675	-1.21532
H	-2.55721	2.01720	-0.52573
O	1.71631	-1.29955	0.36791
O	2.07473	0.62715	-0.63761
O	-0.26816	-0.82347	-1.53586
O	-1.47812	0.89032	-2.38629
P	0.73808	0.97234	2.32032
P	-1.15905	2.00642	-0.25525
Ru	0.08836	0.11276	0.30615
C	-1.38424	-0.64231	1.06823
C	-2.45336	-1.22069	1.60336
H	-3.41594	-0.67740	1.49722
C	-2.46982	-2.57516	2.28397
H	-2.85798	-2.49791	3.32572
H	-1.45205	-3.01648	2.32423
H	-3.12865	-3.28728	1.73584

Vibrational Spectrum

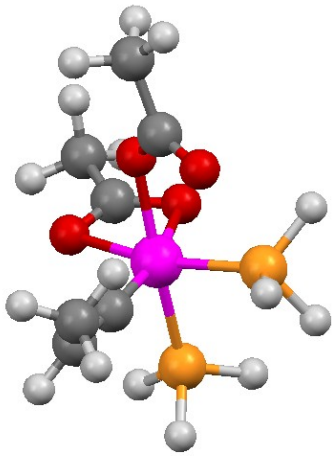
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	25.17	0.12139	YES	YES
8	a	41.50	0.82709	YES	YES
9	a	43.21	0.62849	YES	YES
10	a	49.77	0.48156	YES	YES
11	a	57.95	0.06082	YES	YES
12	a	70.20	0.91121	YES	YES
13	a	74.47	0.44939	YES	YES
14	a	75.35	0.18986	YES	YES
15	a	92.88	2.08596	YES	YES
16	a	106.20	7.91089	YES	YES
17	a	111.84	5.52514	YES	YES
18	a	136.24	0.60060	YES	YES
19	a	161.96	9.69634	YES	YES
20	a	167.23	9.15060	YES	YES
21	a	176.08	2.12773	YES	YES
22	a	204.07	6.94698	YES	YES
23	a	212.69	3.83812	YES	YES
24	a	219.41	5.28791	YES	YES
25	a	260.81	3.21632	YES	YES
26	a	272.90	21.14835	YES	YES
27	a	306.88	25.47337	YES	YES
28	a	343.63	1.23999	YES	YES
29	a	355.87	15.33865	YES	YES
30	a	403.34	1.35536	YES	YES
31	a	456.52	1.27033	YES	YES
32	a	467.39	1.57907	YES	YES
33	a	503.44	8.68448	YES	YES
34	a	513.80	0.30025	YES	YES
35	a	552.50	4.43756	YES	YES
36	a	565.07	0.21766	YES	YES
37	a	586.12	9.25764	YES	YES
38	a	593.49	9.61889	YES	YES
39	a	606.63	18.47299	YES	YES
40	a	612.01	5.74737	YES	YES
41	a	647.50	11.85135	YES	YES
42	a	657.82	14.50563	YES	YES
43	a	672.87	55.28173	YES	YES
44	a	680.41	59.03550	YES	YES
45	a	935.08	3.43469	YES	YES
46	a	938.13	13.31620	YES	YES

47	a	941.00	43.12239	YES	YES
48	a	982.91	40.31877	YES	YES
49	a	985.17	23.54374	YES	YES
50	a	995.36	22.86514	YES	YES
51	a	1007.19	0.19863	YES	YES
52	a	1023.24	128.87000	YES	YES
53	a	1024.09	7.55502	YES	YES
54	a	1027.24	53.16192	YES	YES
55	a	1049.15	3.36983	YES	YES
56	a	1088.12	75.05447	YES	YES
57	a	1093.49	23.76789	YES	YES
58	a	1097.93	17.95251	YES	YES
59	a	1147.98	8.00999	YES	YES
60	a	1189.14	41.49968	YES	YES
61	a	1320.13	31.38025	YES	YES
62	a	1327.25	1.85426	YES	YES
63	a	1354.60	22.33021	YES	YES
64	a	1376.56	319.92489	YES	YES
65	a	1398.42	42.22300	YES	YES
66	a	1405.98	20.11865	YES	YES
67	a	1409.32	40.70506	YES	YES
68	a	1418.64	19.19867	YES	YES
69	a	1421.98	6.07757	YES	YES
70	a	1428.81	7.53613	YES	YES
71	a	1456.89	309.39943	YES	YES
72	a	1553.01	102.40488	YES	YES
73	a	1629.15	256.60239	YES	YES
74	a	1712.02	214.20125	YES	YES
75	a	2211.22	190.64165	YES	YES
76	a	2331.49	154.60289	YES	YES
77	a	2335.94	43.66431	YES	YES
78	a	2341.20	26.74095	YES	YES
79	a	2414.48	35.38426	YES	YES
80	a	2441.42	9.03159	YES	YES
81	a	2929.35	65.19806	YES	YES
82	a	2961.03	9.48750	YES	YES
83	a	2961.30	3.48978	YES	YES
84	a	2996.14	12.65505	YES	YES
85	a	3019.85	5.17050	YES	YES
86	a	3044.83	5.47214	YES	YES
87	a	3047.40	3.31995	YES	YES
88	a	3048.55	6.13867	YES	YES
89	a	3077.96	3.00147	YES	YES
90	a	3078.88	9.41896	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2120158 Hartree *

Cis 5_afn



bp86_svp SCF energy = -1354.5255450130
pbe0_tzvpp SCF energy = -1354.301572542

xyz Coordinates

30

C	1.08186	-0.43439	2.40561
C	2.03560	-0.76922	3.52814
H	3.06671	-0.82719	3.11360
H	1.78846	-1.75361	3.97532
H	2.02099	0.02676	4.30072
C	1.92369	0.24731	-1.73298
C	3.34138	-0.09973	-2.18023
H	3.59980	0.45396	-3.10472
H	3.40299	-1.19206	-2.38306
H	4.07259	0.12601	-1.37588
H	-2.44351	1.64347	2.04977
H	-2.31715	-0.41031	2.74431
H	-3.46986	0.06686	0.96611
H	-1.79148	2.71996	-0.51940
H	0.23344	2.87848	-1.23474
H	-1.29175	1.73708	-2.37272
O	0.52755	-1.37444	1.73298
O	0.83829	0.78066	2.08992
O	1.64893	-0.13910	-0.51883
O	1.13264	0.82940	-2.50041
P	-2.17244	0.33380	1.52183
P	-0.75271	1.85970	-1.05828
Ru	-0.26452	0.03387	0.26972
C	-1.11065	-1.03467	-0.93809
C	-1.69279	-1.85695	-1.80318
H	-2.41084	-2.59959	-1.39761
C	-1.38131	-1.88534	-3.28862
H	-0.98130	-2.88094	-3.58958
H	-0.62464	-1.11506	-3.54672
H	-2.29749	-1.69904	-3.89522

Vibrational Spectrum

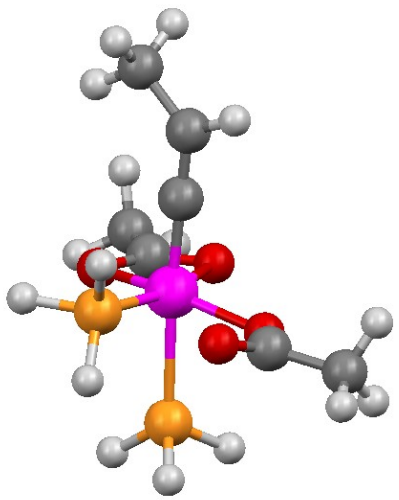
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	32.16	0.60070	YES	YES
8	a	38.40	0.84260	YES	YES
9	a	49.78	0.96864	YES	YES
10	a	57.70	0.29234	YES	YES
11	a	68.29	1.67141	YES	YES
12	a	71.50	0.89217	YES	YES
13	a	75.35	0.32558	YES	YES
14	a	83.69	0.44995	YES	YES
15	a	90.80	3.06393	YES	YES
16	a	98.40	4.55963	YES	YES
17	a	122.74	4.75623	YES	YES
18	a	132.45	3.18877	YES	YES
19	a	159.06	13.65933	YES	YES
20	a	174.86	2.38797	YES	YES
21	a	196.43	0.14433	YES	YES
22	a	198.46	4.71896	YES	YES
23	a	206.20	5.47959	YES	YES
24	a	216.24	2.56671	YES	YES
25	a	259.26	5.22014	YES	YES
26	a	274.41	19.80046	YES	YES
27	a	305.51	23.91612	YES	YES
28	a	336.06	1.12805	YES	YES
29	a	343.01	1.95371	YES	YES
30	a	355.99	16.11389	YES	YES
31	a	457.14	3.53928	YES	YES
32	a	469.16	1.18449	YES	YES
33	a	499.43	4.02432	YES	YES
34	a	514.20	1.27248	YES	YES
35	a	555.69	2.57016	YES	YES
36	a	563.71	8.58781	YES	YES
37	a	584.38	7.04168	YES	YES
38	a	596.94	8.32083	YES	YES
39	a	603.02	7.49440	YES	YES
40	a	607.07	24.66162	YES	YES
41	a	634.63	11.13924	YES	YES
42	a	646.69	13.33404	YES	YES
43	a	676.11	45.85345	YES	YES
44	a	679.18	63.30485	YES	YES
45	a	931.23	4.60142	YES	YES

46	a	935.70	21.35176	YES	YES
47	a	941.31	42.01564	YES	YES
48	a	983.60	1.26066	YES	YES
49	a	992.10	10.26854	YES	YES
50	a	1007.83	36.16007	YES	YES
51	a	1010.89	82.99536	YES	YES
52	a	1024.21	8.33345	YES	YES
53	a	1024.94	94.94984	YES	YES
54	a	1028.06	65.44279	YES	YES
55	a	1048.43	4.17586	YES	YES
56	a	1085.49	81.58565	YES	YES
57	a	1094.16	8.14168	YES	YES
58	a	1101.10	6.09788	YES	YES
59	a	1128.24	6.51451	YES	YES
60	a	1185.48	36.92696	YES	YES
61	a	1313.32	92.76519	YES	YES
62	a	1324.95	1.27674	YES	YES
63	a	1350.53	81.81655	YES	YES
64	a	1355.89	214.49553	YES	YES
65	a	1399.13	34.03233	YES	YES
66	a	1406.39	15.30654	YES	YES
67	a	1408.95	48.27221	YES	YES
68	a	1418.38	16.31658	YES	YES
69	a	1427.14	7.48393	YES	YES
70	a	1432.70	5.58134	YES	YES
71	a	1456.70	320.10336	YES	YES
72	a	1543.26	90.99592	YES	YES
73	a	1636.32	206.07872	YES	YES
74	a	1706.50	211.40249	YES	YES
75	a	2242.07	168.27050	YES	YES
76	a	2340.97	136.23608	YES	YES
77	a	2347.85	39.22569	YES	YES
78	a	2358.76	25.99400	YES	YES
79	a	2399.69	47.29000	YES	YES
80	a	2425.29	14.04534	YES	YES
81	a	2927.08	65.50677	YES	YES
82	a	2959.86	8.98978	YES	YES
83	a	2961.44	3.17474	YES	YES
84	a	2994.49	12.89073	YES	YES
85	a	3027.20	3.63444	YES	YES
86	a	3043.98	5.59893	YES	YES
87	a	3047.71	3.86885	YES	YES
88	a	3050.27	1.72401	YES	YES
89	a	3076.81	3.43597	YES	YES
90	a	3078.59	8.39835	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2119131 Hartree *

Cis 5_pfex



bp86_svp SCF energy = -1354.5075557010
pbe0_tzvpp SCF energy = -1354.279668639

xyz Coordinates

30

C	2.56437	0.76537	-0.41928
C	4.02546	1.08986	-0.61841
H	4.59151	0.14219	-0.76132
H	4.43923	1.60026	0.27548
H	4.16281	1.71404	-1.52439
C	-2.74172	-0.08306	-0.73773
C	-3.80284	0.12478	-1.81660
H	-4.80823	0.18753	-1.35339
H	-3.79138	-0.75123	-2.50336
H	-3.59356	1.02863	-2.42471
H	-0.36089	3.38542	-0.73775
H	0.46167	3.39561	1.25798
H	-1.62058	2.92722	0.94771
H	-1.48858	-1.91742	2.01117
H	-0.04443	-0.67981	3.05391
H	-1.97450	0.16505	2.56695
O	2.12985	0.48401	0.76522
O	1.74819	0.73432	-1.39256
O	-1.55105	0.32865	-1.09942
O	-3.02269	-0.62222	0.34239
P	-0.34046	2.54279	0.42410
P	-0.94824	-0.59821	1.92335
Ru	0.14635	0.08237	0.05773
C	0.41892	-1.68653	-0.31365
C	0.60004	-2.97116	-0.59441
H	-0.17321	-3.45138	-1.23141
C	1.78049	-3.81195	-0.15051
H	1.44183	-4.69942	0.43217
H	2.47573	-3.22603	0.48667
H	2.35262	-4.19208	-1.02805

Vibrational Spectrum

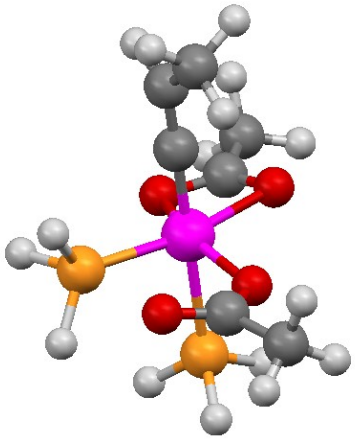
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	29.69	0.38599	YES	YES
8	a	37.59	1.22490	YES	YES
9	a	48.33	0.62728	YES	YES
10	a	59.41	0.25644	YES	YES
11	a	61.52	0.30737	YES	YES
12	a	64.37	1.17786	YES	YES
13	a	74.62	0.97710	YES	YES
14	a	74.73	2.94815	YES	YES
15	a	76.96	0.48528	YES	YES
16	a	96.84	3.35099	YES	YES
17	a	114.35	1.73688	YES	YES
18	a	129.88	0.55043	YES	YES
19	a	151.91	2.66040	YES	YES
20	a	158.64	14.87665	YES	YES
21	a	169.43	5.00824	YES	YES
22	a	191.46	1.06770	YES	YES
23	a	197.29	4.33519	YES	YES
24	a	207.10	0.76702	YES	YES
25	a	227.06	5.40520	YES	YES
26	a	276.85	8.85162	YES	YES
27	a	286.09	16.77468	YES	YES
28	a	324.04	28.18961	YES	YES
29	a	339.31	0.33527	YES	YES
30	a	370.34	14.06979	YES	YES
31	a	386.95	1.42587	YES	YES
32	a	411.12	0.64944	YES	YES
33	a	471.46	2.05309	YES	YES
34	a	480.98	1.59788	YES	YES
35	a	490.72	3.60283	YES	YES
36	a	517.88	1.34105	YES	YES
37	a	592.59	3.57001	YES	YES
38	a	601.30	0.75618	YES	YES
39	a	610.57	6.27558	YES	YES
40	a	623.11	5.58691	YES	YES
41	a	630.87	25.24192	YES	YES
42	a	646.78	1.53248	YES	YES
43	a	673.93	65.06882	YES	YES
44	a	676.04	53.90468	YES	YES
45	a	928.52	4.05444	YES	YES

46	a	937.93	15.85971	YES	YES
47	a	939.12	26.96468	YES	YES
48	a	981.69	2.15156	YES	YES
49	a	990.66	9.07154	YES	YES
50	a	993.53	166.55705	YES	YES
51	a	1005.56	0.01979	YES	YES
52	a	1022.56	33.16902	YES	YES
53	a	1023.55	49.95036	YES	YES
54	a	1027.24	10.84172	YES	YES
55	a	1045.11	1.35118	YES	YES
56	a	1074.39	80.03269	YES	YES
57	a	1098.48	3.24167	YES	YES
58	a	1102.00	4.43101	YES	YES
59	a	1124.95	9.91577	YES	YES
60	a	1186.02	34.28177	YES	YES
61	a	1303.31	256.30256	YES	YES
62	a	1326.98	3.11148	YES	YES
63	a	1341.77	143.84973	YES	YES
64	a	1351.83	23.64690	YES	YES
65	a	1396.36	53.51045	YES	YES
66	a	1408.98	40.45364	YES	YES
67	a	1409.47	21.88536	YES	YES
68	a	1419.37	16.01121	YES	YES
69	a	1421.50	3.88491	YES	YES
70	a	1427.69	2.55622	YES	YES
71	a	1445.10	255.29243	YES	YES
72	a	1554.03	106.15393	YES	YES
73	a	1666.93	212.34035	YES	YES
74	a	1706.60	134.23826	YES	YES
75	a	2263.41	148.02577	YES	YES
76	a	2353.95	95.01690	YES	YES
77	a	2375.76	41.41493	YES	YES
78	a	2377.78	46.75091	YES	YES
79	a	2379.24	35.31985	YES	YES
80	a	2407.47	20.79874	YES	YES
81	a	2928.74	66.50234	YES	YES
82	a	2959.47	9.50326	YES	YES
83	a	2960.68	2.44974	YES	YES
84	a	2995.67	12.17980	YES	YES
85	a	3016.73	3.40469	YES	YES
86	a	3044.70	6.89116	YES	YES
87	a	3045.76	7.94613	YES	YES
88	a	3046.43	2.05334	YES	YES
89	a	3077.22	7.31874	YES	YES
90	a	3080.12	2.39897	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2108592 Hartree *

Cis 5_pfey



bp86_svp SCF energy = -1354.5074089560
pbe0_tzvpp SCF energy = -1354.279832483

xyz Coordinates

30

C	2.72171	0.47142	-0.26798
C	4.19280	0.70842	-0.51079
H	4.40614	0.58348	-1.59591
H	4.80525	-0.03308	0.04240
H	4.47125	1.74127	-0.21978
C	-2.56090	0.75107	0.64916
C	-3.53569	1.87861	0.98436
H	-4.37770	1.48218	1.58847
H	-3.95893	2.27861	0.03583
H	-3.03238	2.71291	1.51347
H	1.61393	0.98602	3.04848
H	1.32966	-1.14066	3.18935
H	-0.35347	0.18902	3.42916
H	-1.85942	-2.38880	-0.84447
H	-0.06609	-3.17261	0.08857
H	-1.65303	-2.43276	1.35418
O	2.29130	-0.73533	-0.08978
O	1.88295	1.42515	-0.25686
O	-1.31683	1.14867	0.56076
O	-2.96597	-0.40547	0.45771
P	0.73354	-0.01992	2.51704
P	-0.93982	-2.01929	0.18367
Ru	0.24383	-0.08807	0.03060
C	-0.09095	-0.14528	-1.76628
C	-0.32223	-0.19963	-3.07212
H	0.41926	-0.76001	-3.68142
C	-1.47809	0.46251	-3.79535
H	-2.06884	-0.28625	-4.37131
H	-1.11051	1.22443	-4.52080
H	-2.16264	0.96772	-3.08295

Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	15.90	0.76810	YES	YES
8	a	17.28	0.66475	YES	YES
9	a	41.98	0.31102	YES	YES
10	a	48.17	0.17258	YES	YES
11	a	48.21	1.21019	YES	YES
12	a	50.10	1.11001	YES	YES
13	a	62.11	0.30353	YES	YES
14	a	73.00	3.63470	YES	YES
15	a	85.69	0.60166	YES	YES
16	a	96.16	3.37053	YES	YES
17	a	109.71	0.85772	YES	YES
18	a	128.31	0.12774	YES	YES
19	a	153.99	14.08390	YES	YES
20	a	158.67	2.85274	YES	YES
21	a	167.37	4.06198	YES	YES
22	a	184.74	4.04991	YES	YES
23	a	198.51	4.13502	YES	YES
24	a	207.21	0.15791	YES	YES
25	a	233.59	3.04879	YES	YES
26	a	277.80	8.56908	YES	YES
27	a	285.72	18.16172	YES	YES
28	a	325.12	28.25546	YES	YES
29	a	332.94	0.00877	YES	YES
30	a	367.18	14.63039	YES	YES
31	a	375.66	4.27317	YES	YES
32	a	410.66	0.55590	YES	YES
33	a	475.30	2.48181	YES	YES
34	a	483.04	0.51357	YES	YES
35	a	487.66	1.62691	YES	YES
36	a	516.97	1.33404	YES	YES
37	a	590.76	3.47593	YES	YES
38	a	600.46	0.83867	YES	YES
39	a	611.82	5.16210	YES	YES
40	a	621.09	9.97488	YES	YES
41	a	632.13	18.02860	YES	YES
42	a	642.10	3.10047	YES	YES
43	a	674.79	108.83347	YES	YES
44	a	676.21	18.76922	YES	YES
45	a	929.30	4.08242	YES	YES

46	a	936.95	16.59415	YES	YES
47	a	939.37	25.71349	YES	YES
48	a	981.29	2.43066	YES	YES
49	a	989.49	6.60749	YES	YES
50	a	992.86	162.55447	YES	YES
51	a	1005.26	0.17017	YES	YES
52	a	1021.14	44.08503	YES	YES
53	a	1022.13	39.99235	YES	YES
54	a	1026.49	10.61826	YES	YES
55	a	1044.88	0.96379	YES	YES
56	a	1074.09	83.68380	YES	YES
57	a	1093.04	4.68650	YES	YES
58	a	1106.12	7.90755	YES	YES
59	a	1125.10	11.28962	YES	YES
60	a	1187.37	36.98760	YES	YES
61	a	1305.10	213.29458	YES	YES
62	a	1325.58	3.15458	YES	YES
63	a	1339.27	157.21466	YES	YES
64	a	1350.17	20.75773	YES	YES
65	a	1396.28	57.85290	YES	YES
66	a	1408.49	47.62991	YES	YES
67	a	1410.54	17.28304	YES	YES
68	a	1419.14	5.64695	YES	YES
69	a	1419.87	17.12120	YES	YES
70	a	1424.79	7.04287	YES	YES
71	a	1443.28	247.18042	YES	YES
72	a	1554.63	108.94812	YES	YES
73	a	1663.93	209.65364	YES	YES
74	a	1706.94	133.13582	YES	YES
75	a	2261.19	153.10913	YES	YES
76	a	2344.30	104.19863	YES	YES
77	a	2368.83	17.70556	YES	YES
78	a	2376.40	80.90788	YES	YES
79	a	2388.56	24.75424	YES	YES
80	a	2409.39	19.70863	YES	YES
81	a	2930.66	61.49531	YES	YES
82	a	2959.09	10.02848	YES	YES
83	a	2961.33	2.40443	YES	YES
84	a	2997.45	11.84473	YES	YES
85	a	3010.96	2.41891	YES	YES
86	a	3044.41	6.92871	YES	YES
87	a	3046.94	2.73755	YES	YES
88	a	3052.28	6.55898	YES	YES
89	a	3075.69	6.98079	YES	YES
90	a	3080.18	2.42288	YES	YES

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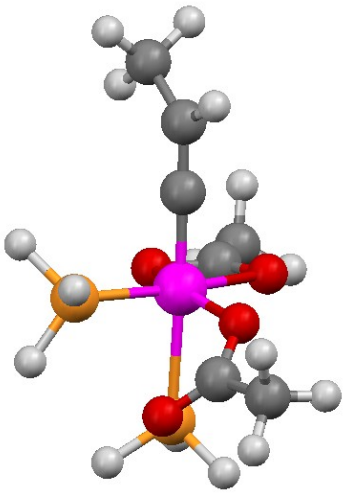
* zero point VIBRATIONAL energy : 0.2105451 Hartree *

Cis 5_pftx



bp86_svp SCF energy = -1354.5079515490
pbe0_tzvpp SCF energy = -1354.280648898

xyz Coordinates

30

C	-1.45648	-2.17531	0.39420
C	-2.27432	-3.43040	0.57428
H	-1.59174	-4.28049	0.79830
H	-2.83119	-3.67239	-0.35398
H	-2.97093	-3.31602	1.42957
C	0.32352	2.70305	0.76981
C	0.72280	3.76322	1.79320
H	0.38236	4.76351	1.45970
H	1.82981	3.77363	1.90373
H	0.29889	3.52352	2.79136
H	-2.68056	2.06293	0.25311
H	-3.29499	0.26978	-0.77477
H	-2.23334	1.80520	-1.85136
H	2.16276	1.72381	-1.55909
H	1.76812	-0.09529	-2.66641
H	0.35057	1.55003	-2.76524
O	-1.01212	-1.86076	-0.77745
O	-1.16451	-1.42057	1.37523
O	0.48360	1.48066	1.20038
O	-0.10363	3.01490	-0.35879
P	-2.11296	1.08173	-0.62075
P	1.07906	0.80715	-1.77986
Ru	0.02015	-0.13638	-0.01937
C	1.56431	-1.05606	0.35308
C	2.66912	-1.74905	0.59715
H	3.37997	-1.30305	1.32570
C	3.01369	-3.09764	-0.00447
H	3.97571	-3.05295	-0.56547
H	2.22175	-3.43990	-0.70342
H	3.13135	-3.87033	0.78984

Vibrational Spectrum

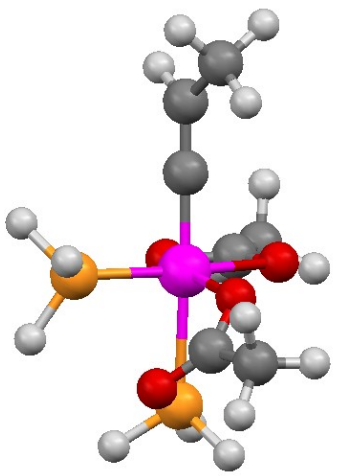
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	24.69	0.60796	YES	YES
8	a	33.14	0.49193	YES	YES
9	a	47.83	0.47831	YES	YES
10	a	56.05	0.37945	YES	YES
11	a	57.87	2.11201	YES	YES
12	a	69.23	0.63659	YES	YES
13	a	73.40	5.24009	YES	YES
14	a	102.58	3.91794	YES	YES
15	a	108.89	5.03363	YES	YES
16	a	122.96	1.81686	YES	YES
17	a	129.89	6.88471	YES	YES
18	a	153.54	4.67571	YES	YES
19	a	158.93	1.74471	YES	YES
20	a	170.41	1.00083	YES	YES
21	a	182.93	6.10710	YES	YES
22	a	189.98	0.24132	YES	YES
23	a	203.30	1.93643	YES	YES
24	a	217.51	0.52331	YES	YES
25	a	235.11	0.15538	YES	YES
26	a	243.85	2.04709	YES	YES
27	a	273.43	3.78688	YES	YES
28	a	293.93	19.91454	YES	YES
29	a	324.10	26.01440	YES	YES
30	a	368.70	11.00927	YES	YES
31	a	411.05	1.35135	YES	YES
32	a	452.87	2.21244	YES	YES
33	a	475.64	3.94244	YES	YES
34	a	486.05	1.62533	YES	YES
35	a	502.28	0.18173	YES	YES
36	a	513.31	0.55612	YES	YES
37	a	589.84	4.98288	YES	YES
38	a	597.93	1.43173	YES	YES
39	a	600.57	4.57198	YES	YES
40	a	613.00	5.70976	YES	YES
41	a	629.87	25.68260	YES	YES
42	a	645.70	2.78160	YES	YES
43	a	674.65	44.21124	YES	YES
44	a	676.07	66.68828	YES	YES
45	a	928.07	5.94584	YES	YES

46	a	934.52	19.38653	YES	YES
47	a	940.76	27.73532	YES	YES
48	a	980.54	1.96957	YES	YES
49	a	990.07	6.98288	YES	YES
50	a	1000.45	138.85130	YES	YES
51	a	1004.95	0.29477	YES	YES
52	a	1022.53	6.50672	YES	YES
53	a	1027.32	7.98142	YES	YES
54	a	1039.00	81.65734	YES	YES
55	a	1043.20	50.01639	YES	YES
56	a	1077.49	19.18080	YES	YES
57	a	1080.67	9.20129	YES	YES
58	a	1107.50	6.95865	YES	YES
59	a	1113.27	6.37251	YES	YES
60	a	1180.79	39.88138	YES	YES
61	a	1311.73	111.78012	YES	YES
62	a	1326.98	2.41599	YES	YES
63	a	1349.56	99.58797	YES	YES
64	a	1351.33	181.26073	YES	YES
65	a	1396.01	56.03403	YES	YES
66	a	1406.32	21.44436	YES	YES
67	a	1409.01	31.88535	YES	YES
68	a	1417.55	11.42244	YES	YES
69	a	1422.12	3.71615	YES	YES
70	a	1427.13	2.54750	YES	YES
71	a	1449.41	254.27346	YES	YES
72	a	1549.59	104.24251	YES	YES
73	a	1635.69	213.18836	YES	YES
74	a	1706.58	156.08595	YES	YES
75	a	2324.99	112.24904	YES	YES
76	a	2326.87	84.81728	YES	YES
77	a	2347.18	81.42057	YES	YES
78	a	2380.75	27.60613	YES	YES
79	a	2385.98	54.24699	YES	YES
80	a	2404.98	18.47801	YES	YES
81	a	2928.00	66.98523	YES	YES
82	a	2959.36	8.60561	YES	YES
83	a	2961.16	2.10694	YES	YES
84	a	2994.70	12.39779	YES	YES
85	a	3013.88	3.03460	YES	YES
86	a	3042.22	4.56734	YES	YES
87	a	3044.95	7.15207	YES	YES
88	a	3047.18	2.09010	YES	YES
89	a	3078.84	7.80759	YES	YES
90	a	3079.53	2.21944	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2110991 Hartree *

Cis 5_pfty



bp86_svp SCF energy = -1354.5079972080
pbe0_tzvpp SCF energy = -1354.280873660

xyz Coordinates

30

C	2.53373	0.48266	0.86863
C	3.94190	0.74985	1.33902
H	4.62556	0.74622	0.46068
H	4.27777	-0.04275	2.03851
H	4.00505	1.74762	1.81877
C	-2.60769	0.79580	0.11543
C	-3.70821	1.78126	-0.27128
H	-4.61243	1.60518	0.34435
H	-3.96754	1.64555	-1.34481
H	-3.35718	2.82799	-0.15112
H	-1.33438	0.90981	2.95181
H	0.53455	-0.06891	3.39858
H	-1.21310	-1.25321	2.96509
H	-2.10089	-1.94584	-1.30657
H	-0.25937	-3.05976	-1.06219
H	-1.55412	-2.73566	0.65436
O	2.10465	-0.73318	0.78407
O	1.75199	1.42495	0.52446
O	-1.44278	1.09415	-0.39319
O	-2.84205	-0.18861	0.84280
P	-0.51480	-0.13166	2.41145
P	-0.97200	-1.98561	-0.41913
Ru	0.21411	-0.10389	-0.01053
C	0.77525	-0.14072	-1.75754
C	1.20468	-0.18561	-3.01229
H	2.10285	-0.81032	-3.20713
C	0.59260	0.56711	-4.17753
H	1.33210	1.26720	-4.62985
H	-0.28762	1.16069	-3.85403
H	0.26626	-0.13398	-4.97993

Vibrational Spectrum

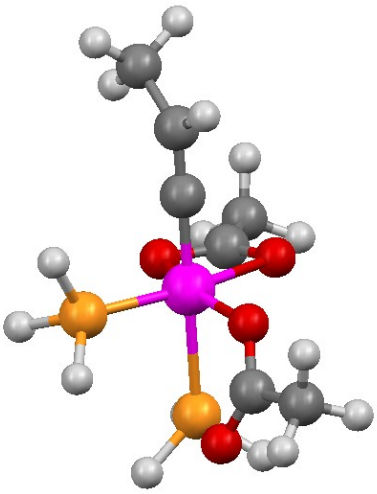
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	29.50	0.33021	YES	YES
8	a	34.90	0.65226	YES	YES
9	a	51.19	0.80760	YES	YES
10	a	55.04	0.60754	YES	YES
11	a	59.10	2.66443	YES	YES
12	a	65.98	0.27507	YES	YES
13	a	75.58	6.90871	YES	YES
14	a	93.95	1.60096	YES	YES
15	a	114.99	3.49418	YES	YES
16	a	119.22	3.49365	YES	YES
17	a	131.12	6.57591	YES	YES
18	a	152.08	5.20492	YES	YES
19	a	161.84	3.06720	YES	YES
20	a	167.77	0.68471	YES	YES
21	a	186.50	1.54086	YES	YES
22	a	195.34	2.64069	YES	YES
23	a	199.27	0.72675	YES	YES
24	a	211.64	0.87998	YES	YES
25	a	230.47	0.04745	YES	YES
26	a	239.53	2.86708	YES	YES
27	a	272.40	4.54468	YES	YES
28	a	292.35	20.51608	YES	YES
29	a	324.27	22.93178	YES	YES
30	a	363.50	12.58763	YES	YES
31	a	410.80	3.73611	YES	YES
32	a	455.27	2.70587	YES	YES
33	a	478.98	3.60096	YES	YES
34	a	483.36	0.95832	YES	YES
35	a	503.14	0.27618	YES	YES
36	a	512.85	0.53038	YES	YES
37	a	590.11	2.97340	YES	YES
38	a	596.91	2.18180	YES	YES
39	a	601.59	4.40391	YES	YES
40	a	615.66	9.20487	YES	YES
41	a	624.83	21.16610	YES	YES
42	a	643.85	4.16526	YES	YES
43	a	674.56	35.19707	YES	YES
44	a	676.92	80.68595	YES	YES
45	a	927.97	4.58425	YES	YES

46	a	934.72	16.26167	YES	YES
47	a	940.82	29.67929	YES	YES
48	a	981.03	1.91099	YES	YES
49	a	990.19	6.40220	YES	YES
50	a	1001.53	138.66655	YES	YES
51	a	1005.62	0.54787	YES	YES
52	a	1022.62	7.21217	YES	YES
53	a	1027.20	7.55355	YES	YES
54	a	1039.41	90.95072	YES	YES
55	a	1045.11	44.99063	YES	YES
56	a	1076.30	17.46771	YES	YES
57	a	1081.03	9.64368	YES	YES
58	a	1107.32	6.87855	YES	YES
59	a	1112.97	6.33527	YES	YES
60	a	1182.42	43.79010	YES	YES
61	a	1311.83	107.85238	YES	YES
62	a	1327.67	2.81561	YES	YES
63	a	1350.46	202.23208	YES	YES
64	a	1351.09	67.07823	YES	YES
65	a	1396.05	52.80617	YES	YES
66	a	1406.29	20.26727	YES	YES
67	a	1409.63	35.60424	YES	YES
68	a	1418.05	11.51582	YES	YES
69	a	1422.74	6.36761	YES	YES
70	a	1425.91	7.52716	YES	YES
71	a	1449.60	254.33386	YES	YES
72	a	1550.02	109.79626	YES	YES
73	a	1636.64	215.84773	YES	YES
74	a	1705.73	152.07175	YES	YES
75	a	2325.28	103.47200	YES	YES
76	a	2327.66	99.65717	YES	YES
77	a	2346.95	78.81539	YES	YES
78	a	2380.56	29.61306	YES	YES
79	a	2386.95	51.76038	YES	YES
80	a	2405.68	17.89440	YES	YES
81	a	2929.80	65.74236	YES	YES
82	a	2958.93	8.52941	YES	YES
83	a	2961.20	2.05221	YES	YES
84	a	2996.61	12.93523	YES	YES
85	a	3011.52	2.64159	YES	YES
86	a	3041.93	4.87107	YES	YES
87	a	3047.19	2.28489	YES	YES
88	a	3051.27	5.76076	YES	YES
89	a	3079.21	7.71783	YES	YES
90	a	3080.13	2.24940	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2111069 Hartree *

Cis 5_pfpx



bp86_svp SCF energy = -1354.5060607760

pbe0_tzvpp SCF energy = -1354.278450226

xyz Coordinates

30

C	1.61243	-1.98244	-0.48444
C	2.55133	-3.13294	-0.74980
H	1.95877	-4.02392	-1.05651
H	3.11906	-3.39444	0.16633
H	3.24281	-2.88091	-1.57929
C	-0.42104	2.71494	-0.81944
C	-1.04716	3.71036	-1.79496
H	-1.14795	4.70160	-1.30733
H	-2.02905	3.35559	-2.16814
H	-0.36911	3.82832	-2.66999
H	2.69102	1.99993	-0.29307
H	3.09456	0.36552	1.04902
H	2.07268	2.10258	1.79855
H	-2.52557	0.20478	2.06541
H	-0.67948	0.09546	3.20554
H	-1.23193	1.95630	2.22654
O	1.14547	-1.79370	0.70502
O	1.23947	-1.19506	-1.41172
O	-0.77921	1.48033	-1.03604
O	0.37940	3.10489	0.05174
P	1.98600	1.22178	0.67622
P	-1.13887	0.55481	1.92018
Ru	-0.05353	-0.13469	0.07357
C	-1.50296	-1.17899	-0.36260
C	-2.54132	-1.95045	-0.65414
H	-3.30823	-1.50715	-1.32524
C	-2.73661	-3.37995	-0.18855
H	-3.68897	-3.48902	0.37939
H	-1.90305	-3.70631	0.46816
H	-2.78742	-4.07768	-1.05588

Vibrational Spectrum

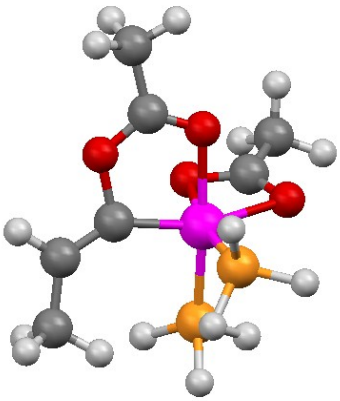
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.14	0.21766	YES	YES
8	a	34.12	0.36893	YES	YES
9	a	37.85	0.17943	YES	YES
10	a	50.33	0.22350	YES	YES
11	a	52.65	0.37226	YES	YES
12	a	54.26	0.61730	YES	YES
13	a	64.09	2.46029	YES	YES
14	a	73.92	1.46315	YES	YES
15	a	93.89	4.88134	YES	YES
16	a	104.47	3.47380	YES	YES
17	a	123.86	1.59118	YES	YES
18	a	141.30	5.17273	YES	YES
19	a	157.57	1.95420	YES	YES
20	a	167.52	2.07516	YES	YES
21	a	172.04	0.37622	YES	YES
22	a	177.41	0.64051	YES	YES
23	a	186.03	15.47937	YES	YES
24	a	214.94	0.38295	YES	YES
25	a	236.22	2.35499	YES	YES
26	a	272.13	7.33966	YES	YES
27	a	289.11	17.96520	YES	YES
28	a	319.07	4.19377	YES	YES
29	a	324.10	23.60342	YES	YES
30	a	374.48	12.26140	YES	YES
31	a	431.81	1.41219	YES	YES
32	a	474.25	4.09644	YES	YES
33	a	483.72	1.81420	YES	YES
34	a	494.30	1.16215	YES	YES
35	a	512.34	1.65862	YES	YES
36	a	542.16	1.11677	YES	YES
37	a	584.78	1.59069	YES	YES
38	a	593.26	1.21269	YES	YES
39	a	602.59	4.00959	YES	YES
40	a	604.19	0.71823	YES	YES
41	a	633.36	31.24173	YES	YES
42	a	646.11	3.79459	YES	YES
43	a	670.75	16.70427	YES	YES
44	a	676.89	85.08393	YES	YES
45	a	929.77	5.25977	YES	YES

46	a	935.05	18.18070	YES	YES
47	a	940.32	27.10413	YES	YES
48	a	981.31	1.53787	YES	YES
49	a	992.60	4.41664	YES	YES
50	a	999.54	138.93228	YES	YES
51	a	1006.95	0.26313	YES	YES
52	a	1022.05	6.16987	YES	YES
53	a	1027.18	5.32580	YES	YES
54	a	1029.44	137.11072	YES	YES
55	a	1042.89	11.60993	YES	YES
56	a	1072.80	27.93116	YES	YES
57	a	1091.42	7.75468	YES	YES
58	a	1101.51	10.82205	YES	YES
59	a	1125.14	9.76776	YES	YES
60	a	1179.99	37.23795	YES	YES
61	a	1315.61	112.95706	YES	YES
62	a	1328.08	2.01682	YES	YES
63	a	1347.64	238.21257	YES	YES
64	a	1351.14	20.54848	YES	YES
65	a	1395.40	56.20522	YES	YES
66	a	1409.47	26.22882	YES	YES
67	a	1410.02	29.91250	YES	YES
68	a	1420.40	19.20266	YES	YES
69	a	1423.03	4.14922	YES	YES
70	a	1427.65	2.78078	YES	YES
71	a	1450.85	247.17136	YES	YES
72	a	1547.52	99.44552	YES	YES
73	a	1642.19	284.68962	YES	YES
74	a	1709.06	133.90410	YES	YES
75	a	2277.16	157.03382	YES	YES
76	a	2326.04	74.33602	YES	YES
77	a	2342.84	92.21562	YES	YES
78	a	2349.70	17.86448	YES	YES
79	a	2398.32	53.23189	YES	YES
80	a	2417.53	16.26566	YES	YES
81	a	2929.98	65.30578	YES	YES
82	a	2958.54	10.48023	YES	YES
83	a	2961.09	1.95150	YES	YES
84	a	2997.74	11.60720	YES	YES
85	a	3014.97	3.68735	YES	YES
86	a	3044.65	7.02807	YES	YES
87	a	3046.24	7.06027	YES	YES
88	a	3047.33	1.67380	YES	YES
89	a	3077.24	6.64956	YES	YES
90	a	3080.90	1.97811	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2109817 Hartree *

Cis 6_afx



bp86_svp SCF energy = -1354.5415808940
pbe0_tzvpp SCF energy = -1354.320518640

xyz Coordinates

30

C	2.58648	-0.46552	-0.23214
C	3.97647	-0.86757	-0.67710
H	4.07705	-0.68325	-1.77023
H	4.14767	-1.94890	-0.49737
H	4.74152	-0.25966	-0.15269
C	-0.82517	0.00625	-2.40702
C	-0.98668	-0.02821	-3.90294
H	-2.05827	-0.06027	-4.18591
H	-0.50160	-0.94859	-4.29927
H	-0.48725	0.85071	-4.35596
H	1.63429	-0.28073	3.00318
H	0.16857	-1.84208	2.69255
H	-0.44146	0.08556	3.46206
H	-2.02751	2.06619	1.77866
H	-0.30941	3.25559	1.23699
H	-1.77690	2.72668	-0.25892
O	1.61690	-1.30496	-0.33367
O	2.35502	0.70485	0.21466
O	0.12222	0.62179	-1.85897
O	-1.72187	-0.66505	-1.72808
P	0.34384	-0.44825	2.37623
P	-0.99656	2.07538	0.76670
Ru	0.15747	0.22937	0.24418
C	-1.57217	-0.67497	-0.24363
C	-2.63123	-1.34673	0.28143
H	-3.34921	-1.78609	-0.43810
C	-2.91404	-1.57706	1.73789
H	-2.34888	-0.87960	2.39219
H	-2.66177	-2.61769	2.05833
H	-3.99614	-1.43443	1.96284

Vibrational Spectrum

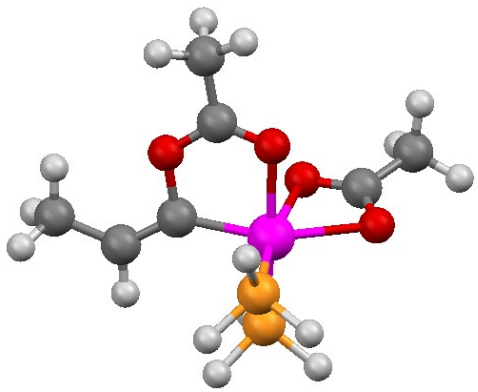
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	37.47	0.42445	YES	YES
8	a	56.41	0.36072	YES	YES
9	a	60.52	0.36787	YES	YES
10	a	65.26	1.13936	YES	YES
11	a	70.51	0.07621	YES	YES
12	a	77.60	2.63138	YES	YES
13	a	85.20	1.55241	YES	YES
14	a	105.68	2.08837	YES	YES
15	a	113.30	0.99373	YES	YES
16	a	123.70	1.93289	YES	YES
17	a	142.75	4.15852	YES	YES
18	a	151.13	4.20767	YES	YES
19	a	167.37	0.62666	YES	YES
20	a	179.17	0.77293	YES	YES
21	a	198.65	0.33205	YES	YES
22	a	216.46	0.18697	YES	YES
23	a	254.18	1.77680	YES	YES
24	a	258.57	3.46008	YES	YES
25	a	261.33	1.60771	YES	YES
26	a	289.99	11.24116	YES	YES
27	a	316.45	14.80322	YES	YES
28	a	374.50	19.49082	YES	YES
29	a	378.93	21.38931	YES	YES
30	a	392.34	2.13167	YES	YES
31	a	460.38	0.74795	YES	YES
32	a	480.65	5.93379	YES	YES
33	a	512.86	2.90867	YES	YES
34	a	548.85	7.96894	YES	YES
35	a	580.95	0.97174	YES	YES
36	a	581.94	4.93595	YES	YES
37	a	594.49	7.98034	YES	YES
38	a	601.45	5.50418	YES	YES
39	a	605.71	1.68595	YES	YES
40	a	609.74	3.44439	YES	YES
41	a	670.59	58.62352	YES	YES
42	a	673.22	18.95640	YES	YES
43	a	771.31	95.51690	YES	YES
44	a	771.65	37.97295	YES	YES
45	a	935.10	19.28279	YES	YES
46	a	937.21	26.44400	YES	YES
47	a	981.90	4.68254	YES	YES
48	a	983.54	14.70926	YES	YES
49	a	1004.58	11.76250	YES	YES

50	a	1013.84	3.21986	YES	YES
51	a	1025.33	10.52735	YES	YES
52	a	1027.05	8.38605	YES	YES
53	a	1038.74	244.54531	YES	YES
54	a	1062.48	143.73149	YES	YES
55	a	1087.89	4.58493	YES	YES
56	a	1090.46	11.14149	YES	YES
57	a	1098.96	7.74471	YES	YES
58	a	1105.50	8.57923	YES	YES
59	a	1109.18	2.03908	YES	YES
60	a	1263.42	18.06311	YES	YES
61	a	1324.44	2.08707	YES	YES
62	a	1332.87	24.92134	YES	YES
63	a	1357.57	8.24465	YES	YES
64	a	1387.46	114.10080	YES	YES
65	a	1399.82	39.87876	YES	YES
66	a	1409.23	25.27737	YES	YES
67	a	1410.60	54.76612	YES	YES
68	a	1419.49	4.89511	YES	YES
69	a	1422.85	11.66782	YES	YES
70	a	1427.58	46.21503	YES	YES
71	a	1446.10	306.21057	YES	YES
72	a	1555.02	101.40101	YES	YES
73	a	1609.41	101.66860	YES	YES
74	a	1632.29	203.50292	YES	YES
75	a	2285.79	46.05899	YES	YES
76	a	2292.56	95.14560	YES	YES
77	a	2296.01	66.02707	YES	YES
78	a	2298.35	151.85510	YES	YES
79	a	2308.40	144.96471	YES	YES
80	a	2326.53	72.09497	YES	YES
81	a	2908.69	54.93251	YES	YES
82	a	2958.80	5.73483	YES	YES
83	a	2964.10	2.41076	YES	YES
84	a	2974.21	17.86084	YES	YES
85	a	3027.36	10.00055	YES	YES
86	a	3044.35	4.40628	YES	YES
87	a	3046.64	25.79086	YES	YES
88	a	3050.94	2.55684	YES	YES
89	a	3076.06	4.35579	YES	YES
90	a	3091.06	1.18623	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2134438 Hartree *

Cis 6_afy



bp86_svp SCF energy = -1354.5438064730

pbe0_tzvpp SCF energy = -1354.322326097

xyz Coordinates

30

C	2.44096	-0.59718	-0.95692
C	3.59960	-1.05878	-1.81538
H	3.40566	-0.77493	-2.87408
H	3.70225	-2.16287	-1.77369
H	4.54023	-0.56801	-1.49248
C	-1.46234	0.33559	-1.94220
C	-2.10611	0.48869	-3.29383
H	-3.20499	0.60476	-3.19999
H	-1.91135	-0.42770	-3.89517
H	-1.66462	1.35481	-3.82467
H	2.18390	-0.30601	2.85617
H	1.19726	-2.12046	2.21847
H	0.12074	-0.64446	3.38522
H	-1.35875	1.99377	2.37516
H	0.42779	3.05453	1.77557
H	-1.27636	2.96588	0.45009
O	1.40134	-1.34610	-0.83739
O	2.46709	0.53438	-0.37424
O	-0.32497	0.80237	-1.69481
O	-2.16474	-0.33731	-1.05898
P	0.95321	-0.70057	2.20889
P	-0.47045	2.06063	1.23667
Ru	0.32419	0.20712	0.26121
C	-1.53404	-0.54623	0.26644
C	-2.35352	-1.23837	1.10235
H	-1.95527	-1.42100	2.11712
C	-3.71775	-1.80684	0.80972
H	-3.72862	-2.91686	0.92765
H	-4.05087	-1.57247	-0.22137
H	-4.48473	-1.41104	1.51751

Vibrational Spectrum

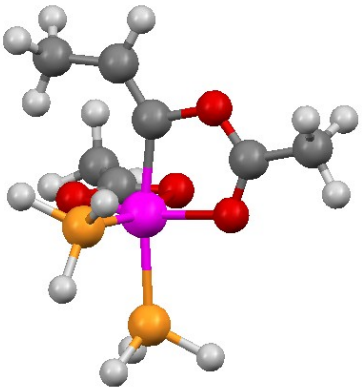
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	40.53	0.39263	YES	YES
8	a	50.97	0.28162	YES	YES
9	a	55.74	0.85105	YES	YES
10	a	59.13	0.26162	YES	YES
11	a	67.32	0.34783	YES	YES
12	a	75.47	3.45106	YES	YES
13	a	82.69	1.36348	YES	YES
14	a	115.27	4.91658	YES	YES
15	a	121.26	1.29749	YES	YES
16	a	128.89	0.40855	YES	YES
17	a	129.87	3.04630	YES	YES
18	a	137.73	0.38800	YES	YES
19	a	148.87	0.25473	YES	YES
20	a	167.25	0.17410	YES	YES
21	a	174.90	1.12458	YES	YES
22	a	195.69	0.30745	YES	YES
23	a	217.54	0.16718	YES	YES
24	a	257.75	7.01822	YES	YES
25	a	281.20	9.20442	YES	YES
26	a	294.99	7.47556	YES	YES
27	a	320.37	15.31038	YES	YES
28	a	330.26	4.38588	YES	YES
29	a	382.31	20.99729	YES	YES
30	a	390.18	7.23591	YES	YES
31	a	461.78	16.09272	YES	YES
32	a	465.42	8.49870	YES	YES
33	a	551.18	0.50564	YES	YES
34	a	578.42	7.39824	YES	YES
35	a	584.22	0.69589	YES	YES
36	a	595.70	4.56143	YES	YES
37	a	601.78	3.62305	YES	YES
38	a	610.93	4.60926	YES	YES
39	a	618.96	1.69679	YES	YES
40	a	633.69	0.00596	YES	YES
41	a	670.75	80.77882	YES	YES
42	a	676.05	3.37803	YES	YES
43	a	755.29	11.27776	YES	YES
44	a	791.89	126.35458	YES	YES
45	a	934.55	12.68988	YES	YES
46	a	935.51	37.03026	YES	YES
47	a	982.42	2.47625	YES	YES
48	a	992.99	34.81309	YES	YES
49	a	1005.17	12.14267	YES	YES

50	a	1012.76	0.05353	YES	YES
51	a	1025.79	6.29679	YES	YES
52	a	1026.70	10.95918	YES	YES
53	a	1038.46	258.24522	YES	YES
54	a	1064.74	133.71280	YES	YES
55	a	1083.76	5.54192	YES	YES
56	a	1090.31	3.25412	YES	YES
57	a	1092.60	10.93113	YES	YES
58	a	1100.15	9.30722	YES	YES
59	a	1104.56	6.09392	YES	YES
60	a	1242.27	30.08208	YES	YES
61	a	1323.87	2.71765	YES	YES
62	a	1332.63	22.03953	YES	YES
63	a	1356.37	1.08458	YES	YES
64	a	1384.40	119.37649	YES	YES
65	a	1399.70	43.91674	YES	YES
66	a	1409.54	25.57131	YES	YES
67	a	1410.19	48.15960	YES	YES
68	a	1421.80	10.20564	YES	YES
69	a	1425.50	15.88965	YES	YES
70	a	1428.24	36.54547	YES	YES
71	a	1445.51	307.51384	YES	YES
72	a	1558.44	105.28386	YES	YES
73	a	1607.60	115.17472	YES	YES
74	a	1643.22	193.08971	YES	YES
75	a	2279.26	62.94096	YES	YES
76	a	2284.46	120.80887	YES	YES
77	a	2291.01	78.00364	YES	YES
78	a	2299.79	153.18974	YES	YES
79	a	2311.09	118.67037	YES	YES
80	a	2324.29	69.67470	YES	YES
81	a	2914.76	80.95137	YES	YES
82	a	2958.19	6.06187	YES	YES
83	a	2964.54	1.95022	YES	YES
84	a	2967.33	19.37916	YES	YES
85	a	3043.48	4.73412	YES	YES
86	a	3050.82	2.26986	YES	YES
87	a	3053.04	0.82567	YES	YES
88	a	3069.44	21.63470	YES	YES
89	a	3075.13	4.56129	YES	YES
90	a	3091.46	1.14527	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2134190 Hartree *

Cis 6_pfx



bp86_svp SCF energy = -1354.5319313360
pbe0_tzvpp SCF energy = -1354.308605660

xyz Coordinates

30

C	2.20215	-0.69936	-0.89527
C	3.41930	-1.41718	-1.42412
H	3.21325	-2.51050	-1.46162
H	4.29060	-1.25311	-0.75760
H	3.64920	-1.07764	-2.45491
C	-2.47558	-0.04740	-0.94520
C	-3.79647	0.10078	-1.64765
H	-4.61335	-0.33428	-1.03275
H	-3.77650	-0.45639	-2.61015
H	-3.99887	1.17076	-1.84673
H	0.46428	3.44967	-1.07110
H	2.42279	2.73379	-0.57171
H	1.12571	3.46385	0.96532
H	-1.95741	0.51220	2.56155
H	-0.02558	-0.18871	3.21993
H	-0.36421	1.92289	2.91188
O	2.06979	-0.48585	0.36731
O	1.26385	-0.31499	-1.67114
O	-1.71092	0.93489	-0.75549
O	-2.17218	-1.26211	-0.55495
P	1.06015	2.52891	-0.13442
P	-0.56539	0.67863	2.20274
Ru	0.12920	0.37081	0.10143
C	-0.86783	-1.41748	0.12053
C	-0.70981	-2.69183	0.55521
H	-1.52861	-3.40994	0.34674
C	0.48686	-3.20839	1.30382
H	0.20816	-3.55424	2.32841
H	1.27284	-2.43029	1.39590
H	0.93180	-4.09440	0.79141

Vibrational Spectrum

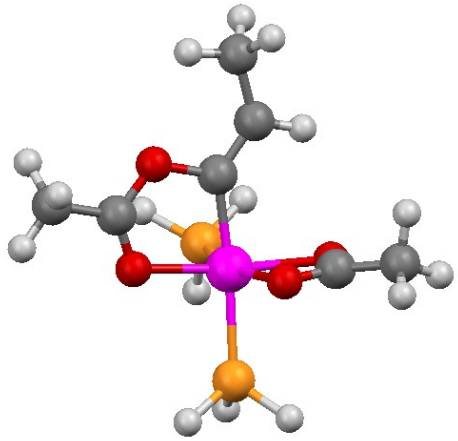
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	37.73	1.55547	YES	YES
8	a	50.07	0.23666	YES	YES
9	a	60.68	0.08438	YES	YES
10	a	63.02	0.29137	YES	YES
11	a	67.64	0.81199	YES	YES
12	a	71.54	0.10133	YES	YES
13	a	83.64	4.11094	YES	YES
14	a	100.13	3.60493	YES	YES
15	a	109.10	0.73494	YES	YES
16	a	114.84	1.06017	YES	YES
17	a	121.08	0.78162	YES	YES
18	a	150.16	1.01238	YES	YES
19	a	172.24	1.93912	YES	YES
20	a	189.03	0.45094	YES	YES
21	a	200.46	1.15245	YES	YES
22	a	203.01	0.67554	YES	YES
23	a	247.00	1.37648	YES	YES
24	a	258.98	0.67647	YES	YES
25	a	278.23	14.37293	YES	YES
26	a	296.89	11.15295	YES	YES
27	a	316.79	10.15531	YES	YES
28	a	328.68	5.35952	YES	YES
29	a	383.82	12.50891	YES	YES
30	a	388.65	5.59450	YES	YES
31	a	443.10	2.70785	YES	YES
32	a	462.65	2.95772	YES	YES
33	a	479.10	5.14903	YES	YES
34	a	491.42	2.27808	YES	YES
35	a	531.64	3.17389	YES	YES
36	a	554.95	4.84618	YES	YES
37	a	593.02	5.60901	YES	YES
38	a	594.99	4.69575	YES	YES
39	a	604.23	0.62146	YES	YES
40	a	610.27	6.79009	YES	YES
41	a	669.53	56.37992	YES	YES
42	a	682.32	2.20281	YES	YES
43	a	797.90	56.10703	YES	YES
44	a	800.64	42.43778	YES	YES
45	a	934.32	16.10792	YES	YES
46	a	940.42	25.76013	YES	YES
47	a	980.07	18.80271	YES	YES
48	a	981.02	5.34866	YES	YES
49	a	1006.43	24.39167	YES	YES
50	a	1021.38	29.12726	YES	YES

51	a	1023.36	186.85974	YES	YES
52	a	1023.76	35.46593	YES	YES
53	a	1025.40	13.08440	YES	YES
54	a	1058.86	177.96554	YES	YES
55	a	1092.42	8.38094	YES	YES
56	a	1096.33	3.94349	YES	YES
57	a	1096.80	3.01104	YES	YES
58	a	1101.08	6.75903	YES	YES
59	a	1116.61	1.86457	YES	YES
60	a	1260.27	15.32897	YES	YES
61	a	1326.65	1.42937	YES	YES
62	a	1332.66	25.02817	YES	YES
63	a	1356.66	3.21692	YES	YES
64	a	1397.00	138.09501	YES	YES
65	a	1399.14	32.67752	YES	YES
66	a	1405.51	25.52455	YES	YES
67	a	1408.90	30.34765	YES	YES
68	a	1414.24	15.04394	YES	YES
69	a	1420.94	12.05620	YES	YES
70	a	1435.58	3.76323	YES	YES
71	a	1454.50	234.55470	YES	YES
72	a	1540.75	80.16081	YES	YES
73	a	1602.43	182.12806	YES	YES
74	a	1637.29	39.04846	YES	YES
75	a	2269.70	122.23466	YES	YES
76	a	2280.30	88.74096	YES	YES
77	a	2289.54	195.85242	YES	YES
78	a	2295.42	94.43526	YES	YES
79	a	2312.17	127.85279	YES	YES
80	a	2316.47	74.72436	YES	YES
81	a	2911.00	67.25714	YES	YES
82	a	2958.05	4.41815	YES	YES
83	a	2963.45	5.39051	YES	YES
84	a	2964.61	18.76815	YES	YES
85	a	3025.33	20.52777	YES	YES
86	a	3041.77	0.98797	YES	YES
87	a	3043.44	2.88545	YES	YES
88	a	3052.04	5.94123	YES	YES
89	a	3076.17	3.11312	YES	YES
90	a	3091.68	1.65018	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2127605 Hartree *

Cis 6_pfy



bp86_svp SCF energy = -1354.5324970740
pbe0_tzvpp SCF energy = -1354.308605660

xyz Coordinates

30

C	-0.59675	-1.66022	1.78140
C	-0.92510	-2.35395	3.08065
H	-0.84822	-1.62292	3.91660
H	-0.20963	-3.17894	3.27517
H	-1.96549	-2.73856	3.05911
C	-0.99966	2.15912	-0.94088
C	-1.76587	3.29691	-1.55549
H	-1.14332	4.21655	-1.58231
H	-2.66247	3.52365	-0.93643
H	-2.08932	3.02401	-2.57830
H	-1.47033	-2.12999	-2.65170
H	-0.76588	-3.51048	-1.17363
H	0.57892	-2.74251	-2.64836
H	2.35162	1.33576	-1.83350
H	3.22577	0.06018	-0.32698
H	2.65515	-0.75811	-2.24591
O	0.61124	-1.64729	1.33857
O	-1.49212	-1.04821	1.10670
O	-0.92847	1.03024	-1.49122
O	-0.42822	2.42015	0.21512
P	-0.38465	-2.22137	-1.70534
P	2.08037	0.06060	-1.20231
Ru	0.08744	-0.38398	-0.29529
C	0.28584	1.29747	0.83608
C	0.87275	1.61120	2.01633
H	1.40975	0.77310	2.49646
C	0.86143	2.93394	2.73756
H	0.39101	2.84199	3.74521
H	0.30478	3.70943	2.17224
H	1.89723	3.31093	2.91153

Vibrational Spectrum

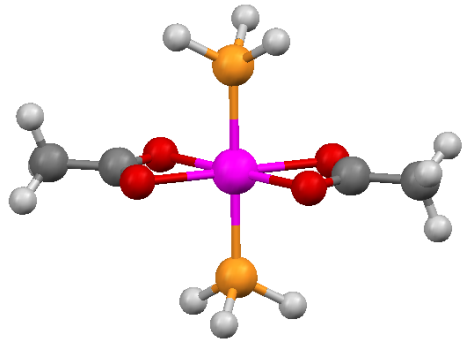
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	29.14	1.36070	YES	YES
8	a	52.16	0.09605	YES	YES
9	a	53.92	0.26613	YES	YES
10	a	59.48	0.60557	YES	YES
11	a	60.92	0.38925	YES	YES
12	a	70.89	0.33935	YES	YES
13	a	78.54	4.38194	YES	YES
14	a	101.68	3.78209	YES	YES
15	a	111.63	1.31562	YES	YES
16	a	115.00	0.55015	YES	YES
17	a	125.72	0.50302	YES	YES
18	a	148.30	0.04265	YES	YES
19	a	155.70	0.45342	YES	YES
20	a	158.02	0.18445	YES	YES
21	a	191.69	0.86610	YES	YES
22	a	202.86	0.92454	YES	YES
23	a	218.68	0.50335	YES	YES
24	a	267.79	1.38551	YES	YES
25	a	275.74	12.99432	YES	YES
26	a	298.15	13.14821	YES	YES
27	a	311.56	6.32372	YES	YES
28	a	323.34	6.92554	YES	YES
29	a	341.70	6.24416	YES	YES
30	a	388.20	9.80057	YES	YES
31	a	462.62	4.82459	YES	YES
32	a	478.87	1.42511	YES	YES
33	a	482.85	6.71581	YES	YES
34	a	500.26	6.99519	YES	YES
35	a	561.54	3.51310	YES	YES
36	a	592.04	5.02566	YES	YES
37	a	593.87	4.02541	YES	YES
38	a	604.64	4.18373	YES	YES
39	a	615.96	8.25611	YES	YES
40	a	633.25	1.46469	YES	YES
41	a	669.53	57.55477	YES	YES
42	a	680.35	3.52537	YES	YES
43	a	796.42	13.86861	YES	YES
44	a	817.96	82.32044	YES	YES
45	a	932.13	10.72372	YES	YES
46	a	940.30	25.77146	YES	YES
47	a	981.04	1.44353	YES	YES
48	a	990.57	36.02008	YES	YES
49	a	1006.08	19.28300	YES	YES

50	a	1015.42	0.12189	YES	YES
51	a	1021.58	8.02139	YES	YES
52	a	1023.68	4.25798	YES	YES
53	a	1027.39	260.15442	YES	YES
54	a	1059.46	181.90448	YES	YES
55	a	1085.04	8.48313	YES	YES
56	a	1092.86	8.31246	YES	YES
57	a	1095.29	4.99779	YES	YES
58	a	1098.07	2.51075	YES	YES
59	a	1102.25	5.76488	YES	YES
60	a	1233.56	29.41728	YES	YES
61	a	1326.83	1.99229	YES	YES
62	a	1330.34	21.43080	YES	YES
63	a	1352.90	0.83444	YES	YES
64	a	1391.32	120.30119	YES	YES
65	a	1399.16	33.17108	YES	YES
66	a	1405.46	21.30516	YES	YES
67	a	1409.33	28.02143	YES	YES
68	a	1413.96	16.18565	YES	YES
69	a	1423.92	11.72927	YES	YES
70	a	1425.37	12.27272	YES	YES
71	a	1455.60	246.47354	YES	YES
72	a	1541.29	76.51384	YES	YES
73	a	1599.79	177.82242	YES	YES
74	a	1650.50	52.71291	YES	YES
75	a	2260.37	135.61086	YES	YES
76	a	2283.82	68.76833	YES	YES
77	a	2289.91	238.65205	YES	YES
78	a	2292.71	77.64008	YES	YES
79	a	2309.33	135.13284	YES	YES
80	a	2313.64	82.70368	YES	YES
81	a	2918.18	75.77951	YES	YES
82	a	2958.09	4.68435	YES	YES
83	a	2961.68	4.85598	YES	YES
84	a	2973.02	17.78876	YES	YES
85	a	3040.56	1.08150	YES	YES
86	a	3043.49	3.31433	YES	YES
87	a	3047.22	6.70334	YES	YES
88	a	3075.96	3.20336	YES	YES
89	a	3077.63	7.60237	YES	YES
90	a	3092.44	1.56650	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2127798 Hartree *

Trans 1



bp86_svp SCF energy = -1237.9149011260
pbe0_tzvpp SCF energy = -1237.711601913

xyz Coordinates

23

H	-0.66423	3.02034	-1.08694
H	-0.64027	3.01999	1.07838
H	1.21747	3.05049	-0.02554
H	-1.21960	-3.04769	0.02210
H	0.64091	-3.01856	-1.07716
H	0.65953	-3.01969	1.08811
C	0.00243	-0.02112	-2.54256
C	0.00047	0.00529	-4.05129
H	-0.79792	-0.65671	-4.44652
H	0.98925	-0.30375	-4.44574
H	-0.21503	1.03764	-4.40733
C	-0.00104	0.01978	2.54273
C	0.00167	-0.01576	4.05119
H	0.85873	0.56548	4.44932
H	-0.95432	0.38000	4.44989
H	0.11422	-1.06701	4.39974
O	1.09353	0.02416	-1.87316
O	-1.08962	-0.06306	-1.87430
O	-1.09268	-0.02315	1.87315
O	1.09075	0.06378	1.87394
P	-0.01889	2.31254	-0.01127
P	0.01744	-2.31088	0.01116
Ru	-0.00018	0.00101	0.00010

Vibrational Spectrum

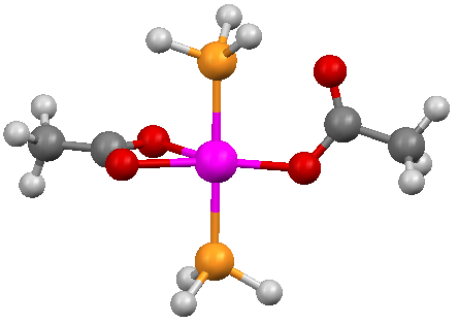
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	28.44	0.56833	YES	YES
8	a	30.33	0.33620	YES	YES
9	a	54.32	0.02146	YES	YES
10	a	55.17	0.57342	YES	YES
11	a	58.51	0.01334	YES	YES
12	a	72.16	2.32014	YES	YES
13	a	88.44	0.00031	YES	YES
14	a	98.88	11.12632	YES	YES
15	a	105.91	6.55072	YES	YES
16	a	108.39	0.00754	YES	YES
17	a	158.86	0.00041	YES	YES
18	a	176.86	0.14275	YES	YES
19	a	214.09	2.89357	YES	YES
20	a	267.74	0.00172	YES	YES
21	a	279.41	0.00040	YES	YES
22	a	298.86	21.62071	YES	YES
23	a	320.07	0.00139	YES	YES
24	a	327.53	4.38411	YES	YES
25	a	363.98	71.30563	YES	YES
26	a	449.72	0.00003	YES	YES
27	a	469.58	0.00019	YES	YES
28	a	480.92	2.45103	YES	YES
29	a	484.97	0.00371	YES	YES
30	a	544.76	5.50427	YES	YES
31	a	545.55	3.21572	YES	YES
32	a	597.67	0.01381	YES	YES
33	a	604.34	2.88795	YES	YES
34	a	663.93	125.39075	YES	YES
35	a	676.18	0.01532	YES	YES
36	a	942.84	0.00538	YES	YES
37	a	948.89	44.28866	YES	YES
38	a	980.37	2.63104	YES	YES
39	a	980.99	1.89499	YES	YES
40	a	996.57	469.47474	YES	YES
41	a	1025.16	1.03888	YES	YES
42	a	1026.20	32.12935	YES	YES
43	a	1031.01	0.00235	YES	YES
44	a	1089.38	0.00416	YES	YES
45	a	1091.54	13.27068	YES	YES
46	a	1094.72	0.00326	YES	YES
47	a	1096.84	11.24099	YES	YES
48	a	1329.93	0.87995	YES	YES
49	a	1330.47	0.01265	YES	YES
50	a	1398.28	75.24827	YES	YES
51	a	1399.03	3.13943	YES	YES
52	a	1410.57	41.53624	YES	YES
53	a	1410.91	10.90773	YES	YES
54	a	1458.90	482.73481	YES	YES
55	a	1462.21	2.87715	YES	YES
56	a	1534.41	204.54543	YES	YES
57	a	1558.65	0.23780	YES	YES
58	a	2322.34	384.54585	YES	YES
59	a	2329.46	0.00753	YES	YES
60	a	2331.32	72.26419	YES	YES
61	a	2332.31	0.53801	YES	YES

62	a	2335.04	28.54643	YES	YES
63	a	2335.10	39.55634	YES	YES
64	a	2958.64	5.07792	YES	YES
65	a	2959.10	3.99568	YES	YES
66	a	3043.19	2.35972	YES	YES
67	a	3043.67	2.50608	YES	YES
68	a	3079.00	2.69653	YES	YES
69	a	3079.44	2.51430	YES	YES

$end

* zero point VIBRATIONAL energy : 0.1534849 Hartree *

Trans I_{12}



bp86_svp SCF energy = -1237.8878855860
pbe0_tzvpp SCF energy = -1237.683565050

xyz Coordinates

23

H	1.06441	-2.90297	-1.40153
H	0.06620	-3.37768	0.46285
H	-1.07427	-3.11781	-1.36040
H	0.84045	2.88372	0.68509
H	-0.75097	2.88203	-0.77971
H	-1.24454	2.68329	1.31615
C	0.27722	0.46181	-2.52355
C	0.64516	0.80563	-3.94047
H	1.51376	1.49583	-3.95872
H	-0.22242	1.26222	-4.45797
H	0.93481	-0.11865	-4.48923
C	0.26225	0.09393	2.83754
C	0.28002	-0.64778	4.16760
H	0.24235	0.07085	5.01018
H	-0.57078	-1.35937	4.22940
H	1.21361	-1.24902	4.24183
O	-0.91797	0.25083	-2.13903
O	1.17947	0.33027	-1.61008
O	0.08894	-0.71945	1.80023
O	0.42274	1.31347	2.76406
P	-0.04853	-2.43277	-0.61480
P	-0.32679	2.11646	0.37565
Ru	-0.20151	-0.16544	-0.11506

Vibrational Spectrum

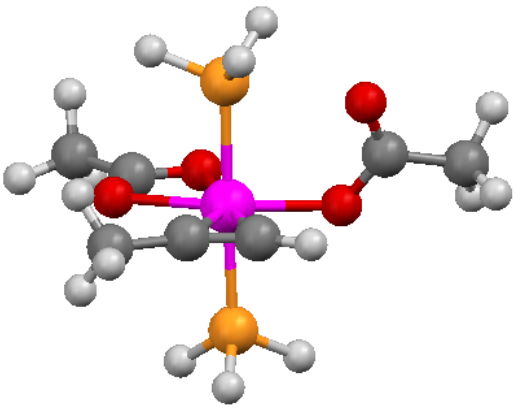
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.33	0.22801	YES	YES
8	a	28.47	0.19260	YES	YES
9	a	45.96	0.09762	YES	YES
10	a	51.27	1.88948	YES	YES
11	a	74.10	1.65740	YES	YES
12	a	82.87	1.05929	YES	YES
13	a	86.39	3.81042	YES	YES
14	a	103.47	1.66893	YES	YES
15	a	138.82	0.60044	YES	YES
16	a	150.55	1.65169	YES	YES
17	a	167.87	14.58307	YES	YES
18	a	188.64	0.84928	YES	YES
19	a	223.87	5.19041	YES	YES
20	a	270.75	3.11114	YES	YES
21	a	290.71	20.40524	YES	YES
22	a	296.27	14.41757	YES	YES
23	a	313.75	1.42533	YES	YES
24	a	320.99	1.31311	YES	YES
25	a	353.40	26.77237	YES	YES
26	a	450.18	0.64275	YES	YES
27	a	487.45	0.75491	YES	YES
28	a	495.93	4.74824	YES	YES
29	a	527.73	6.37564	YES	YES
30	a	539.71	1.80672	YES	YES
31	a	574.01	7.62447	YES	YES
32	a	594.70	2.19686	YES	YES
33	a	596.88	2.52708	YES	YES
34	a	663.36	78.78890	YES	YES
35	a	670.94	37.65848	YES	YES
36	a	916.65	1.53893	YES	YES
37	a	948.42	25.44278	YES	YES
38	a	976.87	2.64442	YES	YES
39	a	982.92	66.50065	YES	YES
40	a	992.95	374.17336	YES	YES
41	a	1020.25	2.05276	YES	YES
42	a	1022.31	7.15447	YES	YES
43	a	1025.51	17.99910	YES	YES
44	a	1071.91	22.82798	YES	YES
45	a	1087.87	4.45047	YES	YES
46	a	1097.91	15.04352	YES	YES
47	a	1115.95	10.65397	YES	YES
48	a	1257.75	506.08462	YES	YES
49	a	1332.46	2.73852	YES	YES
50	a	1336.04	96.65367	YES	YES
51	a	1395.43	42.43102	YES	YES
52	a	1405.24	14.38689	YES	YES
53	a	1408.76	20.00336	YES	YES
54	a	1416.49	11.51163	YES	YES
55	a	1460.93	209.08246	YES	YES
56	a	1547.70	96.84106	YES	YES
57	a	1685.10	198.48533	YES	YES
58	a	2270.74	162.75838	YES	YES
59	a	2318.27	102.62564	YES	YES
60	a	2322.14	105.91419	YES	YES
61	a	2350.71	48.72849	YES	YES

62	a	2384.04	64.42304	YES	YES
63	a	2397.65	18.77242	YES	YES
64	a	2957.82	5.90440	YES	YES
65	a	2959.89	2.15647	YES	YES
66	a	3039.70	4.64082	YES	YES
67	a	3045.22	0.98995	YES	YES
68	a	3079.14	8.82017	YES	YES
69	a	3082.00	0.94174	YES	YES

$end

* zero point VIBRATIONAL energy : 0.1538131 Hartree *

Trans 2_x



bp86_svp SCF energy = -1354.5081832400
pbe0_tzvpp SCF energy = -1354.283970709

xyz Coordinates

30

H	2.65740	-1.10563	-1.97324
H	3.17210	-1.12889	0.13145
H	1.99558	-2.74726	-0.71816
H	-1.91032	2.24136	1.13655
H	-2.67509	1.36030	-0.67493
H	-2.95581	0.29212	1.18910
C	0.29788	1.40536	-2.14050
C	0.37932	2.32367	-3.33459
H	-0.32463	3.17470	-3.19728
H	0.10650	1.78413	-4.26370
H	1.40107	2.74905	-3.42151
C	0.30751	0.50980	2.77361
C	1.19928	0.73602	3.99396
H	0.77618	1.54856	4.61984
H	1.21329	-0.19152	4.60947
H	2.24182	0.97498	3.70135
O	-0.34791	0.29434	-2.20818
O	0.83859	1.71049	-1.02575
O	0.97067	0.14926	1.70493
O	-0.92369	0.64398	2.85515
P	2.01374	-1.30673	-0.70024
P	-1.90660	0.96589	0.49203
Ru	0.05828	-0.16273	-0.13185
C	-1.10776	-1.95862	-0.39329
C	-0.69395	-1.93190	0.81087
H	-0.60687	-2.31408	1.82982
C	-1.79437	-2.46592	-1.59470
H	-2.54292	-1.73410	-1.97232
H	-2.31632	-3.42526	-1.37483
H	-1.07573	-2.63797	-2.42717

Vibrational Spectrum

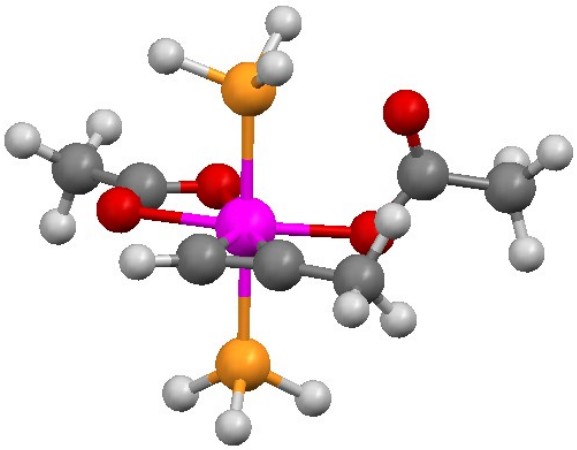
mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.65	0.56737	YES	YES
8	a	31.49	0.53355	YES	YES
9	a	48.82	0.30008	YES	YES
10	a	65.92	0.67080	YES	YES
11	a	71.52	1.08929	YES	YES
12	a	76.28	1.53718	YES	YES
13	a	87.37	0.14780	YES	YES
14	a	100.93	1.21396	YES	YES
15	a	109.00	0.32345	YES	YES
16	a	117.35	5.05423	YES	YES
17	a	119.94	1.20665	YES	YES
18	a	131.64	0.67079	YES	YES
19	a	158.82	13.66354	YES	YES
20	a	184.12	5.50696	YES	YES
21	a	190.53	7.60952	YES	YES
22	a	193.16	3.04529	YES	YES
23	a	223.91	1.67602	YES	YES
24	a	236.91	2.56711	YES	YES
25	a	266.72	8.93746	YES	YES
26	a	278.42	3.53566	YES	YES
27	a	307.11	9.06622	YES	YES
28	a	312.00	4.63707	YES	YES
29	a	330.48	5.19467	YES	YES
30	a	332.65	12.33312	YES	YES
31	a	338.89	1.09142	YES	YES
32	a	418.20	14.74102	YES	YES
33	a	453.32	2.20539	YES	YES
34	a	482.33	5.21164	YES	YES
35	a	485.81	1.09084	YES	YES
36	a	496.99	2.74597	YES	YES
37	a	516.35	0.96415	YES	YES
38	a	558.85	14.85075	YES	YES
39	a	586.50	10.24807	YES	YES
40	a	603.56	0.25008	YES	YES
41	a	605.24	2.24821	YES	YES
42	a	638.46	11.79740	YES	YES
43	a	669.88	79.09261	YES	YES
44	a	675.68	12.57943	YES	YES
45	a	789.03	5.29372	YES	YES
46	a	927.70	4.26438	YES	YES
47	a	931.36	12.81090	YES	YES
48	a	944.68	17.63263	YES	YES
49	a	981.79	2.36581	YES	YES
50	a	986.27	101.87711	YES	YES
51	a	990.69	233.53552	YES	YES
52	a	1006.02	36.12385	YES	YES

53	a	1020.73	4.94575	YES	YES
54	a	1021.02	20.91185	YES	YES
55	a	1022.11	1.39349	YES	YES
56	a	1026.08	8.08970	YES	YES
57	a	1071.67	39.45701	YES	YES
58	a	1088.74	6.10082	YES	YES
59	a	1095.88	3.34707	YES	YES
60	a	1127.35	10.32213	YES	YES
61	a	1306.02	194.16483	YES	YES
62	a	1330.66	1.57983	YES	YES
63	a	1338.83	181.12769	YES	YES
64	a	1356.02	2.62430	YES	YES
65	a	1396.09	51.81980	YES	YES
66	a	1403.21	11.01220	YES	YES
67	a	1409.21	24.86288	YES	YES
68	a	1410.92	13.46863	YES	YES
69	a	1411.76	8.79368	YES	YES
70	a	1420.63	15.56789	YES	YES
71	a	1460.09	251.44462	YES	YES
72	a	1545.06	84.69847	YES	YES
73	a	1658.79	205.22974	YES	YES
74	a	1913.69	19.39531	YES	YES
75	a	2255.05	170.75864	YES	YES
76	a	2321.16	158.25481	YES	YES
77	a	2334.29	41.89426	YES	YES
78	a	2357.86	38.30470	YES	YES
79	a	2396.19	58.34065	YES	YES
80	a	2417.60	16.72768	YES	YES
81	a	2930.08	30.03122	YES	YES
82	a	2956.90	11.31945	YES	YES
83	a	2959.61	3.30417	YES	YES
84	a	3012.49	4.64126	YES	YES
85	a	3015.43	5.92471	YES	YES
86	a	3042.78	7.43852	YES	YES
87	a	3043.47	1.94993	YES	YES
88	a	3074.85	6.58841	YES	YES
89	a	3078.29	2.51543	YES	YES
90	a	3243.70	6.95226	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2103993 Hartree *

Trans 2_y



bp86_svp SCF energy = -1237.9314592950
pbe0_tzvpp SCF energy = -1237.728387502

xyz Coordinates

23

C	-2.07667	1.19314	0.23695
C	-3.23981	2.11525	0.50183
H	-2.87606	3.01243	1.05102
H	-4.00620	1.60951	1.12345
H	-3.68093	2.46157	-0.45573
C	2.07541	1.19264	-0.23469
C	3.23645	2.11433	-0.51001
H	3.67770	2.47112	0.44348
H	2.87035	3.00444	-1.06914
H	4.00304	1.60393	-1.12774
H	-0.42926	-2.04770	-2.57755
H	-2.35696	-1.55400	-1.71925
H	-1.15829	-3.12874	-0.84995
H	0.55607	-3.13143	1.29695
H	2.41452	-2.03205	1.16134
H	0.97866	-1.54092	2.70690
O	-1.83504	0.20114	1.01783
O	-1.28025	1.39176	-0.74511
O	1.29673	1.38167	0.76256
O	1.81845	0.20946	-1.02326
P	-0.99470	-1.75913	-1.28238
P	0.99880	-1.75765	1.28172
Ru	-0.00062	-0.21972	-0.00083

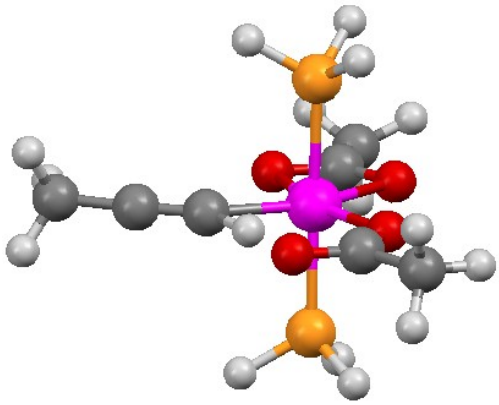
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	37.15	0.03003	YES	YES
8	a	58.88	1.11538	YES	YES
9	a	68.40	2.61367	YES	YES
10	a	72.05	0.92873	YES	YES
11	a	77.03	0.94652	YES	YES
12	a	82.35	1.82046	YES	YES
13	a	105.37	7.05842	YES	YES
14	a	114.81	0.91202	YES	YES
15	a	133.03	2.46980	YES	YES
16	a	139.47	0.50793	YES	YES
17	a	158.00	0.04920	YES	YES
18	a	185.27	0.90430	YES	YES
19	a	194.01	0.34785	YES	YES
20	a	290.42	0.38508	YES	YES
21	a	295.95	13.42836	YES	YES
22	a	311.39	18.55712	YES	YES
23	a	344.72	33.31621	YES	YES
24	a	384.14	21.77195	YES	YES
25	a	391.40	0.12299	YES	YES
26	a	481.40	3.37582	YES	YES
27	a	483.18	8.74037	YES	YES
28	a	571.76	1.22975	YES	YES
29	a	584.84	3.57237	YES	YES
30	a	589.33	11.40966	YES	YES
31	a	595.51	2.25546	YES	YES
32	a	604.12	1.71298	YES	YES
33	a	607.09	1.23719	YES	YES
34	a	671.07	100.96362	YES	YES
35	a	679.34	31.87422	YES	YES
36	a	941.05	29.25767	YES	YES
37	a	942.03	23.04113	YES	YES
38	a	981.32	2.76724	YES	YES
39	a	981.50	0.69072	YES	YES
40	a	1025.84	3.45840	YES	YES
41	a	1026.13	10.77844	YES	YES
42	a	1036.36	262.78208	YES	YES
43	a	1063.09	137.97042	YES	YES
44	a	1084.33	9.84006	YES	YES
45	a	1089.15	7.78967	YES	YES
46	a	1093.80	5.91348	YES	YES
47	a	1099.16	6.13631	YES	YES
48	a	1326.52	2.10673	YES	YES
49	a	1327.39	0.05748	YES	YES
50	a	1396.25	37.46914	YES	YES
51	a	1397.10	46.70170	YES	YES
52	a	1408.92	28.07404	YES	YES
53	a	1409.43	28.26224	YES	YES
54	a	1456.14	337.74845	YES	YES
55	a	1460.71	183.59787	YES	YES
56	a	1527.64	156.45013	YES	YES
57	a	1541.95	26.18927	YES	YES
58	a	2271.83	138.08784	YES	YES

59	a	2283.33	78.20134	YES	YES
60	a	2288.89	84.19137	YES	YES
61	a	2301.03	87.29394	YES	YES
62	a	2309.08	164.67007	YES	YES
63	a	2316.68	75.55176	YES	YES
64	a	2959.75	3.53000	YES	YES
65	a	2959.85	3.22869	YES	YES
66	a	3045.38	2.44813	YES	YES
67	a	3045.53	2.13673	YES	YES
68	a	3077.84	3.16169	YES	YES
69	a	3077.94	2.58645	YES	YES

zero point VIBRATIONAL energy : 0.1546066 Hartree

Trans TS_{34}



bp86_svp SCF energy = -1354.4808728260
pbe0_tzvpp SCF energy = -1354.254210119

xyz Coordinates

30

H	3.13752	-0.47128	-1.34739
H	3.04892	-0.99497	0.75148
H	2.08196	-2.26307	-0.72665
H	-1.94375	2.01295	1.73503
H	-2.02912	2.77458	-0.29137
H	-3.01722	0.90448	0.20307
C	0.59147	1.66878	-2.20075
C	0.84825	2.41836	-3.48447
H	0.97417	3.50183	-3.28511
H	0.01668	2.24733	-4.19837
H	1.78517	2.04216	-3.95315
C	0.54518	-0.09235	2.85307
C	1.08039	0.30674	4.22351
H	0.23297	0.44936	4.92884
H	1.70951	-0.51303	4.63275
H	1.67434	1.24064	4.16449
O	-0.08943	0.58542	-2.20276
O	1.07078	2.07841	-1.08232
O	0.83325	0.72772	1.89356
O	-0.12127	-1.14733	2.71554
P	2.15804	-0.87314	-0.37121
P	-1.74278	1.53957	0.39208
Ru	0.20905	0.35883	-0.05841
C	-1.57610	-2.26914	-0.53104
C	-0.87786	-1.38154	0.00313
H	-0.49963	-1.20367	1.17189
C	-2.36559	-3.20998	-1.31674
H	-1.95267	-4.24496	-1.29389
H	-2.37652	-2.89038	-2.38799
H	-3.42878	-3.26305	-0.98586

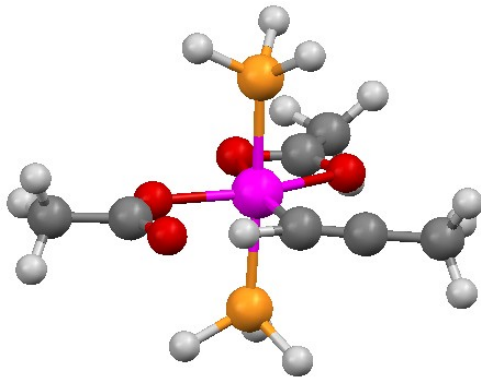
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-66.74	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	18.84	0.19506	YES	YES
9	a	30.20	0.24921	YES	YES
10	a	33.80	1.58445	YES	YES
11	a	50.76	0.50208	YES	YES
12	a	56.05	0.39082	YES	YES
13	a	58.66	0.77536	YES	YES
14	a	58.91	0.98054	YES	YES
15	a	65.91	0.15107	YES	YES
16	a	77.09	1.09124	YES	YES
17	a	85.03	0.38787	YES	YES
18	a	96.44	3.67587	YES	YES
19	a	109.01	15.15432	YES	YES
20	a	137.10	0.00261	YES	YES
21	a	146.17	10.31156	YES	YES
22	a	167.86	0.02961	YES	YES
23	a	201.96	34.29348	YES	YES
24	a	212.48	2.77750	YES	YES
25	a	226.95	4.39244	YES	YES
26	a	265.60	4.97204	YES	YES
27	a	294.61	6.08319	YES	YES
28	a	295.69	7.62673	YES	YES
29	a	315.20	3.08486	YES	YES
30	a	334.96	51.61106	YES	YES
31	a	348.33	16.38725	YES	YES
32	a	389.39	59.59878	YES	YES
33	a	397.16	7.89706	YES	YES
34	a	468.24	1.10686	YES	YES
35	a	474.94	3.01589	YES	YES
36	a	476.96	0.78972	YES	YES
37	a	507.57	11.37578	YES	YES
38	a	550.17	12.14111	YES	YES
39	a	558.23	10.91112	YES	YES
40	a	601.49	1.35841	YES	YES
41	a	605.62	0.54962	YES	YES
42	a	670.71	86.99998	YES	YES
43	a	679.79	44.85772	YES	YES
44	a	872.09	28.10797	YES	YES
45	a	878.85	107.37014	YES	YES
46	a	929.33	106.98014	YES	YES
47	a	942.50	18.93132	YES	YES
48	a	962.41	93.52777	YES	YES
49	a	980.06	2.34550	YES	YES
50	a	991.00	400.97016	YES	YES
51	a	992.75	3.12144	YES	YES

52	a	1007.46	13.49514	YES	YES
53	a	1024.31	11.59489	YES	YES
54	a	1025.66	9.25086	YES	YES
55	a	1026.42	0.76939	YES	YES
56	a	1027.87	7.27796	YES	YES
57	a	1089.32	2.11835	YES	YES
58	a	1089.55	0.24722	YES	YES
59	a	1092.36	5.66522	YES	YES
60	a	1093.47	6.04462	YES	YES
61	a	1324.43	21.34658	YES	YES
62	a	1328.48	0.72134	YES	YES
63	a	1357.08	3.96005	YES	YES
64	a	1364.36	134.46165	YES	YES
65	a	1397.86	110.72017	YES	YES
66	a	1404.83	8.67247	YES	YES
67	a	1408.45	730.63956	YES	YES
68	a	1409.84	27.58373	YES	YES
69	a	1417.37	340.86789	YES	YES
70	a	1419.44	48.75955	YES	YES
71	a	1421.59	44.95013	YES	YES
72	a	1456.03	251.06733	YES	YES
73	a	1543.36	28.88629	YES	YES
74	a	1749.93	757.68841	YES	YES
75	a	2089.45	65.96195	YES	YES
76	a	2327.86	255.86157	YES	YES
77	a	2332.73	40.50782	YES	YES
78	a	2344.52	43.78618	YES	YES
79	a	2348.34	44.90881	YES	YES
80	a	2357.05	26.16123	YES	YES
81	a	2360.00	23.49071	YES	YES
82	a	2902.18	69.82311	YES	YES
83	a	2959.39	4.56377	YES	YES
84	a	2960.37	12.20819	YES	YES
85	a	2970.50	15.67250	YES	YES
86	a	2990.86	7.51701	YES	YES
87	a	3042.72	3.71295	YES	YES
88	a	3045.26	2.54568	YES	YES
89	a	3075.01	5.76958	YES	YES
90	a	3079.64	2.10645	YES	YES

* zero point VIBRATIONAL energy : 0.2044503 Hartree *

Trans TS_{24}



bp86_svp SCF energy = -1354.4706087670
pbe0_tzvpp SCF energy = -1354.247609611

xyz Coordinates

30

H	-2.10545	2.06723	-1.27558
H	-0.88317	3.09281	0.19243
H	-0.18486	2.87804	-1.84270
H	0.56908	-3.12824	0.53772
H	2.47866	-2.36173	-0.12477
H	1.78884	-1.94251	1.88196
C	1.80355	0.16981	-2.21619
C	2.70355	0.25856	-3.42592
H	2.79999	-0.73876	-3.90524
H	3.70308	0.64260	-3.13981
H	2.25457	0.94447	-4.17838
C	-0.22208	0.79037	2.78736
C	0.31300	1.48187	4.04063
H	0.44268	0.72787	4.84766
H	1.27838	1.98990	3.84566
H	-0.43694	2.21786	4.40344
O	2.13826	0.71406	-1.10452
O	0.67488	-0.43469	-2.27591
O	0.53787	0.86556	1.75097
O	-1.33938	0.20912	2.86431
P	-0.74729	2.05764	-0.79782
P	1.28903	-1.88164	0.53363
Ru	0.27803	0.07382	-0.18323
C	-2.32313	-1.35189	-0.51391
C	-1.69253	-0.75252	0.38120
H	-1.64610	-0.37992	1.50361
C	-2.96067	-2.02754	-1.63122
H	-3.92392	-1.55099	-1.92402
H	-3.14604	-3.10624	-1.42479
H	-2.27927	-1.97050	-2.51253

Vibrational Spectrum

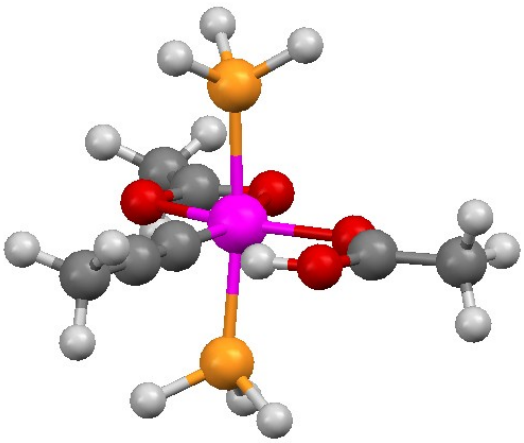
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1	a	-196.36	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	25.18	1.34415	YES	YES
9	a	30.62	0.76356	YES	YES
10	a	40.16	1.74835	YES	YES
11	a	53.39	0.35062	YES	YES
12	a	58.72	0.75546	YES	YES
13	a	67.33	0.42312	YES	YES
14	a	71.23	0.16225	YES	YES
15	a	74.62	0.26232	YES	YES
16	a	77.95	0.13725	YES	YES
17	a	80.23	0.62422	YES	YES
18	a	99.57	2.74217	YES	YES
19	a	100.77	2.52956	YES	YES
20	a	125.31	9.22990	YES	YES
21	a	140.79	0.05707	YES	YES
22	a	166.00	0.00416	YES	YES
23	a	188.61	0.28638	YES	YES
24	a	218.07	1.62259	YES	YES
25	a	232.04	30.93090	YES	YES
26	a	264.40	19.16472	YES	YES
27	a	276.14	17.14596	YES	YES
28	a	296.23	15.57957	YES	YES
29	a	308.50	8.55426	YES	YES
30	a	314.26	6.21513	YES	YES
31	a	320.13	0.50875	YES	YES
32	a	330.46	46.54617	YES	YES
33	a	369.81	2.43633	YES	YES
34	a	467.68	0.03052	YES	YES
35	a	474.77	3.06664	YES	YES
36	a	479.68	0.02464	YES	YES
37	a	517.82	22.32960	YES	YES
38	a	560.39	8.55514	YES	YES
39	a	563.81	10.62296	YES	YES
40	a	598.23	0.44691	YES	YES
41	a	604.81	0.57719	YES	YES
42	a	662.64	48.57635	YES	YES
43	a	666.43	82.88824	YES	YES
44	a	898.80	131.25213	YES	YES
45	a	934.48	40.33774	YES	YES
46	a	940.03	13.53347	YES	YES
47	a	971.25	3.55814	YES	YES
48	a	980.03	1.36266	YES	YES
49	a	985.32	9.35478	YES	YES
50	a	992.47	1.95071	YES	YES
51	a	1002.16	426.72966	YES	YES
52	a	1021.84	18.80734	YES	YES

53	a	1024.87	15.94030	YES	YES
54	a	1033.46	7.09817	YES	YES
55	a	1041.78	9.18414	YES	YES
56	a	1065.58	223.45568	YES	YES
57	a	1089.94	0.58057	YES	YES
58	a	1090.77	1.41569	YES	YES
59	a	1093.61	3.69862	YES	YES
60	a	1095.42	20.90003	YES	YES
61	a	1320.96	10.02149	YES	YES
62	a	1328.49	1.23656	YES	YES
63	a	1343.51	11.85834	YES	YES
64	a	1372.32	177.62025	YES	YES
65	a	1393.34	8.14659	YES	YES
66	a	1397.91	44.69901	YES	YES
67	a	1411.89	17.07408	YES	YES
68	a	1416.11	17.11832	YES	YES
69	a	1416.60	34.54738	YES	YES
70	a	1418.51	34.53863	YES	YES
71	a	1451.54	262.46039	YES	YES
72	a	1511.37	498.31929	YES	YES
73	a	1543.25	3.35198	YES	YES
74	a	1899.68	718.49134	YES	YES
75	a	2204.71	1025.58573	YES	YES
76	a	2312.33	237.80870	YES	YES
77	a	2319.08	75.86902	YES	YES
78	a	2329.50	111.73655	YES	YES
79	a	2334.28	32.12072	YES	YES
80	a	2336.33	18.53544	YES	YES
81	a	2339.92	60.88086	YES	YES
82	a	2923.42	17.87438	YES	YES
83	a	2958.03	14.60870	YES	YES
84	a	2958.70	4.69074	YES	YES
85	a	3004.36	9.82379	YES	YES
86	a	3007.05	2.43020	YES	YES
87	a	3039.55	4.71323	YES	YES
88	a	3040.59	2.58804	YES	YES
89	a	3076.24	7.50448	YES	YES
90	a	3078.46	2.38906	YES	YES

* zero point VIBRATIONAL energy : 0.2052184 Hartree *

Trans 4



bp86_svp SCF energy = -1354.4957394750
pbe0_tzvpp SCF energy = -1354.280357262

xyz Coordinates

30

H	3.16761	0.33660	-1.26547
H	3.04859	0.21346	0.88598
H	2.80163	-1.57340	-0.30961
H	-3.04332	1.08412	0.41511
H	-3.04224	0.18433	-1.54693
H	-3.00424	-1.07408	0.22162
C	0.00590	0.09890	-2.88007
C	0.05133	0.02203	-4.38988
H	-0.40618	0.92989	-4.83343
H	-0.46467	-0.89052	-4.75252
H	1.11099	-0.02641	-4.72784
C	0.07248	1.53396	2.38981
C	0.13874	2.79832	3.21231
H	1.03124	2.76883	3.87475
H	0.18702	3.68599	2.55302
H	-0.75326	2.86413	3.87274
O	-0.04465	-0.98915	-2.18880
O	0.04833	1.21152	-2.26566
O	0.08069	1.59638	1.13759
O	0.00869	0.42474	3.08313
P	2.30012	-0.22982	-0.26134
P	-2.31591	0.07024	-0.30731
Ru	-0.00045	0.05503	-0.31688
C	-0.11120	-2.33701	1.84015
C	-0.06765	-1.40634	1.00840
H	-0.02714	-0.42280	2.44611
C	-0.17171	-3.47172	2.76688
H	-0.59377	-4.37895	2.27340
H	-0.81486	-3.26054	3.65371
H	0.83443	-3.75471	3.15695

Vibrational Spectrum

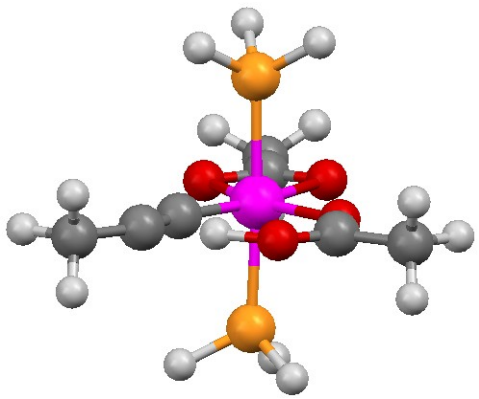
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	30.65	0.51719	YES	YES
8	a	34.47	0.07017	YES	YES
9	a	43.24	0.38430	YES	YES
10	a	44.85	0.43903	YES	YES
11	a	51.83	0.40060	YES	YES
12	a	55.65	0.13224	YES	YES
13	a	62.15	0.62274	YES	YES
14	a	65.07	0.96443	YES	YES
15	a	77.29	0.45141	YES	YES
16	a	79.95	0.61243	YES	YES
17	a	80.31	0.28878	YES	YES
18	a	101.03	6.89383	YES	YES
19	a	115.21	13.95882	YES	YES
20	a	130.85	0.03703	YES	YES
21	a	159.78	0.03772	YES	YES
22	a	172.70	0.04990	YES	YES
23	a	210.20	4.08055	YES	YES
24	a	221.88	3.06536	YES	YES
25	a	239.47	1.10934	YES	YES
26	a	257.34	17.15345	YES	YES
27	a	288.16	7.95883	YES	YES
28	a	298.39	10.18731	YES	YES
29	a	309.10	15.77014	YES	YES
30	a	319.75	1.25049	YES	YES
31	a	371.95	14.30520	YES	YES
32	a	426.98	1.46355	YES	YES
33	a	432.03	7.35196	YES	YES
34	a	477.00	0.14720	YES	YES
35	a	480.16	2.32765	YES	YES
36	a	496.01	7.69119	YES	YES
37	a	501.42	22.60319	YES	YES
38	a	558.69	10.93148	YES	YES
39	a	566.83	7.66502	YES	YES
40	a	587.44	0.03201	YES	YES
41	a	602.75	1.39841	YES	YES
42	a	650.46	5.46549	YES	YES
43	a	671.89	63.37906	YES	YES
44	a	899.74	8.82027	YES	YES
45	a	930.18	17.98314	YES	YES
46	a	938.87	22.20149	YES	YES
47	a	981.03	10.95287	YES	YES
48	a	981.40	0.09086	YES	YES
49	a	999.31	3.32313	YES	YES
50	a	1002.66	441.39960	YES	YES

51	a	1013.20	3.29811	YES	YES
52	a	1023.67	0.04517	YES	YES
53	a	1025.55	10.23950	YES	YES
54	a	1026.74	18.03419	YES	YES
55	a	1034.95	8.81416	YES	YES
56	a	1089.79	3.83272	YES	YES
57	a	1090.86	4.58327	YES	YES
58	a	1095.73	4.40943	YES	YES
59	a	1099.48	5.18673	YES	YES
60	a	1242.01	57.29827	YES	YES
61	a	1327.22	3.46318	YES	YES
62	a	1332.44	3.87734	YES	YES
63	a	1365.88	32.52602	YES	YES
64	a	1397.83	66.53568	YES	YES
65	a	1405.37	31.48730	YES	YES
66	a	1410.83	37.52583	YES	YES
67	a	1415.01	11.24242	YES	YES
68	a	1415.92	9.16923	YES	YES
69	a	1418.19	4.08360	YES	YES
70	a	1423.08	164.47906	YES	YES
71	a	1444.30	256.27987	YES	YES
72	a	1560.10	94.79151	YES	YES
73	a	1628.20	235.33329	YES	YES
74	a	2092.59	126.97616	YES	YES
75	a	2312.62	305.16354	YES	YES
76	a	2314.03	511.46309	YES	YES
77	a	2321.25	866.42786	YES	YES
78	a	2325.92	52.92623	YES	YES
79	a	2333.26	102.31796	YES	YES
80	a	2356.09	41.60692	YES	YES
81	a	2369.27	52.52050	YES	YES
82	a	2903.76	110.59201	YES	YES
83	a	2957.34	6.60143	YES	YES
84	a	2964.31	5.48850	YES	YES
85	a	2973.21	13.78614	YES	YES
86	a	2974.87	12.62591	YES	YES
87	a	3041.93	1.05454	YES	YES
88	a	3042.43	3.56616	YES	YES
89	a	3076.83	3.45482	YES	YES
90	a	3094.50	1.49574	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2090143 Hartree *

Trans TS_{45}



bp86_svp SCF energy = -1354.4916808020
pbe0_tzvpp SCF energy = -1354.268062859

xyz Coordinates

30

H	3.11395	0.46252	-1.71080
H	3.06076	0.63675	0.44371
H	2.89882	-1.31506	-0.48552
H	-3.01030	1.36066	-0.05077
H	-3.03914	0.19406	-1.87376
H	-3.03566	-0.80831	0.05442
C	0.00968	0.52610	-3.19024
C	0.05741	0.62016	-4.69917
H	-0.44384	1.54908	-5.04057
H	-0.41357	-0.26951	-5.16461
H	1.11793	0.66457	-5.03468
C	0.05132	1.40930	2.21878
C	0.11508	2.67514	3.05917
H	1.00623	2.63346	3.72263
H	0.16259	3.57937	2.42146
H	-0.77727	2.72524	3.72041
O	-0.02510	-0.63399	-2.62719
O	0.03297	1.56391	-2.45638
O	0.06478	1.55619	0.95527
O	-0.01250	0.30539	2.86763
P	2.31804	-0.00842	-0.60636
P	-2.32132	0.23531	-0.62682
Ru	0.00096	0.18181	-0.63949
C	-0.09338	-2.05553	1.57406
C	-0.05740	-1.31194	0.54464
H	-0.05070	-0.76019	2.21129
C	-0.14911	-3.31751	2.34626
H	-0.18544	-4.20093	1.67098
H	-1.04748	-3.36127	3.00435
H	0.73880	-3.43704	3.008783

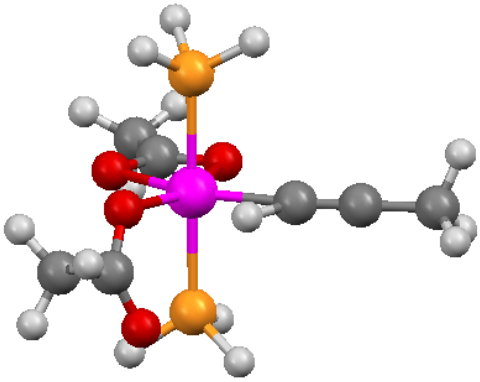
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-799.60	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	2.81	0.67641	YES	YES
9	a	39.59	0.41757	YES	YES
10	a	44.38	0.19466	YES	YES
11	a	47.77	0.29181	YES	YES
12	a	50.79	1.24126	YES	YES
13	a	57.24	0.00788	YES	YES
14	a	61.23	0.10439	YES	YES
15	a	65.97	0.36049	YES	YES
16	a	76.58	1.34982	YES	YES
17	a	83.06	0.79389	YES	YES
18	a	102.36	10.32989	YES	YES
19	a	105.28	4.98315	YES	YES
20	a	124.56	0.04041	YES	YES
21	a	135.05	9.08662	YES	YES
22	a	160.09	0.15188	YES	YES
23	a	183.94	16.52343	YES	YES
24	a	208.03	2.40013	YES	YES
25	a	220.35	3.22029	YES	YES
26	a	244.83	4.21879	YES	YES
27	a	284.93	9.69217	YES	YES
28	a	292.11	7.86981	YES	YES
29	a	305.22	16.57915	YES	YES
30	a	316.48	1.17066	YES	YES
31	a	380.25	8.23335	YES	YES
32	a	416.82	102.52115	YES	YES
33	a	448.43	0.94804	YES	YES
34	a	470.14	0.33872	YES	YES
35	a	476.30	7.06295	YES	YES
36	a	501.33	7.28294	YES	YES
37	a	542.60	22.13464	YES	YES
38	a	558.65	6.30963	YES	YES
39	a	566.63	18.37497	YES	YES
40	a	587.14	49.56883	YES	YES
41	a	591.00	0.40508	YES	YES
42	a	603.19	2.12989	YES	YES
43	a	667.18	1.39468	YES	YES
44	a	673.59	67.02639	YES	YES
45	a	926.26	5.99015	YES	YES
46	a	939.30	17.34712	YES	YES
47	a	981.75	64.49901	YES	YES
48	a	982.77	50.67550	YES	YES
49	a	987.29	4.42812	YES	YES
50	a	998.80	397.41775	YES	YES

51	a	1003.07	18.77475	YES	YES
52	a	1007.02	53.79144	YES	YES
53	a	1024.67	8.83272	YES	YES
54	a	1025.69	17.45066	YES	YES
55	a	1033.11	9.20786	YES	YES
56	a	1043.46	13.22307	YES	YES
57	a	1088.97	5.57988	YES	YES
58	a	1092.61	1.10372	YES	YES
59	a	1096.06	5.17842	YES	YES
60	a	1097.05	11.43839	YES	YES
61	a	1311.56	74.68463	YES	YES
62	a	1327.35	2.13233	YES	YES
63	a	1328.08	2.46466	YES	YES
64	a	1362.83	6.92753	YES	YES
65	a	1396.76	64.01882	YES	YES
66	a	1397.28	106.60469	YES	YES
67	a	1411.32	35.87700	YES	YES
68	a	1416.58	3.39635	YES	YES
69	a	1417.02	13.41450	YES	YES
70	a	1422.97	50.17737	YES	YES
71	a	1425.10	93.47698	YES	YES
72	a	1445.25	266.24036	YES	YES
73	a	1560.31	84.19067	YES	YES
74	a	1669.14	634.55502	YES	YES
75	a	1991.76	202.70348	YES	YES
76	a	2327.93	276.37853	YES	YES
77	a	2333.10	38.09401	YES	YES
78	a	2340.45	14.63982	YES	YES
79	a	2341.94	50.72222	YES	YES
80	a	2357.37	28.30794	YES	YES
81	a	2369.09	30.96149	YES	YES
82	a	2921.78	92.05032	YES	YES
83	a	2958.10	5.88289	YES	YES
84	a	2961.83	7.39325	YES	YES
85	a	2988.96	11.84258	YES	YES
86	a	3009.12	11.74321	YES	YES
87	a	3041.78	2.60579	YES	YES
88	a	3043.21	3.39452	YES	YES
89	a	3077.27	3.40871	YES	YES
90	a	3084.23	4.45324	YES	YES

* zero point VIBRATIONAL energy : 0.2060638 Hartree *

Trans 3_x



bp86_svp SCF energy = -1354.4815827880
pbe0_tzvpp SCF energy = -1354.256514900

xyz Coordinates

30

H	2.67307	-1.24217	1.23858
H	3.00241	-0.17308	-0.61485
H	2.74744	0.96789	1.20833
H	-2.96462	1.33044	-1.10547
H	-2.78382	-0.64437	-1.97941
H	-3.37846	-0.43533	0.09762
C	0.41091	-1.55134	-2.09315
C	0.77208	-2.47545	-3.22789
H	0.59714	-1.97629	-4.20269
H	0.18864	-3.41638	-3.16169
H	1.85235	-2.73619	-3.16338
C	-0.12437	-0.57489	2.81201
C	-0.85542	-1.07725	4.05557
H	-0.12188	-1.46968	4.78876
H	-1.39244	-0.22502	4.52962
H	-1.60443	-1.85427	3.80029
O	0.03757	-2.01845	-0.95427
O	0.49308	-0.28086	-2.21265
O	-0.85489	-0.62663	1.72723
O	1.03679	-0.14138	2.88363
P	2.12469	-0.12488	0.53636
P	-2.36859	0.06089	-0.79571
Ru	-0.12719	-0.03556	-0.12944
C	0.16576	3.21957	-0.50856
C	0.02264	2.01562	-0.22936
H	-0.26832	1.46285	0.80758
C	0.37150	4.60828	-0.90624
H	1.26440	4.71793	-1.56544
H	0.53749	5.26979	-0.02319
H	-0.50379	5.01716	-1.46201

Vibrational Spectrum

mode symmetry wave number IR intensity selection rules

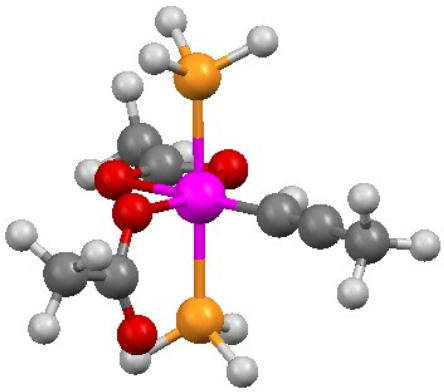
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.41	0.08782	YES	YES
8	a	25.96	0.61168	YES	YES
9	a	28.54	0.03946	YES	YES
10	a	31.39	0.41739	YES	YES
11	a	35.73	0.17878	YES	YES
12	a	43.71	0.40795	YES	YES
13	a	53.21	1.23918	YES	YES
14	a	62.34	0.94186	YES	YES
15	a	78.39	1.42612	YES	YES
16	a	94.88	1.69524	YES	YES
17	a	114.71	8.02938	YES	YES
18	a	143.35	1.44742	YES	YES
19	a	156.70	9.66087	YES	YES
20	a	167.94	12.49042	YES	YES
21	a	178.47	4.44475	YES	YES
22	a	197.88	0.92553	YES	YES
23	a	205.36	3.27355	YES	YES
24	a	216.13	10.73943	YES	YES
25	a	267.33	3.88054	YES	YES
26	a	287.51	12.34084	YES	YES
27	a	296.01	1.51542	YES	YES
28	a	313.68	5.81785	YES	YES
29	a	325.44	8.46742	YES	YES
30	a	332.10	22.72655	YES	YES
31	a	360.01	10.43081	YES	YES
32	a	397.15	0.33670	YES	YES
33	a	409.85	19.62212	YES	YES
34	a	460.13	8.31690	YES	YES
35	a	484.58	5.80604	YES	YES
36	a	494.35	2.03837	YES	YES
37	a	511.14	16.57871	YES	YES
38	a	518.09	1.15208	YES	YES
39	a	564.47	12.37190	YES	YES
40	a	588.86	10.99992	YES	YES
41	a	602.22	0.57224	YES	YES
42	a	604.80	3.04038	YES	YES
43	a	673.18	80.51556	YES	YES
44	a	676.80	13.40754	YES	YES
45	a	930.27	1.96742	YES	YES
46	a	943.68	26.38266	YES	YES
47	a	970.25	72.75034	YES	YES
48	a	981.19	1.86822	YES	YES
49	a	986.35	137.90805	YES	YES
50	a	990.64	212.22667	YES	YES
51	a	1007.58	3.35482	YES	YES
52	a	1016.58	11.59794	YES	YES

53	a	1017.68	1.20167	YES	YES
54	a	1020.92	7.08095	YES	YES
55	a	1026.41	10.28369	YES	YES
56	a	1068.50	36.07952	YES	YES
57	a	1090.17	3.84297	YES	YES
58	a	1095.70	3.63508	YES	YES
59	a	1127.82	8.10246	YES	YES
60	a	1218.54	263.88875	YES	YES
61	a	1307.68	178.99252	YES	YES
62	a	1330.45	1.14133	YES	YES
63	a	1340.32	171.93472	YES	YES
64	a	1362.58	23.67277	YES	YES
65	a	1397.33	33.30728	YES	YES
66	a	1409.14	34.71348	YES	YES
67	a	1409.42	13.42571	YES	YES
68	a	1410.28	8.82934	YES	YES
69	a	1410.80	8.07921	YES	YES
70	a	1420.30	14.42986	YES	YES
71	a	1459.78	268.19603	YES	YES
72	a	1536.86	68.86207	YES	YES
73	a	1658.70	208.34919	YES	YES
74	a	2037.85	131.74560	YES	YES
75	a	2252.23	50.29879	YES	YES
76	a	2278.55	152.09364	YES	YES
77	a	2338.63	126.69267	YES	YES
78	a	2357.44	50.40071	YES	YES
79	a	2365.48	17.87582	YES	YES
80	a	2402.03	49.19561	YES	YES
81	a	2433.16	13.92915	YES	YES
82	a	2910.79	79.46432	YES	YES
83	a	2957.88	11.30122	YES	YES
84	a	2960.19	2.34827	YES	YES
85	a	2980.51	7.11409	YES	YES
86	a	2991.07	7.08689	YES	YES
87	a	3044.21	7.33150	YES	YES
88	a	3046.14	1.81945	YES	YES
89	a	3077.26	6.21195	YES	YES
90	a	3080.11	1.67036	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2084165 Hartree *

Trans 3_y



bp86_svp SCF energy = -1354.4799988420
pbe0_tzvpp SCF energy = -1354.255185730

xyz Coordinates

30

H	1.36513	-0.19877	2.85683
H	2.69452	-1.00966	1.36594
H	2.52903	1.14236	1.52150
H	-1.27344	-0.18777	-3.23534
H	-2.18353	-1.81635	-2.13962
H	-2.77505	0.23237	-1.72333
C	0.14220	-2.80740	0.19061
C	0.16426	-4.30091	0.39140
H	1.13859	-4.72103	0.06977
H	-0.63916	-4.77051	-0.21941
H	-0.03322	-4.54827	1.45491
C	-0.93862	1.84559	1.60916
C	-2.08388	2.75700	2.04617
H	-1.83999	3.23717	3.01466
H	-2.24068	3.54553	1.27729
H	-3.03130	2.18360	2.12923
O	-0.66328	-2.05797	0.84660
O	0.91110	-2.24246	-0.66856
O	-1.26380	1.05802	0.61818
O	0.16775	1.89788	2.17056
P	1.66484	0.00934	1.47652
P	-1.57415	-0.53857	-1.87537
Ru	0.06095	-0.29715	-0.21595
C	1.04695	2.47524	-1.71808
C	0.74811	1.38337	-1.20458
H	1.22698	0.25926	-1.38261
C	1.37773	3.78086	-2.27870
H	0.55325	4.18447	-2.91093
H	2.28843	3.73132	-2.92128
H	1.58447	4.52935	-1.47893

Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	27.73	0.72888	YES	YES
8	a	31.08	0.42554	YES	YES
9	a	36.09	0.41427	YES	YES
10	a	40.26	0.41955	YES	YES
11	a	41.36	0.02203	YES	YES
12	a	56.60	0.54213	YES	YES
13	a	60.71	0.27522	YES	YES
14	a	76.61	0.60978	YES	YES
15	a	80.40	1.40101	YES	YES
16	a	100.54	1.12213	YES	YES
17	a	111.58	6.90282	YES	YES
18	a	138.56	1.19973	YES	YES
19	a	160.32	9.65443	YES	YES
20	a	170.37	10.45930	YES	YES
21	a	186.25	8.06065	YES	YES
22	a	206.13	3.84482	YES	YES
23	a	225.68	7.55171	YES	YES
24	a	235.75	0.91798	YES	YES
25	a	267.37	2.76016	YES	YES
26	a	295.35	16.78847	YES	YES
27	a	295.90	8.48159	YES	YES
28	a	308.97	5.99799	YES	YES
29	a	314.42	2.90071	YES	YES
30	a	348.20	3.93210	YES	YES
31	a	368.94	13.98571	YES	YES
32	a	389.43	0.48735	YES	YES
33	a	426.01	26.01841	YES	YES
34	a	466.48	5.63190	YES	YES
35	a	486.72	2.89546	YES	YES
36	a	501.79	2.93945	YES	YES
37	a	523.24	7.77233	YES	YES
38	a	523.97	8.62662	YES	YES
39	a	557.83	11.69447	YES	YES
40	a	590.13	8.05983	YES	YES
41	a	602.73	5.31426	YES	YES
42	a	604.71	1.45390	YES	YES
43	a	671.99	81.28128	YES	YES
44	a	676.13	20.84373	YES	YES
45	a	930.70	2.76953	YES	YES
46	a	943.97	27.28607	YES	YES
47	a	965.85	86.12000	YES	YES
48	a	980.12	250.60815	YES	YES
49	a	981.75	4.42131	YES	YES
50	a	991.41	41.56440	YES	YES
51	a	1008.53	5.72746	YES	YES

52	a	1013.27	53.60103	YES	YES
53	a	1017.08	3.25390	YES	YES
54	a	1021.26	5.44118	YES	YES
55	a	1027.01	16.06720	YES	YES
56	a	1067.12	52.54692	YES	YES
57	a	1090.46	5.86802	YES	YES
58	a	1098.19	1.51253	YES	YES
59	a	1130.74	7.07689	YES	YES
60	a	1206.58	551.40947	YES	YES
61	a	1308.85	133.39438	YES	YES
62	a	1330.84	1.72139	YES	YES
63	a	1345.52	212.93993	YES	YES
64	a	1361.76	22.36915	YES	YES
65	a	1397.04	37.37217	YES	YES
66	a	1407.46	18.62860	YES	YES
67	a	1409.21	5.82566	YES	YES
68	a	1410.24	27.51691	YES	YES
69	a	1412.21	5.78292	YES	YES
70	a	1418.33	11.23797	YES	YES
71	a	1462.46	283.41940	YES	YES
72	a	1535.83	79.23683	YES	YES
73	a	1658.90	209.81862	YES	YES
74	a	1959.46	95.61756	YES	YES
75	a	2176.45	13.58564	YES	YES
76	a	2248.40	189.53778	YES	YES
77	a	2334.43	123.02557	YES	YES
78	a	2360.72	51.01795	YES	YES
79	a	2371.70	23.65817	YES	YES
80	a	2405.26	45.04138	YES	YES
81	a	2433.52	14.42843	YES	YES
82	a	2913.47	65.17643	YES	YES
83	a	2959.61	3.28128	YES	YES
84	a	2959.81	9.08248	YES	YES
85	a	2984.71	6.70781	YES	YES
86	a	2993.99	5.93376	YES	YES
87	a	3043.72	5.91675	YES	YES
88	a	3044.96	1.65489	YES	YES
89	a	3077.73	8.02787	YES	YES
90	a	3080.09	1.71175	YES	YES

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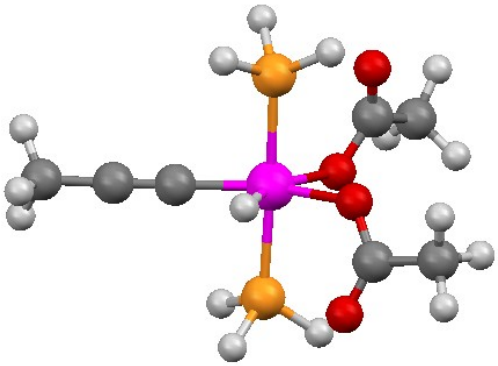
* zero point VIBRATIONAL energy : 0.2084228 Hartree *

Trans 4h _1



bp86_svp SCF energy = -1354.4576723590
pbe0_tzvpp SCF energy = -1354.223805714

xyz Coordinates

30

H	2.72382	-1.32464	1.27892
H	2.35114	0.62888	2.13041
H	1.33214	-1.16357	2.92520
H	-2.58297	0.83465	-1.74671
H	-1.41165	-0.48923	-3.06278
H	-2.68522	-1.32706	-1.53601
C	0.86842	1.77305	-1.95442
C	1.99783	2.67756	-2.43415
H	2.16944	3.48044	-1.68360
H	1.73329	3.13549	-3.40784
H	2.94638	2.10592	-2.52242
C	-0.78442	1.65503	2.06421
C	-1.53320	2.94281	2.40842
H	-1.62850	3.03068	3.50920
H	-0.95176	3.81241	2.02941
H	-2.53203	2.97057	1.92651
O	-0.23619	1.75668	-2.50292
O	1.20807	1.04609	-0.90175
O	-0.97060	1.29543	0.81546
O	-0.07924	1.07215	2.89560
P	1.60413	-0.50603	1.68991
P	-1.69879	-0.28312	-1.67693
Ru	-0.01593	-0.35534	-0.01732
C	-0.05397	-3.53079	-0.10651
C	-0.08454	-2.28421	-0.03482
H	-1.12406	-0.93153	0.99448
C	0.03311	-4.97812	-0.24121
H	-0.14607	-5.31740	-1.28778
H	-0.74857	-5.46348	0.39041
H	1.01677	-5.38136	0.09349

Vibrational Spectrum

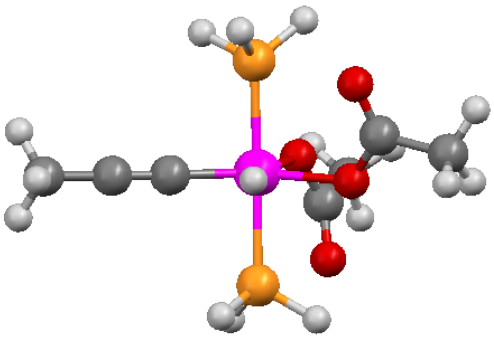
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.21	0.36666	YES	YES
8	a	19.74	0.99680	YES	YES
9	a	32.73	0.37854	YES	YES
10	a	36.48	0.72033	YES	YES
11	a	50.68	1.22283	YES	YES
12	a	56.95	1.46116	YES	YES
13	a	64.55	1.20174	YES	YES
14	a	82.05	0.33568	YES	YES
15	a	88.04	0.44892	YES	YES
16	a	100.44	1.89343	YES	YES
17	a	127.63	0.05923	YES	YES
18	a	153.71	15.24961	YES	YES
19	a	161.04	16.90011	YES	YES
20	a	178.79	10.00739	YES	YES
21	a	180.80	1.82963	YES	YES
22	a	195.56	7.25998	YES	YES
23	a	210.37	4.30218	YES	YES
24	a	215.68	4.73152	YES	YES
25	a	275.40	7.44419	YES	YES
26	a	283.59	11.01167	YES	YES
27	a	290.73	0.56618	YES	YES
28	a	309.89	1.90012	YES	YES
29	a	317.06	1.16173	YES	YES
30	a	324.25	0.09068	YES	YES
31	a	384.74	0.15630	YES	YES
32	a	397.58	7.82701	YES	YES
33	a	423.87	23.41328	YES	YES
34	a	499.45	1.57773	YES	YES
35	a	508.62	0.34530	YES	YES
36	a	521.34	4.53337	YES	YES
37	a	524.39	1.24897	YES	YES
38	a	571.22	4.19382	YES	YES
39	a	586.72	3.52888	YES	YES
40	a	594.15	0.87208	YES	YES
41	a	597.11	13.80392	YES	YES
42	a	644.69	32.15963	YES	YES
43	a	659.78	41.51463	YES	YES
44	a	664.74	43.41277	YES	YES
45	a	816.69	8.49454	YES	YES
46	a	915.32	0.34608	YES	YES
47	a	924.03	2.63982	YES	YES
48	a	979.39	63.51371	YES	YES
49	a	983.36	9.71054	YES	YES
50	a	989.14	244.38082	YES	YES
51	a	991.02	28.83006	YES	YES
52	a	1010.49	13.70516	YES	YES
53	a	1016.51	1.00824	YES	YES

54	a	1020.10	4.89666	YES	YES
55	a	1023.45	7.96292	YES	YES
56	a	1024.10	5.89664	YES	YES
57	a	1073.44	55.99196	YES	YES
58	a	1075.24	2.19729	YES	YES
59	a	1122.22	11.25620	YES	YES
60	a	1122.56	6.93832	YES	YES
61	a	1265.04	513.92104	YES	YES
62	a	1286.25	316.38703	YES	YES
63	a	1326.36	23.56626	YES	YES
64	a	1335.16	112.45159	YES	YES
65	a	1351.27	5.47125	YES	YES
66	a	1393.88	10.21144	YES	YES
67	a	1405.77	12.30741	YES	YES
68	a	1407.10	20.65400	YES	YES
69	a	1415.94	9.32931	YES	YES
70	a	1416.18	27.25052	YES	YES
71	a	1416.67	8.85053	YES	YES
72	a	1673.80	305.52286	YES	YES
73	a	1679.03	109.45891	YES	YES
74	a	2071.15	108.54061	YES	YES
75	a	2085.97	74.71866	YES	YES
76	a	2291.59	122.61496	YES	YES
77	a	2314.23	115.81577	YES	YES
78	a	2394.12	51.06446	YES	YES
79	a	2407.51	41.49740	YES	YES
80	a	2428.19	15.95513	YES	YES
81	a	2438.70	13.40923	YES	YES
82	a	2913.94	35.04041	YES	YES
83	a	2960.03	5.24852	YES	YES
84	a	2962.48	8.52245	YES	YES
85	a	2988.20	16.02450	YES	YES
86	a	2994.63	5.66389	YES	YES
87	a	3042.76	4.04977	YES	YES
88	a	3050.04	4.69626	YES	YES
89	a	3079.61	7.52177	YES	YES
90	a	3081.47	3.96326	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2080375 Hartree *

Trans 4h _2



bp86_svp SCF energy = -1354.4577891780
pbe0_tzvpp SCF energy = -1354.223904424

xyz Coordinates

30

H	-2.37973	-2.10952	0.59422
H	-2.75626	-1.20112	-1.33299
H	-1.38705	-2.87137	-1.22613
H	2.60924	1.67717	0.87636
H	2.70364	1.52509	-1.29049
H	1.45953	3.05085	-0.40769
C	0.75384	-2.10571	1.61249
C	1.55986	-2.50697	2.84748
H	1.60988	-1.67949	3.58487
H	2.60102	-2.74715	2.53642
H	1.10956	-3.41068	3.30452
C	-0.85023	1.94031	1.80790
C	-1.97776	2.43045	2.70893
H	-1.69652	3.39081	3.18493
H	-2.91928	2.54771	2.13105
H	-2.17175	1.67126	3.49857
O	0.05207	-2.91881	1.00087
O	0.93313	-0.84363	1.29693
O	-1.20978	0.91725	1.04877
O	0.27123	2.45384	1.82283
P	-1.63628	-1.64950	-0.53537
P	1.72159	1.65478	-0.24097
Ru	0.01105	0.02680	-0.35062
C	0.06966	0.15789	-3.52458
C	0.09060	0.07058	-2.27884
H	1.10518	-0.99664	-0.93416
C	-0.00773	0.30801	-4.97086
H	0.70465	-0.39726	-5.46158
H	0.26954	1.33311	-5.30940
H	-1.02108	0.07003	-5.36987

Vibrational Spectrum

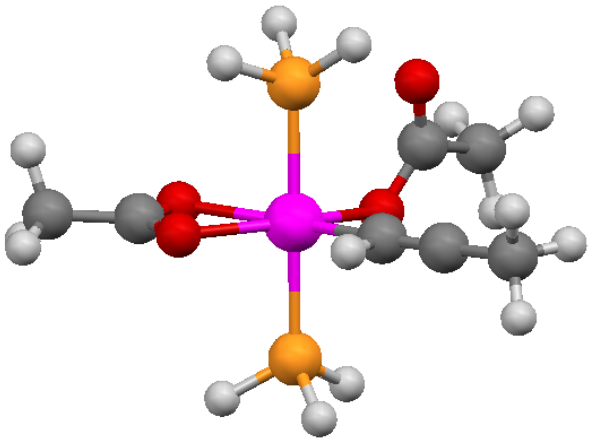
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	33.17	0.39852	YES	YES
8	a	36.36	0.73571	YES	YES
9	a	36.98	0.85821	YES	YES
10	a	51.95	0.76553	YES	YES
11	a	57.89	1.61984	YES	YES
12	a	59.76	1.05105	YES	YES
13	a	67.09	0.76968	YES	YES
14	a	87.27	0.53207	YES	YES
15	a	90.44	0.36348	YES	YES
16	a	100.31	1.77330	YES	YES
17	a	129.61	0.17709	YES	YES
18	a	153.99	16.03420	YES	YES
19	a	160.48	16.58425	YES	YES
20	a	178.68	9.00911	YES	YES
21	a	180.89	1.63458	YES	YES
22	a	196.00	7.40383	YES	YES
23	a	209.80	4.45066	YES	YES
24	a	215.68	4.88122	YES	YES
25	a	274.44	7.45534	YES	YES
26	a	282.58	11.36049	YES	YES
27	a	290.93	0.61019	YES	YES
28	a	310.30	1.87222	YES	YES
29	a	316.55	1.19273	YES	YES
30	a	320.06	0.02510	YES	YES
31	a	384.61	0.12721	YES	YES
32	a	397.42	7.96773	YES	YES
33	a	423.67	23.85414	YES	YES
34	a	498.76	1.32773	YES	YES
35	a	508.71	0.53995	YES	YES
36	a	520.52	3.97358	YES	YES
37	a	524.15	1.96254	YES	YES
38	a	569.17	6.71650	YES	YES
39	a	585.34	2.88403	YES	YES
40	a	594.53	4.58698	YES	YES
41	a	600.49	4.33483	YES	YES
42	a	646.15	30.60531	YES	YES
43	a	657.21	38.96678	YES	YES
44	a	663.60	50.18755	YES	YES
45	a	819.01	8.61987	YES	YES
46	a	915.30	0.25792	YES	YES
47	a	924.29	3.52568	YES	YES
48	a	979.58	71.08100	YES	YES
49	a	984.22	8.65750	YES	YES
50	a	988.97	251.72085	YES	YES
51	a	990.82	21.06623	YES	YES
52	a	1010.32	11.88381	YES	YES
53	a	1016.64	1.98435	YES	YES
54	a	1019.93	7.40039	YES	YES

55	a	1023.52	6.83996	YES	YES
56	a	1024.00	5.41785	YES	YES
57	a	1073.08	52.81180	YES	YES
58	a	1074.78	2.61106	YES	YES
59	a	1121.40	7.37751	YES	YES
60	a	1122.61	10.93875	YES	YES
61	a	1264.75	528.08317	YES	YES
62	a	1286.05	308.49008	YES	YES
63	a	1327.81	24.71720	YES	YES
64	a	1335.04	110.04878	YES	YES
65	a	1351.13	5.71055	YES	YES
66	a	1393.49	9.56935	YES	YES
67	a	1405.88	17.67711	YES	YES
68	a	1407.14	20.41163	YES	YES
69	a	1416.29	26.33877	YES	YES
70	a	1417.04	13.79523	YES	YES
71	a	1417.74	8.18991	YES	YES
72	a	1674.65	322.79772	YES	YES
73	a	1678.26	88.14339	YES	YES
74	a	2071.02	97.79233	YES	YES
75	a	2084.82	85.38220	YES	YES
76	a	2294.05	122.27658	YES	YES
77	a	2314.19	114.87698	YES	YES
78	a	2393.93	51.64963	YES	YES
79	a	2407.48	41.02921	YES	YES
80	a	2426.66	15.55812	YES	YES
81	a	2438.70	13.46413	YES	YES
82	a	2913.29	35.24737	YES	YES
83	a	2959.79	5.27243	YES	YES
84	a	2961.00	7.68767	YES	YES
85	a	2987.46	16.31756	YES	YES
86	a	2993.88	5.49437	YES	YES
87	a	3042.83	4.05484	YES	YES
88	a	3048.37	4.38457	YES	YES
89	a	3079.00	7.59682	YES	YES
90	a	3081.40	4.06848	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2081725 Hartree *

Trans TS_{35}_y



bp86_svp SCF energy = -1354.4610189080
pbe0_tzvpp SCF energy = -1354.236659748

xyz Coordinates

30

H	1.23984	-0.47341	2.94693
H	2.65461	-1.04980	1.42802
H	2.28013	1.05335	1.73225
H	-1.42396	-0.35836	-3.13803
H	-2.05467	-2.16467	-2.14421
H	-2.93596	-0.26145	-1.59151
C	0.53937	-2.98799	-0.08196
C	0.93203	-4.44712	-0.04949
H	1.47956	-4.72674	-0.97218
H	0.03139	-5.08383	0.07439
H	1.59586	-4.63286	0.82429
C	-1.26384	1.39124	1.83271
C	-2.50712	2.07567	2.40225
H	-2.23765	3.08084	2.78823
H	-3.31643	2.15440	1.64838
H	-2.88543	1.47822	3.26197
O	-0.38397	-2.53701	0.67629
O	1.15032	-2.16660	-0.85960
O	-1.50340	0.64501	0.79201
O	-0.15971	1.54928	2.38556
P	1.52386	-0.14829	1.58488
P	-1.63224	-0.83211	-1.79438
Ru	-0.02814	-0.48961	-0.14220
C	0.88088	2.28954	-1.51961
C	0.56574	1.15719	-1.01320
H	1.42279	0.78972	-1.72305
C	1.29997	3.56090	-2.09072
H	0.69646	4.37036	-1.61296
H	1.12251	3.62971	-3.18891
H	2.36899	3.79748	-1.88226

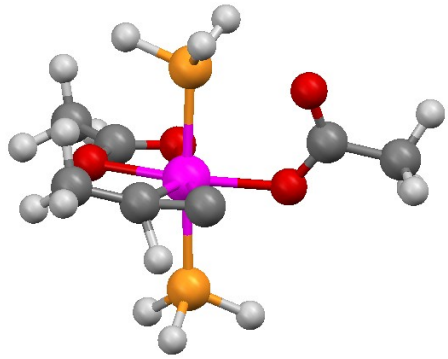
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-795.75	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	33.97	0.88187	YES	YES
9	a	40.84	0.45172	YES	YES
10	a	42.99	1.40487	YES	YES
11	a	44.77	0.65492	YES	YES
12	a	52.03	0.66623	YES	YES
13	a	53.96	0.02554	YES	YES
14	a	65.27	1.17516	YES	YES
15	a	72.35	1.39957	YES	YES
16	a	77.01	0.33003	YES	YES
17	a	98.82	1.28872	YES	YES
18	a	108.89	5.91175	YES	YES
19	a	131.23	0.63658	YES	YES
20	a	156.75	9.44954	YES	YES
21	a	164.75	8.26445	YES	YES
22	a	172.23	12.29840	YES	YES
23	a	185.36	7.35108	YES	YES
24	a	219.49	10.58926	YES	YES
25	a	227.86	1.52643	YES	YES
26	a	267.74	2.47435	YES	YES
27	a	277.24	13.42998	YES	YES
28	a	289.66	14.87253	YES	YES
29	a	300.27	15.85319	YES	YES
30	a	315.76	6.72497	YES	YES
31	a	317.55	20.63368	YES	YES
32	a	357.06	2.01016	YES	YES
33	a	385.07	9.95433	YES	YES
34	a	421.90	49.83428	YES	YES
35	a	429.61	2.68977	YES	YES
36	a	480.75	4.68390	YES	YES
37	a	494.97	2.91876	YES	YES
38	a	507.14	2.69153	YES	YES
39	a	514.60	1.06653	YES	YES
40	a	563.17	18.27822	YES	YES
41	a	596.71	7.40539	YES	YES
42	a	603.55	1.09604	YES	YES
43	a	604.28	4.92165	YES	YES
44	a	668.82	82.90805	YES	YES
45	a	675.35	13.26412	YES	YES
46	a	930.34	3.23262	YES	YES
47	a	938.71	14.98109	YES	YES
48	a	948.74	77.37775	YES	YES
49	a	981.86	1.94645	YES	YES
50	a	987.71	103.67966	YES	YES
51	a	988.47	22.72821	YES	YES

52	a	993.85	227.09295	YES	YES
53	a	1020.01	9.75985	YES	YES
54	a	1021.90	10.38388	YES	YES
55	a	1023.17	37.46671	YES	YES
56	a	1025.99	8.09819	YES	YES
57	a	1069.92	49.47968	YES	YES
58	a	1092.44	7.42477	YES	YES
59	a	1097.58	2.56870	YES	YES
60	a	1129.74	9.22201	YES	YES
61	a	1312.99	99.32722	YES	YES
62	a	1327.97	2.15133	YES	YES
63	a	1342.85	51.55018	YES	YES
64	a	1346.16	194.38277	YES	YES
65	a	1389.58	9.61802	YES	YES
66	a	1398.10	51.36883	YES	YES
67	a	1410.79	33.59521	YES	YES
68	a	1411.61	17.17129	YES	YES
69	a	1415.12	16.00949	YES	YES
70	a	1420.10	16.15049	YES	YES
71	a	1453.03	272.08597	YES	YES
72	a	1546.67	99.18304	YES	YES
73	a	1647.34	220.24322	YES	YES
74	a	1950.07	139.50161	YES	YES
75	a	2235.06	210.16473	YES	YES
76	a	2325.19	172.54992	YES	YES
77	a	2334.39	35.91300	YES	YES
78	a	2350.45	45.25573	YES	YES
79	a	2396.14	59.42005	YES	YES
80	a	2419.19	17.94444	YES	YES
81	a	2640.06	6.66177	YES	YES
82	a	2909.31	45.80865	YES	YES
83	a	2956.02	15.02182	YES	YES
84	a	2958.96	5.18583	YES	YES
85	a	2982.55	11.42832	YES	YES
86	a	2996.41	4.06535	YES	YES
87	a	3040.90	7.29207	YES	YES
88	a	3043.46	3.06215	YES	YES
89	a	3071.10	9.22961	YES	YES
90	a	3076.50	3.67935	YES	YES

* zero point VIBRATIONAL energy : 0.2058120 Hartree *

Trans TS_{25}_xd



bp86_svp SCF energy = -1354.4278134000
pbe0_tzvpp SCF energy = -1354.205019824

xyz Coordinates

30

H	2.53185	0.33088	-2.43152
H	2.36140	-1.74942	-1.81901
H	0.96988	-0.91380	-3.26783
H	-0.86032	0.29512	2.95355
H	-1.63353	1.82706	1.65634
H	-2.67585	-0.06373	1.72539
C	1.38734	2.06776	0.32058
C	2.11504	3.34439	0.65894
H	3.16888	3.12787	0.92838
H	1.62858	3.82563	1.53670
H	2.06970	4.05574	-0.19094
C	-0.10470	-2.51427	1.44358
C	0.37613	-3.92667	1.76321
H	0.11326	-4.19129	2.80715
H	-0.13857	-4.63910	1.08036
H	1.46877	-4.02725	1.59873
O	0.39779	2.07353	-0.50108
O	1.70806	0.95397	0.85795
O	0.56680	-1.94175	0.48209
O	-1.06355	-2.01838	2.06106
P	1.52560	-0.59333	-1.97576
P	-1.33172	0.40310	1.61100
Ru	0.07298	-0.05329	-0.23572
C	-1.59533	0.09045	-1.51902
C	-1.57725	-1.19470	-1.11835
H	-1.34644	-0.68655	-2.44495
C	-2.37734	1.30339	-1.91055
H	-2.76392	1.78813	-0.98835
H	-3.24189	1.03020	-2.55613
H	-1.74123	2.04851	-2.43256

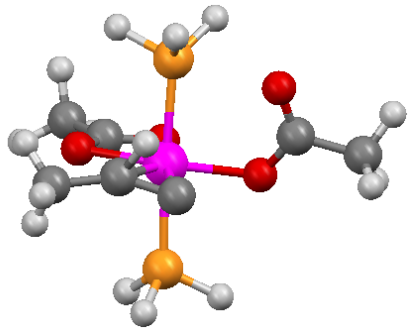
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-671.49	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	40.97	0.26960	YES	YES
9	a	43.56	0.26570	YES	YES
10	a	63.04	0.83418	YES	YES
11	a	68.86	2.52690	YES	YES
12	a	75.95	1.48874	YES	YES
13	a	87.00	1.26151	YES	YES
14	a	91.25	0.15811	YES	YES
15	a	104.02	1.62748	YES	YES
16	a	119.55	5.42472	YES	YES
17	a	127.21	0.39936	YES	YES
18	a	143.24	0.68963	YES	YES
19	a	157.17	1.77363	YES	YES
20	a	166.56	11.59842	YES	YES
21	a	185.49	5.87426	YES	YES
22	a	192.67	9.76809	YES	YES
23	a	202.42	4.83766	YES	YES
24	a	229.26	4.68868	YES	YES
25	a	247.40	1.45218	YES	YES
26	a	268.57	8.85132	YES	YES
27	a	295.28	4.86571	YES	YES
28	a	308.20	8.96687	YES	YES
29	a	312.72	4.12219	YES	YES
30	a	334.46	14.35228	YES	YES
31	a	366.66	1.22364	YES	YES
32	a	409.64	0.92961	YES	YES
33	a	411.74	23.25900	YES	YES
34	a	482.53	5.05940	YES	YES
35	a	494.70	1.25583	YES	YES
36	a	509.18	3.64675	YES	YES
37	a	516.79	0.10570	YES	YES
38	a	545.50	18.65864	YES	YES
39	a	561.28	13.78769	YES	YES
40	a	598.07	9.85099	YES	YES
41	a	603.70	2.12008	YES	YES
42	a	605.63	3.25136	YES	YES
43	a	671.05	83.91831	YES	YES
44	a	676.43	15.88824	YES	YES
45	a	894.79	9.75511	YES	YES
46	a	906.63	6.08355	YES	YES
47	a	933.31	2.19658	YES	YES
48	a	943.49	23.75455	YES	YES
49	a	982.77	3.18204	YES	YES
50	a	986.54	172.34804	YES	YES
51	a	992.91	90.60253	YES	YES
52	a	1013.91	58.60246	YES	YES
53	a	1021.11	7.24409	YES	YES

54	a	1027.04	8.71065	YES	YES
55	a	1034.61	18.16155	YES	YES
56	a	1068.58	32.40659	YES	YES
57	a	1072.54	45.03104	YES	YES
58	a	1087.32	6.31576	YES	YES
59	a	1094.70	3.17395	YES	YES
60	a	1137.62	9.65900	YES	YES
61	a	1310.26	138.70321	YES	YES
62	a	1332.11	1.80038	YES	YES
63	a	1344.82	219.77492	YES	YES
64	a	1347.84	22.97279	YES	YES
65	a	1397.86	38.04002	YES	YES
66	a	1405.17	9.86796	YES	YES
67	a	1408.13	21.98951	YES	YES
68	a	1410.18	27.44054	YES	YES
69	a	1418.25	8.39333	YES	YES
70	a	1420.07	18.68506	YES	YES
71	a	1460.45	268.89218	YES	YES
72	a	1540.17	85.95435	YES	YES
73	a	1633.68	49.38074	YES	YES
74	a	1649.11	175.05041	YES	YES
75	a	2188.00	9.28287	YES	YES
76	a	2225.51	193.01506	YES	YES
77	a	2312.91	110.05544	YES	YES
78	a	2334.89	68.37378	YES	YES
79	a	2371.27	34.31556	YES	YES
80	a	2404.13	41.32441	YES	YES
81	a	2426.54	12.14475	YES	YES
82	a	2948.29	20.38592	YES	YES
83	a	2959.25	9.57745	YES	YES
84	a	2960.75	2.35466	YES	YES
85	a	3036.86	5.75058	YES	YES
86	a	3045.83	7.52221	YES	YES
87	a	3046.43	1.96804	YES	YES
88	a	3052.09	2.73282	YES	YES
89	a	3076.57	7.74714	YES	YES
90	a	3078.99	1.97001	YES	YES

* zero point VIBRATIONAL energy : 0.2074255
Hartree *

Trans TS_{25}_xu



bp86_svp SCF energy = -1354.4286998170
pbe0_tzvpp SCF energy = -1354.205996747

xyz Coordinates

30

H	2.47145	-0.36198	-2.41673
H	2.01831	-2.26929	-1.47286
H	0.76183	-1.51797	-3.07444
H	-0.87753	0.82047	2.92522
H	-1.25374	2.33698	1.43863
H	-2.66407	0.71039	1.61032
C	1.64083	1.93371	-0.02677
C	2.54524	3.13544	0.08276
H	3.55925	2.82679	0.40941
H	2.13683	3.83710	0.84447
H	2.59565	3.67430	-0.88563
C	-0.53877	-2.18247	1.80421
C	-0.25543	-3.57515	2.35889
H	-0.63347	-3.65641	3.39818
H	-0.79137	-4.32203	1.73129
H	0.82771	-3.81234	2.31896
O	0.63373	1.93982	-0.82636
O	1.82606	0.89198	0.68973
O	0.27185	-1.82824	0.84537
O	-1.48146	-1.50235	2.24793
P	1.34767	-1.05664	-1.84343
P	-1.24617	0.88647	1.54762
Ru	0.02712	-0.04283	-0.18749
C	-1.64885	0.08843	-1.46738
C	-1.59992	-1.20219	-1.09126
H	-2.61057	-0.23091	-0.76169
C	-1.94692	1.09785	-2.53056
H	-2.86457	0.82366	-3.09758
H	-1.08835	1.12809	-3.23481
H	-2.05997	2.11747	-2.10681

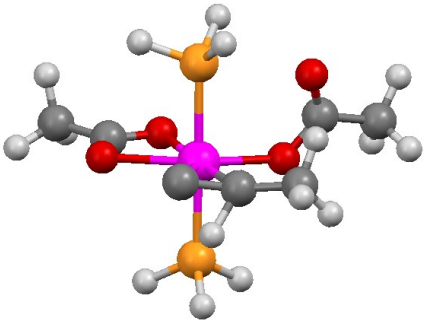
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-685.93	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	43.33	0.52880	YES	YES
9	a	59.35	0.33215	YES	YES
10	a	65.46	1.15049	YES	YES
11	a	68.29	2.58621	YES	YES
12	a	74.10	0.69798	YES	YES
13	a	85.96	0.11705	YES	YES
14	a	90.36	0.94764	YES	YES
15	a	100.05	1.75923	YES	YES
16	a	107.69	1.36361	YES	YES
17	a	117.67	4.46362	YES	YES
18	a	135.56	0.48725	YES	YES
19	a	150.07	0.94964	YES	YES
20	a	163.90	15.68336	YES	YES
21	a	182.09	8.30939	YES	YES
22	a	194.77	0.94661	YES	YES
23	a	199.48	6.68014	YES	YES
24	a	228.28	4.76430	YES	YES
25	a	249.23	2.30366	YES	YES
26	a	269.20	9.55113	YES	YES
27	a	292.97	2.09475	YES	YES
28	a	309.66	11.55485	YES	YES
29	a	313.66	1.72943	YES	YES
30	a	334.66	16.69783	YES	YES
31	a	358.80	1.16729	YES	YES
32	a	406.32	0.76198	YES	YES
33	a	413.56	21.56441	YES	YES
34	a	481.42	6.37715	YES	YES
35	a	486.11	0.91421	YES	YES
36	a	504.84	2.38596	YES	YES
37	a	515.74	0.16740	YES	YES
38	a	544.18	16.86547	YES	YES
39	a	559.22	15.88618	YES	YES
40	a	594.27	11.76825	YES	YES
41	a	601.76	1.46258	YES	YES
42	a	606.24	2.85269	YES	YES
43	a	670.12	87.12391	YES	YES
44	a	676.19	15.77384	YES	YES
45	a	889.26	2.72629	YES	YES
46	a	899.90	10.09955	YES	YES
47	a	933.27	3.06407	YES	YES
48	a	943.39	23.85281	YES	YES
49	a	982.15	2.53634	YES	YES
50	a	984.53	195.15155	YES	YES
51	a	991.51	54.54907	YES	YES
52	a	1012.47	76.90350	YES	YES
53	a	1021.00	7.22946	YES	YES
54	a	1026.25	9.02798	YES	YES

55	a	1033.32	28.52904	YES	YES
56	a	1062.92	16.39748	YES	YES
57	a	1069.25	49.95119	YES	YES
58	a	1091.25	5.60959	YES	YES
59	a	1097.16	2.84048	YES	YES
60	a	1131.65	9.19952	YES	YES
61	a	1310.94	122.48634	YES	YES
62	a	1330.02	1.31897	YES	YES
63	a	1345.17	14.09913	YES	YES
64	a	1346.54	241.55208	YES	YES
65	a	1398.22	36.19665	YES	YES
66	a	1403.51	10.53380	YES	YES
67	a	1407.57	22.12307	YES	YES
68	a	1409.90	28.15037	YES	YES
69	a	1419.71	16.42341	YES	YES
70	a	1419.87	12.19301	YES	YES
71	a	1459.71	269.64092	YES	YES
72	a	1540.03	86.67277	YES	YES
73	a	1633.41	20.05961	YES	YES
74	a	1649.23	194.84464	YES	YES
75	a	2191.94	6.01007	YES	YES
76	a	2235.98	186.90683	YES	YES
77	a	2330.91	136.28192	YES	YES
78	a	2342.43	26.22478	YES	YES
79	a	2376.69	30.74628	YES	YES
80	a	2389.23	43.12078	YES	YES
81	a	2417.43	18.51213	YES	YES
82	a	2949.47	20.76361	YES	YES
83	a	2958.29	9.59985	YES	YES
84	a	2959.05	2.33167	YES	YES
85	a	3039.25	5.90064	YES	YES
86	a	3044.68	2.03844	YES	YES
87	a	3044.93	7.48685	YES	YES
88	a	3053.80	3.25631	YES	YES
89	a	3074.74	7.72097	YES	YES
90	a	3078.18	1.94622	YES	YES

* zero point VIBRATIONAL energy : 0.2071338 Hartree *

Trans TS_{25}_yd



bp86_svp SCF energy = -1354.4326818020
pbe0_tzvpp SCF energy = -1354.209081700

xyz Coordinates

30

H	2.16239	0.44326	2.32594
H	2.95731	-0.57019	0.53322
H	2.81158	1.58778	0.60788
H	-2.24411	1.52272	-2.46791
H	-2.76844	-0.46067	-1.74666
H	-3.27629	1.29916	-0.57558
C	0.18592	-2.24535	0.80945
C	-0.22965	-3.71046	0.68632
H	0.61250	-4.36609	0.98693
H	-0.56027	-3.95140	-0.34476
H	-1.08314	-3.90817	1.37328
C	1.09273	1.54810	-2.20774
C	1.83367	2.09338	-3.40368
H	1.51979	3.13655	-3.61135
H	2.92650	2.09604	-3.19234
H	1.66151	1.45076	-4.29159
O	1.06765	-1.89872	1.61499
O	-0.49385	-1.44776	0.02892
O	0.92445	0.28435	-2.05581
O	0.63793	2.32157	-1.29815
P	2.00466	0.42607	0.90621
P	-2.14114	0.73912	-1.26647
Ru	-0.10360	0.58612	-0.14899
C	-1.06626	0.78915	1.73848
C	-0.57914	1.99084	1.37970
C	-1.42558	-0.16470	2.82760
H	-2.19973	-0.88934	2.49713
H	-1.78293	0.37064	3.73579
H	-0.51408	-0.74960	3.07601
H	-1.93433	1.66549	1.50472

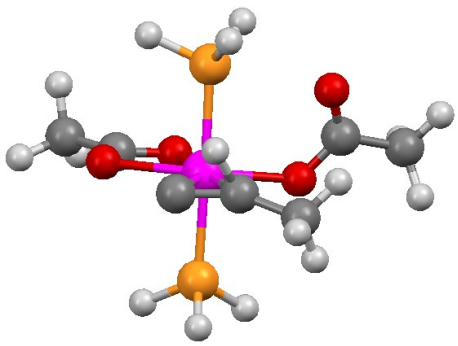
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-727.66	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	40.67	0.43585	YES	YES
9	a	44.80	0.40318	YES	YES
10	a	58.17	0.36986	YES	YES
11	a	71.47	1.52392	YES	YES
12	a	77.76	1.05100	YES	YES
13	a	85.71	1.00614	YES	YES
14	a	98.08	1.91978	YES	YES
15	a	112.44	1.11610	YES	YES
16	a	119.73	5.30131	YES	YES
17	a	129.81	2.03992	YES	YES
18	a	132.13	0.95878	YES	YES
19	a	157.89	13.66305	YES	YES
20	a	174.04	10.50906	YES	YES
21	a	177.38	2.85961	YES	YES
22	a	184.40	1.87461	YES	YES
23	a	209.40	3.45025	YES	YES
24	a	228.84	3.66218	YES	YES
25	a	247.51	7.45768	YES	YES
26	a	263.96	4.84818	YES	YES
27	a	293.50	2.60578	YES	YES
28	a	303.43	5.59504	YES	YES
29	a	311.13	0.40520	YES	YES
30	a	324.50	0.50825	YES	YES
31	a	332.82	28.11901	YES	YES
32	a	404.93	8.79089	YES	YES
33	a	428.99	0.80722	YES	YES
34	a	471.26	0.17218	YES	YES
35	a	487.36	2.47438	YES	YES
36	a	494.58	1.94992	YES	YES
37	a	515.61	3.15100	YES	YES
38	a	544.63	14.80148	YES	YES
39	a	554.97	6.29702	YES	YES
40	a	577.02	11.57283	YES	YES
41	a	602.09	0.73257	YES	YES
42	a	606.28	4.01649	YES	YES
43	a	669.82	69.41544	YES	YES
44	a	674.02	28.95960	YES	YES
45	a	892.37	4.89202	YES	YES
46	a	909.99	10.66750	YES	YES
47	a	928.67	4.12063	YES	YES
48	a	943.18	28.81269	YES	YES
49	a	981.34	2.64513	YES	YES
50	a	986.63	219.94255	YES	YES
51	a	991.25	101.30481	YES	YES
52	a	1014.37	24.09483	YES	YES
53	a	1022.51	6.61299	YES	YES
54	a	1026.66	10.92738	YES	YES

55	a	1043.09	13.93149	YES	YES
56	a	1065.16	35.46330	YES	YES
57	a	1066.74	9.54946	YES	YES
58	a	1087.74	4.13678	YES	YES
59	a	1093.77	3.03791	YES	YES
60	a	1127.60	7.74859	YES	YES
61	a	1309.61	144.04182	YES	YES
62	a	1329.36	1.07119	YES	YES
63	a	1343.02	195.14940	YES	YES
64	a	1347.01	6.41077	YES	YES
65	a	1397.76	33.34531	YES	YES
66	a	1406.07	34.77710	YES	YES
67	a	1408.82	6.05091	YES	YES
68	a	1410.17	28.08027	YES	YES
69	a	1420.50	8.61852	YES	YES
70	a	1429.41	13.86934	YES	YES
71	a	1460.77	288.93819	YES	YES
72	a	1542.09	96.96479	YES	YES
73	a	1637.67	60.34867	YES	YES
74	a	1650.04	155.91337	YES	YES
75	a	2131.76	7.71635	YES	YES
76	a	2298.56	133.56786	YES	YES
77	a	2316.56	97.68014	YES	YES
78	a	2348.26	71.84091	YES	YES
79	a	2362.41	30.91353	YES	YES
80	a	2401.07	46.92079	YES	YES
81	a	2421.89	14.28483	YES	YES
82	a	2944.22	27.92930	YES	YES
83	a	2957.25	9.90652	YES	YES
84	a	2959.63	2.65575	YES	YES
85	a	3032.22	6.78993	YES	YES
86	a	3043.47	6.82319	YES	YES
87	a	3045.11	2.14125	YES	YES
88	a	3047.39	5.40595	YES	YES
89	a	3077.41	5.57423	YES	YES
90	a	3078.25	2.20240	YES	YES

* zero point VIBRATIONAL energy : 0.2071415 Hartree *

Trans TS_{25}_yu



bp86_svp SCF energy = -1354.4327567900
pbe0_tzvpp SCF energy = -1354.209971610

xyz Coordinates

30

H	2.21055	0.12739	2.36100
H	2.86835	-1.08762	0.64199
H	3.02953	1.07165	0.58876
H	-2.05364	1.67423	-2.31990
H	-2.75967	-0.29210	-1.71826
H	-3.16631	1.44729	-0.48044
C	-0.05614	-2.38894	0.90152
C	-0.55656	-3.82064	0.71291
H	-0.18919	-4.21467	-0.26032
H	-1.66644	-3.85048	0.67929
H	-0.18094	-4.46627	1.53140
C	1.21275	1.33110	-2.13718
C	1.98357	1.82485	-3.33666
H	1.78687	2.90284	-3.50723
H	3.07414	1.69712	-3.15372
H	1.71851	1.23337	-4.23706
O	0.80333	-2.11229	1.75474
O	-0.61533	-1.54011	0.07804
O	0.88982	0.09333	-2.02519
O	0.88802	2.11878	-1.18500
P	2.06365	0.05477	0.93897
P	-2.05767	0.82893	-1.15792
Ru	-0.01557	0.44233	-0.06487
C	-0.95264	0.67848	1.82458
C	-0.57443	1.89576	1.39601
C	-1.88977	-0.16936	2.61552
H	-1.37555	-1.07662	2.99613
H	-2.71189	-0.50753	1.94790
H	-2.32912	0.39608	3.46773
H	-0.06043	1.23700	2.50970

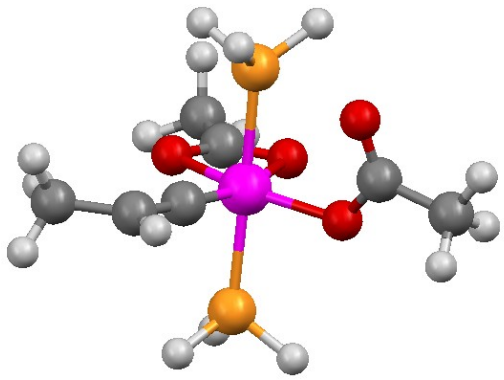
Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-704.95	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	34.38	0.62351	YES	YES
9	a	45.96	0.36943	YES	YES
10	a	56.63	0.39954	YES	YES
11	a	73.12	1.46069	YES	YES
12	a	78.09	0.52996	YES	YES
13	a	85.24	2.04799	YES	YES
14	a	96.64	1.63852	YES	YES
15	a	108.39	0.67956	YES	YES
16	a	112.52	0.92928	YES	YES
17	a	123.96	8.07468	YES	YES
18	a	131.45	1.11215	YES	YES
19	a	151.10	6.59261	YES	YES
20	a	166.71	17.10408	YES	YES
21	a	179.23	1.57363	YES	YES
22	a	187.29	1.64270	YES	YES
23	a	193.34	3.31243	YES	YES
24	a	220.64	3.81187	YES	YES
25	a	246.73	5.87401	YES	YES
26	a	264.31	3.94817	YES	YES
27	a	291.37	2.38417	YES	YES
28	a	303.28	4.85918	YES	YES
29	a	312.74	2.06974	YES	YES
30	a	321.81	0.51656	YES	YES
31	a	333.11	26.99966	YES	YES
32	a	397.28	7.45850	YES	YES
33	a	428.33	1.92022	YES	YES
34	a	471.46	0.64562	YES	YES
35	a	484.75	1.46765	YES	YES
36	a	497.47	1.56743	YES	YES
37	a	517.48	2.41005	YES	YES
38	a	544.37	14.39096	YES	YES
39	a	558.09	8.44037	YES	YES
40	a	580.19	8.65017	YES	YES
41	a	602.27	1.71567	YES	YES
42	a	606.61	3.25742	YES	YES
43	a	668.77	65.04236	YES	YES
44	a	673.80	35.28681	YES	YES
45	a	887.97	5.14749	YES	YES
46	a	905.46	6.70942	YES	YES
47	a	927.05	5.65554	YES	YES
48	a	943.09	29.11612	YES	YES
49	a	981.84	2.54606	YES	YES
50	a	988.19	67.02106	YES	YES
51	a	993.00	255.42393	YES	YES
52	a	1016.73	26.31107	YES	YES
53	a	1021.46	8.14994	YES	YES
54	a	1026.32	12.70164	YES	YES

55	a	1032.19	13.92994	YES	YES
56	a	1057.48	13.77047	YES	YES
57	a	1065.94	24.51023	YES	YES
58	a	1093.94	3.04022	YES	YES
59	a	1097.79	4.19366	YES	YES
60	a	1121.37	8.49712	YES	YES
61	a	1306.96	158.98019	YES	YES
62	a	1329.48	1.17373	YES	YES
63	a	1340.51	18.51363	YES	YES
64	a	1343.09	180.29991	YES	YES
65	a	1397.71	10.64376	YES	YES
66	a	1397.99	32.61748	YES	YES
67	a	1407.75	19.09411	YES	YES
68	a	1410.24	30.74695	YES	YES
69	a	1417.85	9.39636	YES	YES
70	a	1428.43	6.71873	YES	YES
71	a	1460.83	287.64304	YES	YES
72	a	1542.55	97.37289	YES	YES
73	a	1642.06	12.75406	YES	YES
74	a	1656.76	193.35546	YES	YES
75	a	2150.83	5.36682	YES	YES
76	a	2298.86	133.98331	YES	YES
77	a	2339.07	112.81635	YES	YES
78	a	2356.89	48.41066	YES	YES
79	a	2365.53	21.71913	YES	YES
80	a	2384.94	45.22212	YES	YES
81	a	2412.99	21.74968	YES	YES
82	a	2945.11	23.53050	YES	YES
83	a	2959.30	3.19328	YES	YES
84	a	2959.46	9.04200	YES	YES
85	a	3031.60	8.19408	YES	YES
86	a	3042.03	5.34054	YES	YES
87	a	3044.92	2.14858	YES	YES
88	a	3049.60	0.84171	YES	YES
89	a	3077.76	7.24116	YES	YES
90	a	3078.54	2.19610	YES	YES

* zero point VIBRATIONAL energy : 0.2063798 Hartree *

Trans 5_x



bp86_svp SCF energy = -1354.5250906480
pbe0_tzvpp SCF energy = -1354.297309942

xyz Coordinates

30

C	-0.18888	-0.05833	1.80036
C	-0.34606	-0.21274	3.11250
H	-1.35957	0.00016	3.51427
C	0.72205	-0.66938	4.08707
H	-1.32589	-2.76762	0.74209
H	-1.02271	-2.65480	-1.45161
H	0.65049	-2.99385	-0.12213
H	0.87852	2.83168	1.72478
H	1.99400	2.87442	-0.13843
H	-0.11608	3.39458	-0.13004
C	2.27531	-0.31440	-1.36671
C	3.56529	-0.64955	-2.07855
H	4.43871	-0.44888	-1.42466
H	3.64345	-0.07148	-3.02152
H	3.57397	-1.73256	-2.33555
C	-2.72020	0.13389	-0.82858
C	-3.89384	0.92223	-1.40293
H	-4.75828	0.25058	-1.57248
H	-3.59640	1.40460	-2.35920
H	-4.18368	1.73592	-0.70289
O	1.24384	0.08066	-1.99235
O	2.20128	-0.46104	-0.08628
O	-1.64882	0.87462	-0.65514
O	-2.81624	-1.07245	-0.56704
P	-0.50471	-2.12621	-0.22971
P	0.74970	2.36564	0.37318
Ru	0.13788	0.12446	0.02605
H	0.89305	0.09065	4.88436
H	0.42465	-1.61554	4.59634
H	1.68834	-0.84830	3.57005

Vibrational Spectrum

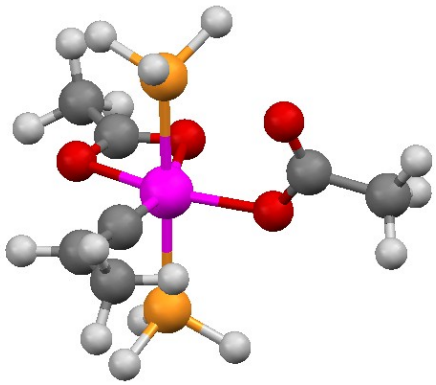
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	33.91	0.14208	YES	YES
8	a	41.58	0.37476	YES	YES
9	a	43.96	1.76256	YES	YES
10	a	45.80	0.15393	YES	YES
11	a	49.24	0.25904	YES	YES
12	a	62.55	0.44981	YES	YES
13	a	69.65	0.51931	YES	YES
14	a	74.21	0.43159	YES	YES
15	a	94.56	1.09022	YES	YES
16	a	110.49	6.69175	YES	YES
17	a	114.54	2.19488	YES	YES
18	a	135.85	1.28653	YES	YES
19	a	156.09	8.00902	YES	YES
20	a	164.08	9.44668	YES	YES
21	a	174.63	5.69705	YES	YES
22	a	182.36	4.46244	YES	YES
23	a	203.40	3.02430	YES	YES
24	a	220.56	4.18262	YES	YES
25	a	256.21	7.32077	YES	YES
26	a	278.51	5.84526	YES	YES
27	a	285.57	1.96291	YES	YES
28	a	310.10	3.72717	YES	YES
29	a	320.79	25.37900	YES	YES
30	a	341.32	2.50375	YES	YES
31	a	459.21	1.35788	YES	YES
32	a	464.03	1.24117	YES	YES
33	a	487.86	6.79006	YES	YES
34	a	499.79	2.65177	YES	YES
35	a	511.99	8.61022	YES	YES
36	a	526.52	0.43030	YES	YES
37	a	556.43	14.11860	YES	YES
38	a	589.82	7.45185	YES	YES
39	a	600.50	0.89232	YES	YES
40	a	601.67	2.81304	YES	YES
41	a	629.46	25.82077	YES	YES
42	a	636.07	3.23684	YES	YES
43	a	672.18	57.60770	YES	YES
44	a	677.13	38.29348	YES	YES
45	a	928.97	0.78501	YES	YES

46	a	939.84	6.01164	YES	YES
47	a	943.54	35.96547	YES	YES
48	a	982.45	247.09663	YES	YES
49	a	983.98	2.77650	YES	YES
50	a	990.00	80.79402	YES	YES
51	a	1007.40	0.25712	YES	YES
52	a	1008.92	18.00459	YES	YES
53	a	1022.10	5.46962	YES	YES
54	a	1026.67	9.09319	YES	YES
55	a	1047.09	0.84681	YES	YES
56	a	1067.87	39.60945	YES	YES
57	a	1089.69	4.34311	YES	YES
58	a	1095.26	4.31037	YES	YES
59	a	1126.68	8.06496	YES	YES
60	a	1197.23	50.67550	YES	YES
61	a	1296.74	261.33803	YES	YES
62	a	1328.65	2.64918	YES	YES
63	a	1338.54	184.98590	YES	YES
64	a	1353.91	18.12875	YES	YES
65	a	1397.98	54.02516	YES	YES
66	a	1407.23	15.91704	YES	YES
67	a	1411.28	33.42750	YES	YES
68	a	1416.42	9.21947	YES	YES
69	a	1422.86	5.59931	YES	YES
70	a	1430.02	4.09232	YES	YES
71	a	1448.26	253.35934	YES	YES
72	a	1565.98	103.11134	YES	YES
73	a	1670.18	194.52685	YES	YES
74	a	1708.33	160.06673	YES	YES
75	a	2276.51	152.11739	YES	YES
76	a	2344.18	126.54883	YES	YES
77	a	2364.00	36.65801	YES	YES
78	a	2372.37	14.68297	YES	YES
79	a	2405.24	43.61599	YES	YES
80	a	2440.08	11.82923	YES	YES
81	a	2924.32	72.98716	YES	YES
82	a	2959.99	9.81052	YES	YES
83	a	2960.04	1.99563	YES	YES
84	a	2988.39	14.40872	YES	YES
85	a	3014.54	2.42597	YES	YES
86	a	3041.76	4.36093	YES	YES
87	a	3043.93	8.53973	YES	YES
88	a	3045.53	2.74325	YES	YES
89	a	3079.43	2.47684	YES	YES
90	a	3081.03	7.81121	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2111361 Hartree *

Trans 5_y



bp86_svp SCF energy = -1354.5250340530
pbe0_tzvpp SCF energy = -1354.297305623

xyz Coordinates

30

C	-0.72028	-1.56220	-0.54989
C	-1.32862	-2.64280	-1.03267
H	-0.69411	-3.37934	-1.56937
C	-2.81286	-2.93376	-0.91900
H	-1.33671	0.51327	-2.79695
H	-0.32788	2.36047	-2.10361
H	0.81881	0.71735	-2.92294
H	0.29977	-2.67713	2.13462
H	1.96933	-1.36909	2.60243
H	-0.03297	-0.84139	3.26164
C	2.71974	0.48182	-0.18699
C	4.18357	0.75831	-0.43953
H	4.75918	-0.18847	-0.49179
H	4.59094	1.41843	0.35285
H	4.29697	1.28083	-1.41578
C	-2.16647	1.58918	0.53552
C	-3.07024	2.30065	1.53933
H	-3.84291	2.88869	1.00631
H	-2.46446	2.97178	2.18597
H	-3.55852	1.55787	2.20703
O	1.97992	1.29692	0.44533
O	2.18953	-0.59958	-0.65183
O	-1.21494	0.89247	1.11391
O	-2.35274	1.68655	-0.68491
P	-0.25340	0.93941	-1.97556
P	0.63601	-1.28280	2.07026
Ru	0.21849	-0.13687	0.06320
H	-3.28051	-3.03635	-1.92550
H	-2.99690	-3.88808	-0.37264
H	-3.34259	-2.12030	-0.38036

Vibrational Spectrum

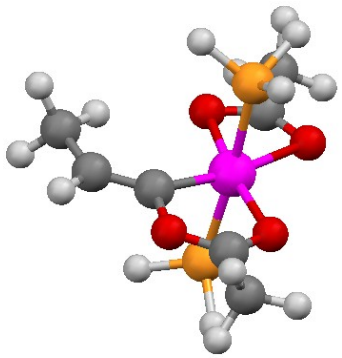
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.67	1.45279	YES	YES
8	a	30.20	0.25921	YES	YES
9	a	34.14	0.32752	YES	YES
10	a	50.89	0.09826	YES	YES
11	a	60.56	0.72053	YES	YES
12	a	65.55	0.47224	YES	YES
13	a	69.55	0.40303	YES	YES
14	a	77.12	0.32705	YES	YES
15	a	94.48	1.09883	YES	YES
16	a	112.84	8.63652	YES	YES
17	a	117.27	0.10990	YES	YES
18	a	124.41	1.54908	YES	YES
19	a	152.18	2.98528	YES	YES
20	a	161.62	9.85690	YES	YES
21	a	168.04	7.90934	YES	YES
22	a	183.28	3.64829	YES	YES
23	a	212.50	7.89944	YES	YES
24	a	219.17	4.40167	YES	YES
25	a	250.10	7.88010	YES	YES
26	a	275.78	5.00551	YES	YES
27	a	286.44	1.84125	YES	YES
28	a	310.89	2.71451	YES	YES
29	a	325.21	24.92793	YES	YES
30	a	334.21	6.71768	YES	YES
31	a	462.49	1.27223	YES	YES
32	a	469.40	1.73854	YES	YES
33	a	483.49	1.38089	YES	YES
34	a	494.22	2.16993	YES	YES
35	a	505.13	3.06019	YES	YES
36	a	527.60	0.59226	YES	YES
37	a	558.08	7.40523	YES	YES
38	a	589.76	9.90097	YES	YES
39	a	601.02	0.84086	YES	YES
40	a	602.97	2.69147	YES	YES
41	a	631.83	23.91009	YES	YES
42	a	642.10	12.02755	YES	YES
43	a	672.28	44.54164	YES	YES
44	a	677.19	47.76120	YES	YES
45	a	928.25	1.96584	YES	YES

46	a	939.00	11.91682	YES	YES
47	a	944.25	35.34132	YES	YES
48	a	983.65	8.20146	YES	YES
49	a	983.98	247.11179	YES	YES
50	a	991.12	80.92835	YES	YES
51	a	1006.28	0.48335	YES	YES
52	a	1010.11	8.66688	YES	YES
53	a	1022.87	5.44278	YES	YES
54	a	1026.20	9.51852	YES	YES
55	a	1048.23	0.56536	YES	YES
56	a	1069.00	40.32151	YES	YES
57	a	1089.97	4.40171	YES	YES
58	a	1096.08	4.32929	YES	YES
59	a	1126.15	8.28917	YES	YES
60	a	1200.11	44.22283	YES	YES
61	a	1297.91	251.33299	YES	YES
62	a	1328.22	2.52244	YES	YES
63	a	1340.08	173.37600	YES	YES
64	a	1353.65	19.15011	YES	YES
65	a	1397.84	52.82710	YES	YES
66	a	1407.42	15.97341	YES	YES
67	a	1411.34	34.76849	YES	YES
68	a	1416.69	8.95115	YES	YES
69	a	1420.64	4.61066	YES	YES
70	a	1429.56	7.49799	YES	YES
71	a	1448.22	254.43819	YES	YES
72	a	1565.74	109.64319	YES	YES
73	a	1668.58	187.39931	YES	YES
74	a	1705.97	157.89859	YES	YES
75	a	2282.22	155.10361	YES	YES
76	a	2344.79	131.72267	YES	YES
77	a	2363.27	31.05645	YES	YES
78	a	2371.29	15.67478	YES	YES
79	a	2404.73	42.87815	YES	YES
80	a	2441.13	11.87930	YES	YES
81	a	2924.98	71.74447	YES	YES
82	a	2960.20	3.82074	YES	YES
83	a	2960.67	8.06131	YES	YES
84	a	2989.45	13.92486	YES	YES
85	a	3017.37	2.06883	YES	YES
86	a	3042.27	4.53849	YES	YES
87	a	3045.80	2.71507	YES	YES
88	a	3045.83	8.95416	YES	YES
89	a	3079.30	2.53522	YES	YES
90	a	3081.47	7.58687	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2110780 Hartree *

Trans 6_x



bp86_svp SCF energy = -1354.5292277840
pbe0_tzvpp SCF energy = -1354.306984555

xyz Coordinates

30

C	-2.76229	0.02049	0.32447
C	-4.27489	-0.01739	0.25648
H	-4.61473	-1.06572	0.09930
H	-4.64301	0.58349	-0.60120
H	-4.71225	0.35396	1.20498
C	2.61263	0.00655	0.81628
C	3.95463	0.02370	1.49653
H	4.51602	0.94065	1.21151
H	4.56392	-0.84662	1.16951
H	3.82033	-0.00201	2.59511
C	1.28085	-0.02994	-1.13777
C	1.40468	-0.05945	-2.48790
H	2.42679	-0.07527	-2.91603
C	0.24181	-0.06933	-3.44228
H	0.25753	-0.97326	-4.09754
H	-0.72636	-0.05275	-2.89870
H	-0.10020	2.94068	-1.20334
H	0.88482	3.07969	0.71381
H	-1.27305	3.08594	0.61012
H	-1.31228	-3.04405	0.71703
H	0.84014	-3.04630	0.88871
H	-0.08272	-2.99032	-1.06356
O	-2.08329	-0.00132	-0.77317
O	-2.14130	0.04563	1.42943
O	1.53629	0.02710	1.47077
O	2.63467	-0.02542	-0.49344
H	0.26953	0.80990	-4.13007
P	-0.16945	2.31848	0.09114
P	-0.18762	-2.30762	0.19784
Ru	-0.17526	0.00730	0.22570

Vibrational Spectrum

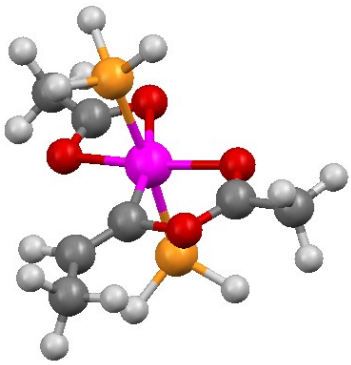
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.41	0.58277	YES	YES
8	a	34.18	0.03409	YES	YES
9	a	46.92	0.33516	YES	YES
10	a	48.99	1.03655	YES	YES
11	a	51.84	0.13714	YES	YES
12	a	60.05	0.17742	YES	YES
13	a	70.91	1.28831	YES	YES
14	a	84.40	0.01385	YES	YES
15	a	91.80	6.14437	YES	YES
16	a	103.27	5.30381	YES	YES
17	a	109.09	0.46704	YES	YES
18	a	129.81	0.32093	YES	YES
19	a	154.55	7.59603	YES	YES
20	a	159.17	0.03140	YES	YES
21	a	162.04	0.41291	YES	YES
22	a	227.66	1.89185	YES	YES
23	a	235.77	2.51391	YES	YES
24	a	254.01	11.22933	YES	YES
25	a	255.51	0.21463	YES	YES
26	a	295.61	18.78403	YES	YES
27	a	303.27	0.68701	YES	YES
28	a	318.59	0.52127	YES	YES
29	a	345.24	14.99272	YES	YES
30	a	385.36	8.65660	YES	YES
31	a	456.05	1.16815	YES	YES
32	a	464.85	0.09374	YES	YES
33	a	474.39	1.00950	YES	YES
34	a	492.24	4.21472	YES	YES
35	a	523.75	0.73264	YES	YES
36	a	547.50	1.00299	YES	YES
37	a	552.64	9.45704	YES	YES
38	a	561.11	11.46803	YES	YES
39	a	599.87	1.14981	YES	YES
40	a	604.62	0.11683	YES	YES
41	a	661.88	1.75656	YES	YES
42	a	670.04	61.86354	YES	YES
43	a	736.13	89.99874	YES	YES
44	a	771.93	14.61440	YES	YES
45	a	934.03	22.20241	YES	YES
46	a	939.07	22.86388	YES	YES
47	a	975.21	18.93806	YES	YES
48	a	981.95	4.45467	YES	YES
49	a	998.84	425.28239	YES	YES

50	a	1001.11	23.26687	YES	YES
51	a	1020.42	2.44581	YES	YES
52	a	1022.91	7.98092	YES	YES
53	a	1025.16	19.53979	YES	YES
54	a	1029.84	5.45262	YES	YES
55	a	1088.91	0.11188	YES	YES
56	a	1092.15	5.08745	YES	YES
57	a	1093.55	0.67099	YES	YES
58	a	1097.23	7.97199	YES	YES
59	a	1111.78	2.73106	YES	YES
60	a	1251.17	15.53155	YES	YES
61	a	1325.56	4.47631	YES	YES
62	a	1332.70	21.51472	YES	YES
63	a	1360.58	2.57098	YES	YES
64	a	1398.42	159.48049	YES	YES
65	a	1400.36	29.32430	YES	YES
66	a	1405.49	29.78282	YES	YES
67	a	1410.72	55.17617	YES	YES
68	a	1412.89	12.91371	YES	YES
69	a	1422.78	3.94560	YES	YES
70	a	1432.06	4.39481	YES	YES
71	a	1437.39	258.38549	YES	YES
72	a	1572.88	140.59576	YES	YES
73	a	1596.98	134.01525	YES	YES
74	a	1638.73	72.15346	YES	YES
75	a	2313.28	285.23107	YES	YES
76	a	2319.41	41.47520	YES	YES
77	a	2326.72	47.31240	YES	YES
78	a	2329.97	63.25813	YES	YES
79	a	2340.45	52.33214	YES	YES
80	a	2344.76	28.13603	YES	YES
81	a	2908.83	70.18831	YES	YES
82	a	2957.17	6.94744	YES	YES
83	a	2961.12	18.32456	YES	YES
84	a	2961.72	5.93805	YES	YES
85	a	3030.28	13.88089	YES	YES
86	a	3038.95	1.04331	YES	YES
87	a	3040.87	4.19442	YES	YES
88	a	3047.75	9.59418	YES	YES
89	a	3077.29	3.97231	YES	YES
90	a	3090.44	1.74875	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2117975 Hartree *

Trans 6_y



bp86_svp SCF energy = -1354.5286581880

pbe0_tzvpp SCF energy = -1354.305484706

xyz Coordinates

30

C	-2.87662	0.02515	-0.12478
C	-4.35772	0.01153	-0.44300
H	-4.66367	-1.01346	-0.75097
H	-4.58257	0.69487	-1.28828
H	-4.94612	0.29733	0.45218
C	2.36436	-0.09852	1.17233
C	3.59797	-0.16292	2.03107
H	4.18895	0.77283	1.92195
H	4.25102	-1.00135	1.70555
H	3.31144	-0.29848	3.09181
C	1.32544	0.06719	-0.94286
C	1.58503	0.16397	-2.27098
H	0.68507	0.21588	-2.91066
C	2.92655	0.20561	-2.95815
H	3.04897	1.13868	-3.55825
H	3.76495	0.15489	-2.23320
H	-0.06973	3.01811	-0.96191
H	0.68863	3.00264	1.06272
H	-1.44266	3.03976	0.71347
H	-1.53329	-3.06555	0.09817
H	0.53164	-3.15396	0.72125
H	0.04969	-2.84525	-1.36412
O	-2.02710	0.10534	-1.09371
O	-2.44594	-0.06723	1.06378
O	1.20774	-0.13091	1.66664
O	2.57220	-0.00288	-0.12077
H	3.04439	-0.64107	-3.67597
P	-0.28831	2.30189	0.26643
P	-0.31968	-2.30936	-0.08027
Ru	-0.30956	-0.01091	0.19281

Vibrational Spectrum

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	42.46	0.47959	YES	YES
8	a	49.47	1.23670	YES	YES
9	a	56.41	0.17523	YES	YES
10	a	58.54	0.02267	YES	YES
11	a	66.05	1.06305	YES	YES
12	a	68.74	0.07470	YES	YES
13	a	80.22	0.18645	YES	YES
14	a	89.68	0.44368	YES	YES
15	a	96.14	7.37024	YES	YES
16	a	105.65	5.98539	YES	YES
17	a	117.80	0.32262	YES	YES
18	a	125.35	0.25331	YES	YES
19	a	151.45	0.39850	YES	YES
20	a	160.02	0.02884	YES	YES
21	a	163.20	2.66376	YES	YES
22	a	206.64	2.03902	YES	YES
23	a	229.00	2.70464	YES	YES
24	a	246.96	12.83414	YES	YES
25	a	255.34	2.27854	YES	YES
26	a	303.07	14.34368	YES	YES
27	a	315.22	2.08992	YES	YES
28	a	315.99	2.95094	YES	YES
29	a	335.41	5.09483	YES	YES
30	a	351.52	13.55671	YES	YES
31	a	461.41	13.56550	YES	YES
32	a	465.80	0.39365	YES	YES
33	a	471.03	2.19107	YES	YES
34	a	478.14	0.92260	YES	YES
35	a	553.73	11.60322	YES	YES
36	a	559.65	10.19351	YES	YES
37	a	563.44	1.44929	YES	YES
38	a	601.10	1.21936	YES	YES
39	a	613.69	3.78604	YES	YES
40	a	617.51	2.59466	YES	YES
41	a	667.99	50.20240	YES	YES
42	a	676.47	8.49560	YES	YES
43	a	746.30	92.16718	YES	YES
44	a	775.17	11.59490	YES	YES
45	a	931.08	20.38218	YES	YES
46	a	937.91	19.75078	YES	YES
47	a	981.41	3.27769	YES	YES
48	a	987.61	26.41645	YES	YES
49	a	999.01	416.38629	YES	YES

50	a	1003.16	22.17909	YES	YES
51	a	1013.79	6.46474	YES	YES
52	a	1023.05	10.72093	YES	YES
53	a	1025.29	19.83531	YES	YES
54	a	1032.22	2.37613	YES	YES
55	a	1077.46	6.73343	YES	YES
56	a	1089.77	0.48591	YES	YES
57	a	1092.62	4.04303	YES	YES
58	a	1093.63	2.54331	YES	YES
59	a	1097.26	7.34698	YES	YES
60	a	1231.82	30.05673	YES	YES
61	a	1325.71	4.41216	YES	YES
62	a	1332.82	18.94216	YES	YES
63	a	1353.01	1.23827	YES	YES
64	a	1395.66	143.52883	YES	YES
65	a	1400.42	41.10528	YES	YES
66	a	1405.86	24.30691	YES	YES
67	a	1411.28	53.04114	YES	YES
68	a	1413.67	13.35036	YES	YES
69	a	1424.34	5.41880	YES	YES
70	a	1426.46	16.10440	YES	YES
71	a	1436.93	249.71326	YES	YES
72	a	1573.55	132.72599	YES	YES
73	a	1597.10	127.24270	YES	YES
74	a	1648.88	94.87896	YES	YES
75	a	2310.31	287.10092	YES	YES
76	a	2316.73	48.86805	YES	YES
77	a	2326.12	72.42765	YES	YES
78	a	2329.25	64.36196	YES	YES
79	a	2332.48	30.25501	YES	YES
80	a	2340.06	34.60486	YES	YES
81	a	2914.19	83.75890	YES	YES
82	a	2957.30	7.27885	YES	YES
83	a	2962.41	5.69602	YES	YES
84	a	2966.85	19.11631	YES	YES
85	a	3040.11	1.01373	YES	YES
86	a	3041.26	4.29982	YES	YES
87	a	3045.67	7.13146	YES	YES
88	a	3075.83	9.51153	YES	YES
89	a	3076.21	3.86729	YES	YES
90	a	3090.40	1.70616	YES	YES

$end

* zero point VIBRATIONAL energy : 0.2121651 Hartree *

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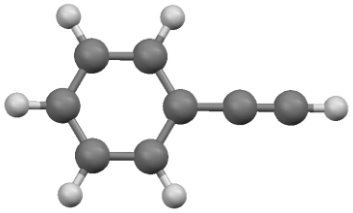
Model ii Data

alkyne2



bp86-SVP SCF energy: -308.1699041423
pbe-TZVPP SCF energy: -308.1232340947

XYZ Coordinates
14

C	3.39435	-0.00022	0.00000
C	2.16836	-0.00003	0.00000
H	4.47650	0.00083	0.00000
C	0.73594	-0.00014	0.00000
C	-2.09408	-0.00004	0.00000
C	-1.38835	1.21642	0.00000
C	0.01356	1.22138	0.00000
C	0.01331	-1.22165	0.00000
C	-1.38827	-1.21656	0.00000
H	-3.19658	-0.00016	0.00000
H	-1.93644	2.17325	0.00000
H	0.56892	2.17277	0.00000
H	0.56928	-2.17260	0.00000
H	-1.93650	-2.17324	0.00000

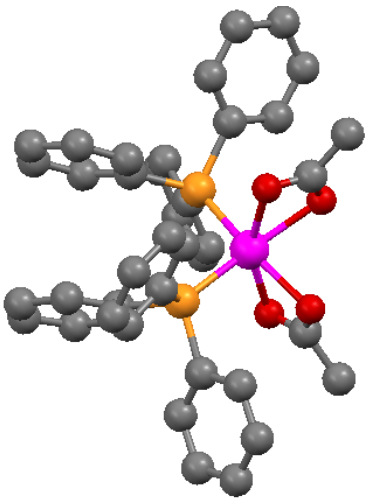
Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	138.58	1.56350	YES	YES
8	a	153.36	1.02614	YES	YES
9	a	360.71	2.76431	YES	YES
10	a	399.55	0.00000	YES	YES
11	a	458.65	0.36259	YES	YES
12	a	517.43	2.58233	YES	YES
13	a	545.25	5.43247	YES	YES
14	a	599.84	35.57001	YES	YES
15	a	614.17	0.56729	YES	YES
16	a	644.20	35.27145	YES	YES
17	a	691.70	31.10686	YES	YES
18	a	758.28	2.37088	YES	YES
19	a	760.51	32.33700	YES	YES
20	a	830.67	0.00002	YES	YES
21	a	909.89	3.36655	YES	YES
22	a	956.97	0.00005	YES	YES
23	a	982.21	0.09086	YES	YES
24	a	984.04	0.15727	YES	YES
25	a	1025.46	3.71812	YES	YES
26	a	1071.46	5.60308	YES	YES
27	a	1142.13	0.00024	YES	YES
28	a	1158.82	0.00064	YES	YES
29	a	1204.59	0.87849	YES	YES
30	a	1290.68	0.07755	YES	YES
31	a	1357.29	0.05531	YES	YES
32	a	1438.19	4.75377	YES	YES
33	a	1482.84	13.37436	YES	YES
34	a	1582.10	1.09586	YES	YES
35	a	1614.42	1.68597	YES	YES
36	a	2144.51	3.17526	YES	YES
37	a	3091.71	0.47356	YES	YES
38	a	3100.25	4.81166	YES	YES
39	a	3110.71	14.50562	YES	YES
40	a	3117.91	16.88683	YES	YES
41	a	3121.76	4.58438	YES	YES
42	a	3386.05	81.76982	YES	YES

$end

* zero point VIBRATIONAL energy : 0.1064972 Hartree *

Cis 1



bp86-SVP SCF energy: -2623.2690899190
pbe-TZVPP SCF energy: -2622.871217447

XYZ Coordinates
83

C	2.75404	-1.26451	-1.66952
C	3.63735	-1.94652	-2.68212
H	3.44704	-3.04250	-2.64891
H	4.70516	-1.78252	-2.42484
H	3.42855	-1.57242	-3.70412
C	2.79179	1.25758	1.61601
C	3.68419	1.94625	2.61599
H	3.26175	2.95089	2.84426
H	4.69915	2.08570	2.19187
H	3.73496	1.36675	3.56033
C	0.44556	-3.30310	-0.70686
C	1.52658	-3.95788	-0.07119
H	1.94264	-3.54767	0.86194
C	2.07298	-5.13138	-0.61393
H	2.91137	-5.62942	-0.09901
C	1.55484	-5.66925	-1.80662
H	1.98285	-6.59242	-2.23189
C	0.48474	-5.02438	-2.44746
H	0.06500	-5.43850	-3.37950
C	-0.06678	-3.84970	-1.90156
H	-0.91483	-3.36933	-2.41286
C	-1.85322	-1.53507	-0.73388
C	-1.84284	-1.08112	-2.07424
H	-0.88219	-0.85264	-2.56283
C	-3.04290	-0.91947	-2.78543
H	-3.01345	-0.56998	-3.83067
C	-4.27396	-1.19311	-2.16336
H	-5.21749	-1.06459	-2.71979
C	-4.29451	-1.61688	-0.82445
H	-5.25560	-1.81411	-0.32103
C	-3.09373	-1.78843	-0.11292
H	-3.13189	-2.10781	0.93938
C	-0.58474	-2.44884	1.77539
C	-1.32739	-3.64733	1.89651
H	-1.70466	-4.15703	0.99448
C	-1.57365	-4.20948	3.15890
H	-2.15786	-5.14172	3.23747
C	-1.06247	-3.59517	4.31686
H	-1.24948	-4.04152	5.30798
C	-0.29810	-2.42312	4.20155
H	0.12755	-1.94926	5.10208
C	-0.05768	-1.85033	2.93810
H	0.57191	-0.95078	2.85179
C	-1.86584	1.52844	0.71548
C	-3.09581	1.79932	0.08078
H	-3.11668	2.13627	-0.96649
C	-4.30777	1.62529	0.77228
H	-5.26009	1.83702	0.25815
C	-4.30972	1.17956	2.10423
H	-5.26212	1.04887	2.64478
C	-3.08983	0.88714	2.73936
H	-3.07757	0.51990	3.77883
C	-1.87876	1.05171	2.04768
H	-0.92777	0.80605	2.54630
C	0.44064	3.28672	0.74739
C	-0.06648	3.79989	1.95908
H	-0.91039	3.30404	2.46236
C	0.48426	4.96173	2.53256
H	0.06816	5.35014	3.47728
C	1.54809	5.62751	1.90249
H	1.97513	6.54104	2.34905
C	2.06078	5.12322	0.69316
H	2.89426	5.63766	0.18649
C	1.51558	3.96211	0.12318
H	1.92783	3.57816	-0.82264
C	-0.57091	2.47700	-1.76094
C	-1.29644	3.68751	-1.86574
H	-1.66470	4.19121	-0.95661
C	-1.53824	4.26798	-3.12064
H	-2.10887	5.20957	-3.18641
C	-1.04127	3.65880	-4.28750
H	-1.22522	4.11906	-5.27285
C	-0.29430	2.47425	-4.18831
H	0.12023	2.00395	-5.09586
C	-0.05819	1.88335	-2.93237
H	0.55756	0.97323	-2.85896
O	1.74056	-0.56375	-2.04503
O	2.96608	-1.37946	-0.41713
O	2.97626	1.37669	0.35976
O	1.78816	0.55357	2.01189
P	-0.20008	-1.73150	0.09727
P	-0.20053	1.73048	-0.09125
Ru	1.29869	-0.00159	-0.01085

Vibrational Frequencies

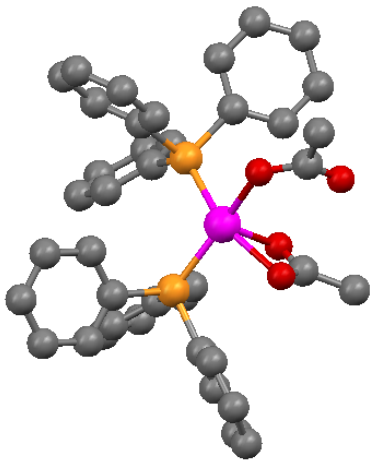
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.34	0.07926	YES	YES
8	a	20.60	0.00981	YES	YES
9	a	33.76	0.15370	YES	YES
10	a	35.89	0.10484	YES	YES
11	a	39.92	0.70976	YES	YES
12	a	44.79	0.37272	YES	YES
13	a	44.94	0.11417	YES	YES
14	a	49.26	0.13678	YES	YES
15	a	51.70	0.05582	YES	YES
16	a	60.35	0.18116	YES	YES
17	a	62.29	0.33556	YES	YES
18	a	63.65	0.03654	YES	YES
19	a	65.15	0.15335	YES	YES
20	a	67.73	0.41754	YES	YES
21	a	70.19	0.47392	YES	YES
22	a	76.04	0.03751	YES	YES
23	a	81.00	0.34589	YES	YES
24	a	81.17	0.48750	YES	YES
25	a	88.19	2.67366	YES	YES
26	a	89.41	0.43497	YES	YES
27	a	100.93	0.12702	YES	YES
28	a	103.49	2.31334	YES	YES
29	a	106.35	0.38024	YES	YES
30	a	107.38	0.18212	YES	YES
31	a	119.40	1.93415	YES	YES

32	a	162.75	0.23747	YES	YES
33	a	165.64	0.61069	YES	YES
34	a	179.46	1.48428	YES	YES
35	a	185.80	0.45168	YES	YES
36	a	194.85	0.92054	YES	YES
37	a	197.61	3.53878	YES	YES
38	a	202.40	1.80640	YES	YES
39	a	209.32	0.01119	YES	YES
40	a	216.57	1.81920	YES	YES
41	a	221.68	0.09558	YES	YES
42	a	224.97	10.05287	YES	YES
43	a	236.07	0.86508	YES	YES
44	a	244.88	0.49778	YES	YES
45	a	246.79	0.18581	YES	YES
46	a	249.43	0.11355	YES	YES
47	a	249.61	0.11189	YES	YES
48	a	266.48	0.47891	YES	YES
49	a	267.12	1.56199	YES	YES
50	a	285.29	1.57303	YES	YES
51	a	311.10	15.78299	YES	YES
52	a	330.82	22.95153	YES	YES
53	a	348.58	34.79836	YES	YES
54	a	395.86	0.07374	YES	YES
55	a	397.78	0.00224	YES	YES
56	a	399.13	0.57848	YES	YES
57	a	402.96	0.13293	YES	YES
58	a	408.86	0.38601	YES	YES
59	a	411.62	13.39915	YES	YES
60	a	412.74	19.58855	YES	YES
61	a	417.45	5.91811	YES	YES
62	a	432.85	31.63538	YES	YES
63	a	442.44	0.01063	YES	YES
64	a	458.43	26.18301	YES	YES
65	a	460.14	1.35194	YES	YES
66	a	480.12	5.98839	YES	YES
67	a	481.79	4.21583	YES	YES
68	a	495.02	0.24421	YES	YES
69	a	499.06	46.40239	YES	YES
70	a	504.80	4.93034	YES	YES
71	a	516.32	40.82239	YES	YES
72	a	520.37	212.25545	YES	YES
73	a	540.54	54.79842	YES	YES
74	a	597.09	5.57525	YES	YES
75	a	599.73	0.30558	YES	YES
76	a	608.19	0.09404	YES	YES
77	a	609.28	0.33567	YES	YES
78	a	609.92	3.66615	YES	YES
79	a	611.49	1.83816	YES	YES
80	a	611.69	0.06284	YES	YES
81	a	611.83	0.10119	YES	YES
82	a	665.24	64.63298	YES	YES
83	a	671.43	27.95228	YES	YES
84	a	672.23	11.72652	YES	YES
85	a	673.33	28.22207	YES	YES
86	a	678.11	3.33330	YES	YES
87	a	680.83	20.24609	YES	YES
88	a	689.16	23.08130	YES	YES
89	a	689.80	6.76028	YES	YES
90	a	696.66	74.33748	YES	YES
91	a	696.81	28.97983	YES	YES
92	a	700.50	47.30515	YES	YES
93	a	704.14	10.39346	YES	YES
94	a	708.25	37.67463	YES	YES
95	a	710.69	1.42552	YES	YES
96	a	737.56	14.85298	YES	YES
97	a	739.60	6.12097	YES	YES
98	a	742.18	0.94494	YES	YES
99	a	744.03	8.37380	YES	YES
100	a	747.31	6.29126	YES	YES
101	a	748.46	0.86310	YES	YES
102	a	833.38	0.70364	YES	YES
103	a	833.96	0.32552	YES	YES
104	a	840.70	2.79526	YES	YES
105	a	842.26	0.01434	YES	YES
106	a	850.25	0.12651	YES	YES
107	a	852.07	0.49024	YES	YES
108	a	905.92	0.62785	YES	YES
109	a	906.34	0.69157	YES	YES
110	a	911.98	3.12121	YES	YES
111	a	912.92	1.22453	YES	YES
112	a	927.85	1.07445	YES	YES
113	a	929.42	0.17234	YES	YES
114	a	943.73	21.11956	YES	YES
115	a	944.60	13.67499	YES	YES
116	a	957.12	0.45135	YES	YES
117	a	957.56	0.10153	YES	YES
118	a	962.71	0.68552	YES	YES
119	a	964.17	0.70836	YES	YES
120	a	974.53	0.14335	YES	YES
121	a	975.47	0.30046	YES	YES
122	a	980.09	0.14663	YES	YES
123	a	980.34	0.11173	YES	YES
124	a	982.12	1.02643	YES	YES
125	a	982.77	0.01714	YES	YES
126	a	983.34	0.20026	YES	YES
127	a	983.59	0.64582	YES	YES
128	a	983.89	0.31114	YES	YES
129	a	983.99	0.38017	YES	YES
130	a	984.73	4.91867	YES	YES
131	a	985.15	3.25368	YES	YES
132	a	985.52	3.77078	YES	YES
133	a	985.61	0.42632	YES	YES
134	a	1000.15	0.86271	YES	YES
135	a	1001.55	1.41688	YES	YES
136	a	1022.80	0.75649	YES	YES
137	a	1022.88	0.96264	YES	YES
138	a	1023.81	0.77102	YES	YES
139	a	1023.85	1.43888	YES	YES
140	a	1024.85	0.62134	YES	YES
141	a	1025.12	0.58324	YES	YES
142	a	1027.00	11.57192	YES	YES
143	a	1028.20	12.17062	YES	YES
144	a	1068.90	16.68279	YES	YES
145	a	1069.06	15.72411	YES	YES
146	a	1071.34	0.33487	YES	YES
147	a	1072.49	4.41540	YES	YES
148	a	1073.76	1.33170	YES	YES
149	a	1074.71	2.20014	YES	YES
150	a	1075.93	43.34718	YES	YES
151	a	1076.14	4.03604	YES	YES
152	a	1077.49	12.16927	YES	YES
153	a	1078.82	2.76069	YES	YES
154	a	1081.05	13.12337	YES	YES
155	a	1082.25	10.08586	YES	YES
156	a	1139.65	0.20492	YES	YES
157	a	1139.88	0.22095	YES	YES
158	a	1141.67	0.06290	YES	YES
159	a	1141.71	0.10694	YES	YES
160	a	1142.00	0.87048	YES	YES
161	a	1142.45	0.04317	YES	YES
162	a	1166.95	0.06036	YES	YES
163	a	1168.53	8.68827	YES	YES
164	a	1171.05	9.63106	YES	YES
165	a	1171.49	7.40543	YES	YES
166	a	1173.40	2.73058	YES	YES
167	a	1174.03	0.47216	YES	YES
168	a	1292.81	0.33100	YES	YES
169	a	1293.85	1.08498	YES	YES
170	a	1294.67	4.69074	YES	YES
171	a	1294.86	7.65177	YES	YES
172	a	1300.96	3.58162	YES	YES
173	a	1301.90	1.21529	YES	YES
174	a	1327.02	0.57705	YES	YES
175	a	1328.71	1.74330	YES	YES
176	a	1357.68	2.06263	YES	YES
177	a	1357.88	0.49219	YES	YES
178	a	1359.23	0.70253	YES	YES
179	a	1359.91	0.35849	YES	YES

180	a	1362.56	3.31119	YES	YES
181	a	1362.98	0.69699	YES	YES
182	a	1394.33	60.69943	YES	YES
183	a	1397.76	33.05943	YES	YES
184	a	1410.35	26.15949	YES	YES
185	a	1410.37	11.25749	YES	YES
186	a	1425.73	4.55159	YES	YES
187	a	1425.83	11.30282	YES	YES
188	a	1426.67	10.60530	YES	YES
189	a	1426.80	18.79244	YES	YES
190	a	1431.34	24.72178	YES	YES
191	a	1431.54	13.75846	YES	YES
192	a	1455.23	229.64546	YES	YES
193	a	1459.56	256.07521	YES	YES
194	a	1472.56	4.90405	YES	YES
195	a	1472.86	8.55697	YES	YES
196	a	1473.49	7.52775	YES	YES
197	a	1473.88	1.76083	YES	YES
198	a	1474.55	6.97462	YES	YES

* zero point VIBRATIONAL energy : 0.6378432 Hartree *

Cis I_{12}_afb



bp86-SVP SCF energy: -2623.2349854410
pbe-TZVPP SCF energy: -2622.836737078

XYZ Coordinates
83

C	0.96560	0.74430	-3.03584
C	1.82532	1.00495	-4.23531
H	1.74058	0.11250	-4.89403
H	2.88690	1.13726	-3.94286
H	1.45685	1.89541	-4.78430
C	-0.83430	-2.04678	-3.43258
C	-1.92223	-2.89458	-4.09545
H	-1.54977	-3.30580	-5.05500
H	-2.82472	-2.27274	-4.28762
H	-2.23104	-3.72641	-3.42535
C	-0.07677	3.36304	-1.00181
C	-1.18478	3.60813	-1.84498
H	-2.05030	2.92546	-1.82713
C	-1.19124	4.70869	-2.71368
H	-2.06511	4.88620	-3.36245
C	-0.08294	5.57402	-2.76815
H	-0.08609	6.43663	-3.45541
C	1.02834	5.32983	-1.94638
H	1.90352	6.00018	-1.98250
C	1.03146	4.23215	-1.06513
H	1.90719	4.05879	-0.42041
C	1.34740	2.18574	1.20001
C	2.57570	1.60899	0.80634
H	2.60893	0.96375	-0.08726
C	3.74600	1.86360	1.54086
H	4.69854	1.40893	1.22206
C	3.70265	2.68604	2.67982
H	4.62164	2.88174	3.25726
C	2.48171	3.25369	3.08256
H	2.43860	3.89642	3.97816
C	1.30998	3.00659	2.34685
H	0.36013	3.45660	2.67700
C	-1.60111	2.29449	1.17816
C	-1.94265	3.63251	1.48372
H	-1.33314	4.46064	1.08722
C	-3.06852	3.91910	2.27386
H	-3.32154	4.96804	2.50232
C	-3.87657	2.87640	2.76160
H	-4.76342	3.10461	3.37600
C	-3.55605	1.54471	2.45048
H	-4.18937	0.71878	2.81335
C	-2.42711	1.25772	1.66287
H	-2.19476	0.20975	1.40875
C	1.17685	-1.39884	1.97038
C	2.43284	-2.03586	2.07143
H	2.76017	-2.73269	1.28476
C	3.27096	-1.79306	3.17386
H	4.24855	-2.29985	3.23445
C	2.86366	-0.91884	4.19443
H	3.51840	-0.73453	5.06222
C	1.61747	-0.27471	4.10013
H	1.29133	0.42033	4.89085
C	0.78612	-0.50392	2.99272
H	-0.18255	0.01884	2.93266
C	-1.49040	-2.37911	1.29244
C	-1.60629	-2.71505	2.65929
H	-0.74807	-2.58485	3.33677
C	-2.81477	-3.22580	3.16653
H	-2.88881	-3.48623	4.23578
C	-3.91940	-3.40889	2.31743
H	-4.86565	-3.80928	2.71816
C	-3.80941	-3.08363	0.95366
H	-4.66829	-3.23156	0.27805
C	-2.60603	-2.57084	0.44166
H	-2.51268	-2.33084	-0.63224
C	0.81833	-3.21065	-0.24697
C	0.61697	-4.48712	0.32393
H	-0.02666	-4.60266	1.21119
C	1.22831	-5.61964	-0.23806
H	1.05840	-6.61206	0.21232
C	2.04586	-5.48902	-1.37512
H	2.51934	-6.38001	-1.82093
C	2.24627	-4.22208	-1.94740
H	2.86802	-4.11140	-2.85078
C	1.63711	-3.08421	-1.38907
H	1.77501	-2.10139	-1.86524
O	1.47560	0.18808	-1.97621
O	-0.27479	1.01243	-2.99464
O	0.24625	-1.82173	-3.98491
O	-1.17790	-1.61189	-2.23685
P	-0.13074	1.86479	0.11412
P	0.06148	-1.68973	0.51287
Ru	-0.36906	-0.09253	-1.07983

Vibrational Frequencies

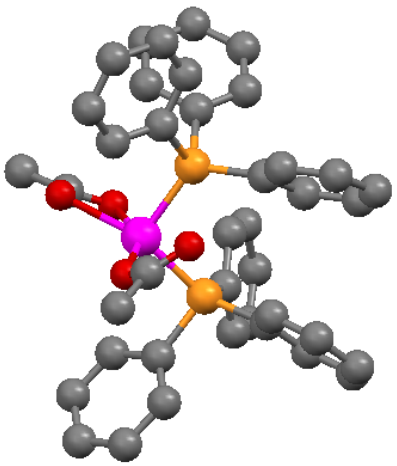
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.98	0.06158	YES	YES
8	a	22.89	0.11597	YES	YES
9	a	27.76	0.09806	YES	YES
10	a	31.50	0.06140	YES	YES
11	a	38.58	0.18951	YES	YES
12	a	41.22	0.06267	YES	YES
13	a	43.76	0.05314	YES	YES
14	a	44.70	0.09167	YES	YES
15	a	51.03	0.20021	YES	YES
16	a	51.57	0.32201	YES	YES
17	a	56.53	0.34328	YES	YES
18	a	57.51	0.10390	YES	YES
19	a	58.36	0.12765	YES	YES
20	a	63.64	0.33633	YES	YES
21	a	66.97	0.34479	YES	YES
22	a	67.83	0.41802	YES	YES
23	a	75.04	0.69683	YES	YES
24	a	79.44	0.35105	YES	YES
25	a	85.00	0.59147	YES	YES
26	a	88.67	0.44665	YES	YES
27	a	93.35	2.35490	YES	YES
28	a	95.43	0.17023	YES	YES
29	a	102.29	2.19331	YES	YES
30	a	106.03	1.72470	YES	YES
31	a	119.52	1.14617	YES	YES
32	a	124.04	2.02435	YES	YES

33	a	158.05	6.97065	YES	YES
34	a	165.18	0.30855	YES	YES
35	a	181.72	2.02004	YES	YES
36	a	184.84	0.95329	YES	YES
37	a	191.58	2.36274	YES	YES
38	a	196.40	1.45176	YES	YES
39	a	201.78	0.66345	YES	YES
40	a	211.40	0.73173	YES	YES
41	a	218.14	0.26553	YES	YES
42	a	220.40	8.39707	YES	YES
43	a	229.16	5.54980	YES	YES
44	a	239.08	0.32176	YES	YES
45	a	244.91	0.12272	YES	YES
46	a	245.20	0.16405	YES	YES
47	a	247.04	0.14377	YES	YES
48	a	248.31	0.41298	YES	YES
49	a	263.56	1.32816	YES	YES
50	a	264.49	0.53984	YES	YES
51	a	283.51	20.89360	YES	YES
52	a	298.79	21.22098	YES	YES
53	a	350.05	10.98615	YES	YES
54	a	395.62	0.03269	YES	YES
55	a	396.47	0.12895	YES	YES
56	a	398.49	0.23100	YES	YES
57	a	399.33	0.35880	YES	YES
58	a	405.59	0.07998	YES	YES
59	a	406.69	0.87831	YES	YES
60	a	420.09	33.32155	YES	YES
61	a	421.45	4.06485	YES	YES
62	a	436.85	24.49625	YES	YES
63	a	438.35	1.44727	YES	YES
64	a	449.19	13.62360	YES	YES
65	a	455.70	9.32627	YES	YES
66	a	489.06	16.04719	YES	YES
67	a	495.57	40.22972	YES	YES
68	a	502.18	6.30948	YES	YES
69	a	507.86	29.35448	YES	YES
70	a	512.19	42.82206	YES	YES
71	a	513.19	128.51930	YES	YES
72	a	517.27	80.37904	YES	YES
73	a	536.40	59.89702	YES	YES
74	a	575.15	6.63521	YES	YES
75	a	579.21	3.25362	YES	YES
76	a	608.53	0.22398	YES	YES
77	a	609.09	0.16605	YES	YES
78	a	609.79	0.33769	YES	YES
79	a	609.96	2.44432	YES	YES
80	a	610.74	0.82802	YES	YES
81	a	610.93	1.02721	YES	YES
82	a	637.75	45.53981	YES	YES
83	a	672.76	16.49180	YES	YES
84	a	674.46	2.68061	YES	YES
85	a	677.74	39.73085	YES	YES
86	a	681.43	13.91014	YES	YES
87	a	686.28	10.76283	YES	YES
88	a	687.57	10.50153	YES	YES
89	a	688.96	17.84019	YES	YES
90	a	695.33	28.75116	YES	YES
91	a	697.35	30.44024	YES	YES
92	a	697.96	65.58336	YES	YES
93	a	700.41	15.35282	YES	YES
94	a	706.50	19.13726	YES	YES
95	a	707.61	22.33602	YES	YES
96	a	740.84	8.86326	YES	YES
97	a	741.63	3.90797	YES	YES
98	a	742.24	5.69437	YES	YES
99	a	744.50	4.03593	YES	YES
100	a	747.13	6.55268	YES	YES
101	a	748.53	5.29968	YES	YES
102	a	831.74	0.33289	YES	YES
103	a	836.25	0.78301	YES	YES
104	a	837.95	0.60500	YES	YES
105	a	840.53	0.58817	YES	YES
106	a	846.36	0.18468	YES	YES
107	a	851.55	0.48039	YES	YES
108	a	904.03	0.49680	YES	YES
109	a	908.67	5.64051	YES	YES
110	a	909.35	0.56438	YES	YES
111	a	913.49	2.37875	YES	YES
112	a	914.31	0.15030	YES	YES
113	a	919.52	0.40461	YES	YES
114	a	924.73	0.14042	YES	YES
115	a	940.11	8.41318	YES	YES
116	a	954.76	0.04115	YES	YES
117	a	960.23	0.00881	YES	YES
118	a	961.36	0.14157	YES	YES
119	a	964.03	0.17516	YES	YES
120	a	968.29	0.29859	YES	YES
121	a	974.95	0.86872	YES	YES
122	a	980.84	0.86527	YES	YES
123	a	981.40	1.08454	YES	YES
124	a	981.78	0.21901	YES	YES
125	a	981.97	2.67714	YES	YES
126	a	982.73	3.63454	YES	YES
127	a	982.92	2.66098	YES	YES
128	a	983.70	4.08725	YES	YES
129	a	984.25	0.59335	YES	YES
130	a	984.29	24.98558	YES	YES
131	a	984.66	6.31300	YES	YES
132	a	986.74	0.37068	YES	YES
133	a	987.89	0.54142	YES	YES
134	a	990.07	0.28223	YES	YES
135	a	999.69	0.97647	YES	YES
136	a	1016.44	10.21081	YES	YES
137	a	1016.91	6.33658	YES	YES
138	a	1022.10	1.63282	YES	YES
139	a	1023.64	1.57135	YES	YES
140	a	1024.06	0.11837	YES	YES
141	a	1024.16	1.08397	YES	YES
142	a	1024.59	1.30989	YES	YES
143	a	1025.67	0.78527	YES	YES
144	a	1068.58	9.43815	YES	YES
145	a	1070.92	15.48981	YES	YES
146	a	1072.65	16.20669	YES	YES
147	a	1073.62	4.86901	YES	YES
148	a	1074.94	19.63173	YES	YES
149	a	1075.38	6.23024	YES	YES
150	a	1076.50	3.38483	YES	YES
151	a	1076.68	13.16495	YES	YES
152	a	1078.06	6.11929	YES	YES
153	a	1079.89	16.95775	YES	YES
154	a	1081.59	17.93274	YES	YES
155	a	1083.40	13.55105	YES	YES
156	a	1141.00	0.20115	YES	YES
157	a	1141.36	0.12993	YES	YES
158	a	1142.09	0.11730	YES	YES
159	a	1142.29	0.61124	YES	YES
160	a	1142.88	0.49248	YES	YES
161	a	1144.20	0.47234	YES	YES
162	a	1162.16	2.16396	YES	YES
163	a	1168.38	6.30278	YES	YES
164	a	1169.29	3.07341	YES	YES
165	a	1171.34	6.11320	YES	YES
166	a	1173.45	4.95497	YES	YES
167	a	1176.37	9.32242	YES	YES
168	a	1280.34	477.22499	YES	YES
169	a	1285.21	4.66827	YES	YES
170	a	1293.51	3.10994	YES	YES
171	a	1294.62	4.48320	YES	YES
172	a	1295.81	1.84114	YES	YES
173	a	1299.59	4.29556	YES	YES
174	a	1304.74	8.31579	YES	YES
175	a	1313.72	2.79881	YES	YES
176	a	1333.68	241.78113	YES	YES
177	a	1358.24	7.32975	YES	YES
178	a	1358.82	0.29058	YES	YES
179	a	1360.20	1.67212	YES	YES
180	a	1360.63	0.86225	YES	YES

181	a	1362.36	1.67674	YES	YES
182	a	1362.99	0.49633	YES	YES
183	a	1390.60	120.34200	YES	YES
184	a	1404.35	17.87548	YES	YES
185	a	1407.23	10.09419	YES	YES
186	a	1418.51	7.22039	YES	YES
187	a	1426.41	12.09889	YES	YES
188	a	1427.12	13.77724	YES	YES
189	a	1429.26	11.93926	YES	YES
190	a	1429.66	15.70410	YES	YES
191	a	1430.37	17.47564	YES	YES
192	a	1431.56	11.62096	YES	YES
193	a	1445.55	158.55970	YES	YES
194	a	1469.15	5.21735	YES	YES
195	a	1471.66	8.06406	YES	YES
196	a	1472.21	7.24361	YES	YES
197	a	1473.84	5.79503	YES	YES
198	a	1474.20	12.55459	YES	YES

* zero point VIBRATIONAL energy : 0.6365277 Hartree *

Cis I_{12}_pfb



bp86-SVP SCF energy: -2623.2455779440
pbe-TZVPP SCF energy: -2622.846757691

XYZ Coordinates
83

C	-1.54160	-2.96271	-0.83595
C	-1.89319	-4.40050	-1.13009
H	-2.46376	-4.82342	-0.27268
H	-0.97288	-5.00634	-1.25794
H	-2.53366	-4.46496	-2.03309
C	-2.56229	2.08876	-0.23720
C	-3.91736	2.71897	0.08881
H	-4.04506	3.65644	-0.48894
H	-3.95968	2.95963	1.17486
H	-4.74943	2.01551	-0.12486
C	1.36565	-1.10311	-2.44885
C	0.70784	-2.19176	-3.06945
H	-0.39375	-2.22310	-3.08339
C	1.43782	-3.21014	-3.69845
H	0.90429	-4.04434	-4.18410
C	2.84376	-3.16356	-3.72040
H	3.41857	-3.96315	-4.21662
C	3.50738	-2.08226	-3.12055
H	4.60835	-2.02253	-3.14934
C	2.77532	-1.05709	-2.49143
H	3.31904	-0.20497	-2.05682
C	1.40582	1.61402	-1.33928
C	2.51366	1.46266	-0.47514
H	2.69164	0.50689	0.04288
C	3.40175	2.52754	-0.25188
H	4.26305	2.38501	0.42105
C	3.17921	3.76971	-0.86823
H	3.87315	4.60835	-0.69113
C	2.05578	3.94186	-1.69460
H	1.85621	4.92091	-2.16104
C	1.17154	2.87581	-1.92713
H	0.27917	3.03413	-2.54829
C	-0.69738	0.67134	-3.17580
C	0.00024	1.01775	-4.35521
H	1.10277	1.03441	-4.36279
C	-0.70153	1.33567	-5.52865
H	-0.14501	1.61007	-6.44050
C	-2.10746	1.29541	-5.54212
H	-2.65865	1.53920	-6.46579
C	-2.80461	0.93797	-4.37655
H	-3.90652	0.89871	-4.37987
C	-2.10502	0.63075	-3.19622
H	-2.65475	0.34773	-2.28655
C	0.81620	1.58106	2.36841
C	1.76636	1.71352	3.40638
H	2.19053	0.82178	3.89311
C	2.19445	2.98602	3.81964
H	2.93703	3.07407	4.63077
C	1.67891	4.14021	3.20396
H	2.01505	5.13857	3.53117
C	0.74720	4.01313	2.16071
H	0.35078	4.90860	1.65440
C	0.32053	2.74228	1.73743
H	-0.37369	2.66261	0.88274
C	-1.19634	-0.42905	3.05266
C	-1.81905	0.57990	3.81888
H	-1.43607	1.61221	3.78227
C	-2.92226	0.27124	4.63118
H	-3.39539	1.06616	5.23144
C	-3.42301	-1.04184	4.68226
H	-4.29068	-1.27825	5.32058
C	-2.81341	-2.05106	3.91738
H	-3.19909	-3.08352	3.95396
C	-1.70610	-1.75017	3.10594
H	-1.22330	-2.54951	2.51785
C	1.46368	-1.29182	2.30247
C	1.70078	-1.63648	3.65399
H	1.08580	-1.19239	4.45400
C	2.69866	-2.56702	3.98903
H	2.87047	-2.82565	5.04748
C	3.46732	-3.17266	2.97924
H	4.24842	-3.90526	3.24264
C	3.21943	-2.85698	1.63280
H	3.79627	-3.34669	0.83097
C	2.21789	-1.93061	1.29605
H	1.99829	-1.72955	0.23589
O	-0.48047	-2.67843	-0.16669
O	-2.29761	-2.00210	-1.21412
O	-1.65846	2.73498	-0.78377
O	-2.47478	0.83956	0.14367
P	0.25959	0.18831	-1.64843
P	0.14755	-0.06715	1.82375
Ru	-1.03914	-0.59839	-0.02119

Vibrational Frequencies

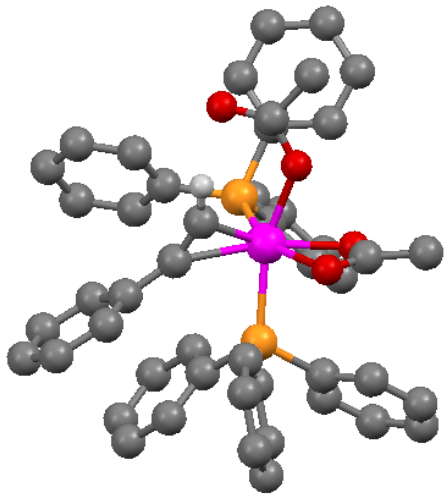
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	20.24	0.19928	YES	YES
8	a	24.53	0.09815	YES	YES
9	a	25.34	0.16179	YES	YES
10	a	35.92	0.25145	YES	YES
11	a	37.70	0.32222	YES	YES
12	a	42.50	0.11674	YES	YES
13	a	44.10	0.20018	YES	YES
14	a	46.44	0.22815	YES	YES
15	a	51.74	0.24278	YES	YES
16	a	53.07	0.24539	YES	YES
17	a	53.95	1.10721	YES	YES
18	a	54.26	0.49993	YES	YES
19	a	56.50	0.94334	YES	YES
20	a	60.17	0.51429	YES	YES
21	a	60.99	0.10748	YES	YES
22	a	66.94	0.96005	YES	YES
23	a	69.91	0.55828	YES	YES
24	a	72.05	0.26934	YES	YES
25	a	77.43	0.04646	YES	YES
26	a	85.35	0.02852	YES	YES
27	a	87.86	1.56159	YES	YES
28	a	92.37	0.12236	YES	YES
29	a	96.87	2.99058	YES	YES
30	a	103.82	1.13267	YES	YES
31	a	111.24	3.33736	YES	YES
32	a	118.13	1.72232	YES	YES

33	a	131.53	1.56956	YES	YES
34	a	155.17	0.66454	YES	YES
35	a	166.48	0.53505	YES	YES
36	a	181.20	2.21155	YES	YES
37	a	184.96	0.80431	YES	YES
38	a	191.29	1.15505	YES	YES
39	a	192.88	0.85137	YES	YES
40	a	204.73	3.21370	YES	YES
41	a	215.00	0.26366	YES	YES
42	a	218.08	1.60067	YES	YES
43	a	226.43	2.01453	YES	YES
44	a	237.85	0.97099	YES	YES
45	a	243.48	0.29950	YES	YES
46	a	244.61	0.32509	YES	YES
47	a	249.10	0.31151	YES	YES
48	a	252.17	0.94000	YES	YES
49	a	263.89	1.14538	YES	YES
50	a	264.96	0.46370	YES	YES
51	a	271.00	4.86094	YES	YES
52	a	303.53	20.57325	YES	YES
53	a	328.81	25.60252	YES	YES
54	a	394.91	0.05534	YES	YES
55	a	397.05	0.15990	YES	YES
56	a	401.47	0.37274	YES	YES
57	a	401.87	0.07967	YES	YES
58	a	407.55	3.82137	YES	YES
59	a	408.13	1.25922	YES	YES
60	a	412.67	12.48955	YES	YES
61	a	421.73	15.31447	YES	YES
62	a	439.43	24.92879	YES	YES
63	a	441.49	1.68244	YES	YES
64	a	446.27	9.46015	YES	YES
65	a	467.13	6.52318	YES	YES
66	a	471.47	6.57056	YES	YES
67	a	486.76	2.33968	YES	YES
68	a	495.77	46.31686	YES	YES
69	a	504.61	15.73630	YES	YES
70	a	514.32	3.89946	YES	YES
71	a	517.52	184.68702	YES	YES
72	a	519.31	77.29459	YES	YES
73	a	546.63	82.92571	YES	YES
74	a	588.25	11.11163	YES	YES
75	a	596.04	2.84300	YES	YES
76	a	607.85	0.09075	YES	YES
77	a	608.72	0.21745	YES	YES
78	a	608.84	0.60065	YES	YES
79	a	609.75	1.96641	YES	YES
80	a	610.98	2.14578	YES	YES
81	a	611.51	0.64132	YES	YES
82	a	652.59	25.93341	YES	YES
83	a	668.25	56.74632	YES	YES
84	a	670.87	19.02126	YES	YES
85	a	673.61	9.68615	YES	YES
86	a	679.09	10.75552	YES	YES
87	a	686.40	6.55591	YES	YES
88	a	689.24	10.80525	YES	YES
89	a	691.95	33.54546	YES	YES
90	a	694.60	62.74663	YES	YES
91	a	696.22	18.71268	YES	YES
92	a	700.10	32.60718	YES	YES
93	a	701.71	47.61173	YES	YES
94	a	703.85	11.23513	YES	YES
95	a	706.17	11.08225	YES	YES
96	a	736.67	9.68831	YES	YES
97	a	739.15	5.39671	YES	YES
98	a	740.34	2.18048	YES	YES
99	a	741.97	6.55997	YES	YES
100	a	744.49	3.21565	YES	YES
101	a	748.73	10.18921	YES	YES
102	a	831.16	1.00549	YES	YES
103	a	833.29	0.82645	YES	YES
104	a	838.01	0.08876	YES	YES
105	a	839.78	0.34868	YES	YES
106	a	843.33	0.48977	YES	YES
107	a	849.98	0.60232	YES	YES
108	a	903.56	0.58950	YES	YES
109	a	905.32	0.23549	YES	YES
110	a	913.01	0.71672	YES	YES
111	a	914.47	0.82549	YES	YES
112	a	916.67	0.16871	YES	YES
113	a	923.37	10.21062	YES	YES
114	a	926.21	0.14403	YES	YES
115	a	937.75	17.07976	YES	YES
116	a	955.14	0.46718	YES	YES
117	a	955.90	1.12992	YES	YES
118	a	962.41	0.10049	YES	YES
119	a	962.67	0.07039	YES	YES
120	a	965.67	0.35065	YES	YES
121	a	973.83	0.27390	YES	YES
122	a	979.14	0.47727	YES	YES
123	a	981.21	0.96240	YES	YES
124	a	981.44	2.84007	YES	YES
125	a	981.71	0.89703	YES	YES
126	a	982.54	0.50712	YES	YES
127	a	983.05	1.57517	YES	YES
128	a	983.33	1.39969	YES	YES
129	a	983.66	0.11882	YES	YES
130	a	983.90	2.07274	YES	YES
131	a	985.51	0.24553	YES	YES
132	a	986.41	0.08602	YES	YES
133	a	988.21	2.57756	YES	YES
134	a	989.01	11.67292	YES	YES
135	a	1008.62	0.28138	YES	YES
136	a	1020.83	6.64853	YES	YES
137	a	1022.36	1.40427	YES	YES
138	a	1022.65	0.92187	YES	YES
139	a	1023.31	0.58542	YES	YES
140	a	1024.04	0.96933	YES	YES
141	a	1025.23	10.54864	YES	YES
142	a	1025.38	1.20744	YES	YES
143	a	1025.97	0.61402	YES	YES
144	a	1068.07	20.83391	YES	YES
145	a	1070.21	5.20269	YES	YES
146	a	1071.69	24.20173	YES	YES
147	a	1072.03	10.55411	YES	YES
148	a	1073.11	8.45902	YES	YES
149	a	1074.35	18.72394	YES	YES
150	a	1075.39	11.74048	YES	YES
151	a	1076.64	12.49863	YES	YES
152	a	1079.00	19.22761	YES	YES
153	a	1080.07	8.72187	YES	YES
154	a	1081.11	10.88706	YES	YES
155	a	1082.46	2.74051	YES	YES
156	a	1140.81	0.28065	YES	YES
157	a	1140.92	0.17048	YES	YES
158	a	1141.89	0.17635	YES	YES
159	a	1142.08	0.61413	YES	YES
160	a	1142.60	0.29144	YES	YES
161	a	1142.73	0.55935	YES	YES
162	a	1163.97	0.81717	YES	YES
163	a	1165.43	8.52291	YES	YES
164	a	1167.14	2.91386	YES	YES
165	a	1170.74	3.50370	YES	YES
166	a	1174.22	2.34929	YES	YES
167	a	1175.76	2.42174	YES	YES
168	a	1287.28	3.59892	YES	YES
169	a	1290.27	9.45662	YES	YES
170	a	1292.56	10.16146	YES	YES
171	a	1293.84	4.39837	YES	YES
172	a	1297.43	103.33880	YES	YES
173	a	1299.88	18.52437	YES	YES
174	a	1301.89	80.77696	YES	YES
175	a	1327.23	1.39895	YES	YES
176	a	1336.17	194.79959	YES	YES
177	a	1357.85	3.07831	YES	YES
178	a	1359.08	1.89085	YES	YES
179	a	1360.14	1.03419	YES	YES
180	a	1361.62	1.60890	YES	YES

181	a	1362.31	2.17611	YES	YES
182	a	1364.02	3.35846	YES	YES
183	a	1396.53	34.73410	YES	YES
184	a	1407.88	13.67150	YES	YES
185	a	1409.65	58.20857	YES	YES
186	a	1418.16	7.90934	YES	YES
187	a	1425.83	7.16873	YES	YES
188	a	1426.06	5.71997	YES	YES
189	a	1428.01	18.09565	YES	YES
190	a	1428.54	22.31378	YES	YES
191	a	1430.08	16.38123	YES	YES
192	a	1431.84	12.69658	YES	YES
193	a	1448.97	240.68756	YES	YES
194	a	1468.95	7.16119	YES	YES
195	a	1470.26	4.75976	YES	YES
196	a	1471.02	4.94395	YES	YES
197	a	1472.53	13.18348	YES	YES
198	a	1473.74	2.23986	YES	YES

* zero point VIBRATIONAL energy : 0.6361895 Hartree *

Cis 2_afax



bp86-SVP SCF energy: -2931.4282081170
pbe-TZVPP SCF energy: -2930.976889142

XYZ Coordinates
97

C	-1.53322	0.65037	-1.61556
C	-0.96606	-0.09818	-2.47399
C	-2.61416	1.53943	-1.23823
H	-1.00148	-0.64203	-3.41904
C	-4.83622	3.22549	-0.70203
C	-4.00661	3.48027	-1.80845
C	-2.90809	2.65028	-2.07525
C	-3.45474	1.30007	-0.12288
C	-4.55361	2.13110	0.13468
H	-5.70194	3.87655	-0.49534
H	-4.21745	4.33230	-2.47633
H	-2.26797	2.84737	-2.94843
H	-3.24864	0.44407	0.53301
H	-5.20019	1.91604	1.00111
C	3.01110	-0.00548	-1.62300
C	4.45204	-0.13238	-2.05014
H	4.55757	-1.06555	-2.64701
H	5.11739	-0.21451	-1.16577
H	4.74895	0.72483	-2.68786
C	0.40371	-2.71382	-3.03492
C	1.28117	-3.57985	-3.94564
H	0.64742	-4.11685	-4.67977
H	1.81867	-4.32742	-3.32137
H	2.04411	-2.96634	-4.46973
C	2.16411	2.04029	1.25194
C	3.38569	2.26184	0.57436
H	3.39958	2.30165	-0.52589
C	4.57536	2.47398	1.28747
H	5.51504	2.64976	0.73779
C	4.56815	2.47435	2.69366
H	5.50183	2.64631	3.25451
C	3.35904	2.26787	3.37621
H	3.33420	2.28338	4.47863
C	2.16578	2.05176	2.66214
H	1.22859	1.90654	3.22009
C	-0.71464	2.26439	1.43209
C	-1.07407	1.35027	2.44701
H	-0.60276	0.35602	2.48204
C	-2.02288	1.69656	3.42348
H	-2.27697	0.97243	4.21525
C	-2.64608	2.95528	3.38782
H	-3.39373	3.22731	4.15142
C	-2.31781	3.85897	2.36424
H	-2.81559	4.84125	2.31132
C	-1.35938	3.51931	1.39439
H	-1.13081	4.23783	0.59412
C	0.77783	3.27365	-0.87752
C	1.18954	4.50849	-0.31965
H	1.40836	4.58346	0.75775
C	1.33570	5.64730	-1.12738
H	1.65476	6.60030	-0.67325
C	1.08752	5.56842	-2.50931
H	1.21094	6.46008	-3.14645
C	0.69448	4.34453	-3.07312
H	0.51421	4.26662	-4.15808
C	0.53964	3.20407	-2.26444
H	0.25025	2.24750	-2.71918
C	-2.19416	-2.04002	0.51881
C	-2.90642	-1.79257	1.71339
H	-2.37098	-1.53625	2.63980
C	-4.31069	-1.86563	1.73392
H	-4.85175	-1.67680	2.67632
C	-5.01981	-2.17368	0.56088
H	-6.12105	-2.22962	0.57798
C	-4.31759	-2.40138	-0.63569
H	-4.86613	-2.63203	-1.56396
C	-2.91500	-2.33133	-0.66518
H	-2.36116	-2.50702	-1.60580
C	0.19989	-3.63332	-0.08053
C	-0.68296	-4.72237	-0.21378
H	-1.77107	-4.56836	-0.15437
C	-0.18188	-6.01972	-0.42668
H	-0.88581	-6.86241	-0.52974
C	1.20171	-6.24013	-0.51148
H	1.59231	-7.25823	-0.67667
C	2.08666	-5.15329	-0.38694
H	3.17563	-5.31522	-0.45510
C	1.59231	-3.85711	-0.17356
H	2.29124	-3.01037	-0.08319
C	0.30514	-2.00086	2.11756
C	-0.22877	-2.92700	3.04543
H	-1.09700	-3.54822	2.77297
C	0.35963	-3.09004	4.30896
H	-0.07375	-3.81107	5.02225
C	1.50780	-2.35486	4.65594
H	1.97501	-2.49168	5.64558
C	2.06712	-1.46490	3.72613
H	2.98109	-0.90041	3.97390
C	1.47023	-1.28851	2.46432
H	1.93666	-0.61320	1.73105
O	2.60394	-0.63206	-0.57190
O	2.17665	0.68401	-2.29085
O	-0.82312	-2.88607	-2.98891
O	1.10201	-1.84721	-2.34854
P	0.61602	1.77130	0.22499
P	-0.35167	-1.90221	0.36831
Ru	0.53574	-0.28503	-1.02350

Vibrational Frequencies

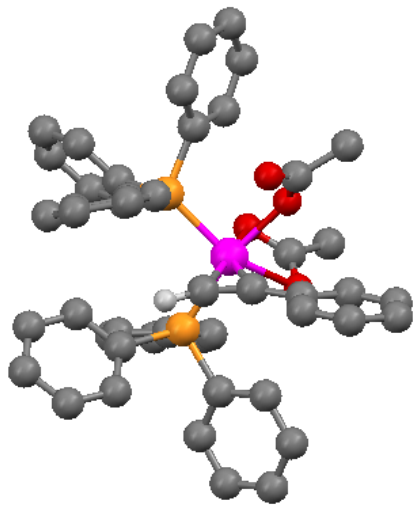
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.56	0.20787	YES	YES
8	a	25.66	0.05175	YES	YES
9	a	28.97	0.88695	YES	YES
10	a	30.10	0.28179	YES	YES
11	a	36.95	0.15582	YES	YES
12	a	45.39	0.08543	YES	YES
13	a	47.82	0.06903	YES	YES
14	a	49.26	0.20562	YES	YES
15	a	52.93	0.02507	YES	YES
16	a	54.57	0.12380	YES	YES
17	a	57.27	0.25011	YES	YES

18	a	60.29	0.03463	YES	YES
19	a	61.45	0.15230	YES	YES
20	a	63.07	0.11570	YES	YES
21	a	65.44	0.15387	YES	YES
22	a	69.58	0.48441	YES	YES
23	a	73.78	0.21458	YES	YES
24	a	80.63	0.52411	YES	YES
25	a	80.99	1.19400	YES	YES
26	a	85.08	0.62259	YES	YES
27	a	87.56	0.34623	YES	YES
28	a	93.43	1.27489	YES	YES
29	a	96.15	4.11550	YES	YES
30	a	99.66	1.11475	YES	YES
31	a	102.02	1.86718	YES	YES
32	a	107.69	1.62780	YES	YES
33	a	111.57	1.02840	YES	YES
34	a	119.31	0.41985	YES	YES
35	a	120.97	0.50722	YES	YES
36	a	127.70	1.37502	YES	YES
37	a	134.23	1.91135	YES	YES
38	a	141.25	0.93559	YES	YES
39	a	157.65	4.64611	YES	YES
40	a	166.13	0.49177	YES	YES
41	a	184.69	5.24852	YES	YES
42	a	188.57	1.99575	YES	YES
43	a	195.86	1.32535	YES	YES
44	a	202.36	4.15755	YES	YES
45	a	205.53	0.49729	YES	YES
46	a	210.35	0.56575	YES	YES
47	a	216.12	2.42741	YES	YES
48	a	222.05	5.21032	YES	YES
49	a	226.11	6.83196	YES	YES
50	a	233.34	6.65592	YES	YES
51	a	246.63	1.02814	YES	YES
52	a	249.96	0.99011	YES	YES
53	a	251.03	0.26297	YES	YES
54	a	253.53	1.53524	YES	YES
55	a	255.68	0.39909	YES	YES
56	a	267.62	0.53525	YES	YES
57	a	270.18	0.85347	YES	YES
58	a	275.78	7.93459	YES	YES
59	a	280.41	11.21321	YES	YES
60	a	320.06	3.14468	YES	YES
61	a	323.95	10.63274	YES	YES
62	a	395.03	0.23160	YES	YES
63	a	397.61	0.28197	YES	YES
64	a	400.88	0.13177	YES	YES
65	a	402.33	0.48422	YES	YES
66	a	404.82	0.62836	YES	YES
67	a	410.43	25.81290	YES	YES
68	a	411.53	5.83628	YES	YES
69	a	412.52	1.40817	YES	YES
70	a	413.93	11.33205	YES	YES
71	a	421.61	22.50297	YES	YES
72	a	432.94	13.61493	YES	YES
73	a	455.20	14.53656	YES	YES
74	a	457.92	9.14318	YES	YES
75	a	472.99	11.70198	YES	YES
76	a	479.54	3.08732	YES	YES
77	a	483.95	10.34420	YES	YES
78	a	489.12	21.25942	YES	YES
79	a	496.67	31.42580	YES	YES
80	a	499.23	8.05344	YES	YES
81	a	506.81	8.41085	YES	YES
82	a	508.47	18.00873	YES	YES
83	a	511.19	72.70108	YES	YES
84	a	516.97	156.67680	YES	YES
85	a	529.20	34.55707	YES	YES
86	a	532.33	12.10641	YES	YES
87	a	592.28	3.50461	YES	YES
88	a	594.17	5.08267	YES	YES
89	a	607.69	0.32492	YES	YES
90	a	609.43	0.34799	YES	YES
91	a	609.52	0.42387	YES	YES
92	a	610.46	1.43157	YES	YES
93	a	610.65	1.78703	YES	YES
94	a	612.04	0.48903	YES	YES
95	a	612.41	0.08139	YES	YES
96	a	641.45	18.09191	YES	YES
97	a	651.48	17.03265	YES	YES
98	a	669.98	65.03409	YES	YES
99	a	670.56	8.68064	YES	YES
100	a	672.97	18.60833	YES	YES
101	a	676.48	9.30734	YES	YES
102	a	678.02	7.96754	YES	YES
103	a	686.71	11.16476	YES	YES
104	a	690.64	19.52985	YES	YES
105	a	693.18	49.70908	YES	YES
106	a	695.51	24.73303	YES	YES
107	a	696.46	28.88635	YES	YES
108	a	699.52	40.05203	YES	YES
109	a	702.65	42.67186	YES	YES
110	a	704.28	15.94041	YES	YES
111	a	710.15	9.66205	YES	YES
112	a	737.32	12.79748	YES	YES
113	a	738.19	8.36320	YES	YES
114	a	741.62	7.46253	YES	YES
115	a	743.03	5.23569	YES	YES
116	a	746.59	3.65219	YES	YES
117	a	747.58	4.11672	YES	YES
118	a	754.85	17.15347	YES	YES
119	a	768.27	1.80647	YES	YES
120	a	828.78	1.56228	YES	YES
121	a	832.14	0.73118	YES	YES
122	a	834.77	1.98976	YES	YES
123	a	836.65	0.76066	YES	YES
124	a	840.44	0.93977	YES	YES
125	a	843.24	0.58940	YES	YES
126	a	853.16	0.78849	YES	YES
127	a	861.51	4.17942	YES	YES
128	a	905.65	4.34582	YES	YES
129	a	905.94	1.45450	YES	YES
130	a	908.17	0.62609	YES	YES
131	a	909.93	0.50439	YES	YES
132	a	913.80	0.32275	YES	YES
133	a	921.10	0.29928	YES	YES
134	a	922.06	1.11186	YES	YES
135	a	925.69	0.99992	YES	YES
136	a	938.14	24.21456	YES	YES
137	a	956.09	0.62219	YES	YES
138	a	957.69	0.39098	YES	YES
139	a	959.22	0.90384	YES	YES
140	a	960.88	0.31589	YES	YES
141	a	964.14	0.80478	YES	YES
142	a	966.20	0.30860	YES	YES
143	a	971.60	0.05003	YES	YES
144	a	979.00	0.21801	YES	YES
145	a	980.27	0.95870	YES	YES
146	a	980.75	0.64926	YES	YES
147	a	981.77	1.16162	YES	YES
148	a	982.62	1.61168	YES	YES
149	a	983.09	0.95055	YES	YES
150	a	983.39	0.11585	YES	YES
151	a	984.22	3.85770	YES	YES
152	a	984.69	0.53586	YES	YES
153	a	984.90	2.72710	YES	YES
154	a	985.48	2.02898	YES	YES
155	a	986.47	0.13069	YES	YES
156	a	987.02	1.06318	YES	YES
157	a	987.66	0.28837	YES	YES
158	a	988.80	7.42616	YES	YES
159	a	1018.29	6.52077	YES	YES
160	a	1020.79	0.70715	YES	YES
161	a	1022.42	0.59141	YES	YES
162	a	1023.43	0.77362	YES	YES
163	a	1024.06	2.15396	YES	YES
164	a	1024.47	2.18387	YES	YES
165	a	1025.35	3.29611	YES	YES

166	a	1025.54	9.12551	YES	YES
167	a	1026.11	0.14885	YES	YES
168	a	1028.25	3.48987	YES	YES
169	a	1068.14	10.89355	YES	YES
170	a	1068.19	15.76737	YES	YES
171	a	1070.53	4.58577	YES	YES
172	a	1072.44	29.50485	YES	YES
173	a	1073.89	2.29376	YES	YES
174	a	1075.17	0.18191	YES	YES
175	a	1075.41	0.57105	YES	YES
176	a	1075.74	5.14657	YES	YES
177	a	1076.27	14.99475	YES	YES
178	a	1079.29	9.43009	YES	YES
179	a	1079.48	11.77802	YES	YES
180	a	1081.45	10.77534	YES	YES
181	a	1083.90	9.54287	YES	YES
182	a	1139.96	0.10316	YES	YES
183	a	1140.89	0.23505	YES	YES
184	a	1141.52	0.32796	YES	YES
185	a	1141.94	0.42124	YES	YES
186	a	1142.34	0.61139	YES	YES
187	a	1142.46	0.31247	YES	YES
188	a	1143.74	0.55162	YES	YES
189	a	1162.01	1.42803	YES	YES
190	a	1166.92	2.35216	YES	YES
191	a	1170.73	6.64447	YES	YES
192	a	1170.98	5.30530	YES	YES
193	a	1173.84	7.17544	YES	YES
194	a	1176.08	0.95303	YES	YES
195	a	1177.74	3.67270	YES	YES
196	a	1183.21	0.37075	YES	YES
197	a	1291.02	5.47187	YES	YES
198	a	1292.40	7.89383	YES	YES

* zero point VIBRATIONAL energy : 0.7456070 Hartree *

Cis 2_afay



bp86-SVP SCF energy: -2931.4401772160
pbe-TZVPP SCF energy: -2930.990027304

XYZ Coordinates
97

C	-0.91000	0.01657	-2.23866
C	-1.56525	0.05644	-1.14805
C	-0.76016	0.01653	-3.67413
H	-2.49358	0.10963	-0.57744
C	-0.58326	0.07499	-6.50191
C	-1.82374	-0.15185	-5.87576
C	-1.91543	-0.18091	-4.47896
C	0.48548	0.24045	-4.31364
C	0.56485	0.27201	-5.71464
H	-0.51313	0.09528	-7.60226
H	-2.72951	-0.31188	-6.48449
H	-2.88429	-0.36440	-3.98787
H	1.38146	0.39094	-3.69334
H	1.54006	0.45109	-6.19802
C	2.95716	0.73347	-0.78868
C	4.43423	0.94044	-1.00900
H	4.82743	0.07952	-1.59466
H	4.97425	0.97347	-0.04068
H	4.61707	1.86596	-1.59251
C	0.99530	-2.47523	-2.43768
C	2.00436	-3.14494	-3.37617
H	3.04576	-3.04049	-3.00866
H	1.93656	-2.65725	-4.37479
H	1.74426	-4.21622	-3.49847
C	1.02275	2.72820	1.78430
C	2.28591	3.15015	1.30629
H	2.52150	3.05397	0.23496
C	3.22421	3.73216	2.17205
H	4.20031	4.05935	1.77687
C	2.91768	3.90934	3.53308
H	3.65367	4.36879	4.21359
C	1.66085	3.50980	4.01420
H	1.39909	3.66081	5.07481
C	0.71911	2.92428	3.14747
H	-0.26522	2.63860	3.54693
C	-1.80600	2.03416	1.36424
C	-2.03471	1.26975	2.53117
H	-1.23080	0.64106	2.94559
C	-3.28324	1.29824	3.17525
H	-3.43193	0.71180	4.09706
C	-4.33821	2.05895	2.64403
H	-5.31958	2.07581	3.14643
C	-4.13499	2.78813	1.46113
H	-4.95945	3.37518	1.02331
C	-2.87923	2.78213	0.82898
H	-2.73773	3.36862	-0.09117
C	-0.25633	3.45093	-0.62096
C	-0.41455	4.74437	-0.06756
H	-0.46215	4.87527	1.02599
C	-0.50998	5.87088	-0.89846
H	-0.63296	6.87078	-0.44958
C	-0.44286	5.72456	-2.29625
H	-0.51340	6.61022	-2.94964
C	-0.27890	4.44669	-2.85242
H	-0.21736	4.31774	-3.94539
C	-0.18542	3.31550	-2.02066
H	-0.04262	2.32544	-2.47228
C	-1.97689	-2.27364	0.81036
C	-2.84072	-2.07274	1.90870
H	-2.45608	-1.65384	2.84985
C	-4.20350	-2.40786	1.81674
H	-4.86229	-2.24676	2.68624
C	-4.72115	-2.94574	0.62717
H	-5.78922	-3.21234	0.55821
C	-3.86992	-3.13418	-0.47579
H	-4.26755	-3.54656	-1.41825
C	-2.50908	-2.79354	-0.39581
H	-1.84026	-2.91937	-1.26610
C	0.74967	-3.36500	0.54538
C	0.12586	-4.62256	0.43119
H	-0.97179	-4.70068	0.41177
C	0.90196	-5.79145	0.33622
H	0.40018	-6.76946	0.24529
C	2.30382	-5.71463	0.35044
H	2.91045	-6.63260	0.27486
C	2.92937	-4.45980	0.45952
H	4.02990	-4.38858	0.46878
C	2.16047	-3.28942	0.55627
H	2.65748	-2.30922	0.63424
C	0.25515	-1.61750	2.63062
C	-0.15276	-2.60581	3.55823
H	-0.78659	-3.44566	3.23040
C	0.26156	-2.54114	4.89744
H	-0.07241	-3.31478	5.60904
C	1.11235	-1.50547	5.32634
H	1.44386	-1.46096	6.37729
C	1.55228	-0.54332	4.40405
H	2.23840	0.25950	4.71985
C	1.12623	-0.59814	3.06354
H	1.50364	0.14129	2.34183
O	2.54177	0.05078	0.21560
O	2.09442	1.20763	-1.60428
O	-0.16973	-2.88704	-2.37334
O	1.49960	-1.46111	-1.78369
P	-0.14262	1.97585	0.52496
P	-0.18854	-1.77635	0.82120
Ru	0.52562	-0.03136	-0.56712

Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	9.71	0.03949	YES	YES
8	a	13.80	0.01155	YES	YES
9	a	22.54	0.07295	YES	YES
10	a	29.50	0.00773	YES	YES
11	a	33.34	0.08410	YES	YES
12	a	35.80	0.19656	YES	YES
13	a	40.64	0.45058	YES	YES
14	a	43.23	0.04366	YES	YES
15	a	44.55	0.08220	YES	YES
16	a	49.05	0.33624	YES	YES
17	a	51.13	0.18704	YES	YES

18	a	51.78	0.00752	YES	YES
19	a	52.81	0.01537	YES	YES
20	a	59.14	0.15040	YES	YES
21	a	60.62	0.17138	YES	YES
22	a	64.40	0.40360	YES	YES
23	a	67.26	0.40687	YES	YES
24	a	67.63	0.12436	YES	YES
25	a	71.55	0.04306	YES	YES
26	a	73.27	0.28078	YES	YES
27	a	81.70	0.48581	YES	YES
28	a	84.06	2.61587	YES	YES
29	a	88.63	1.55127	YES	YES
30	a	93.71	0.14179	YES	YES
31	a	95.05	4.06898	YES	YES
32	a	103.66	2.00446	YES	YES
33	a	106.37	0.58983	YES	YES
34	a	114.13	0.42241	YES	YES
35	a	118.99	0.93499	YES	YES
36	a	125.95	1.38330	YES	YES
37	a	137.05	0.52123	YES	YES
38	a	145.28	5.89436	YES	YES
39	a	170.39	1.08932	YES	YES
40	a	175.00	0.12075	YES	YES
41	a	188.18	1.27883	YES	YES
42	a	193.52	1.63307	YES	YES
43	a	195.62	3.54342	YES	YES
44	a	203.06	0.18050	YES	YES
45	a	204.16	5.66228	YES	YES
46	a	213.05	0.50871	YES	YES
47	a	215.24	1.41093	YES	YES
48	a	219.12	0.41003	YES	YES
49	a	222.84	5.06559	YES	YES
50	a	235.03	11.83657	YES	YES
51	a	245.18	0.81989	YES	YES
52	a	246.95	1.09774	YES	YES
53	a	247.74	3.46025	YES	YES
54	a	249.72	0.18942	YES	YES
55	a	253.72	0.51491	YES	YES
56	a	265.35	1.36632	YES	YES
57	a	268.65	1.05504	YES	YES
58	a	275.41	6.34341	YES	YES
59	a	296.19	5.60586	YES	YES
60	a	316.53	8.36797	YES	YES
61	a	361.23	6.31418	YES	YES
62	a	394.79	0.13753	YES	YES
63	a	397.29	0.30563	YES	YES
64	a	398.71	0.06303	YES	YES
65	a	399.88	0.08900	YES	YES
66	a	403.07	2.00043	YES	YES
67	a	407.50	2.70555	YES	YES
68	a	410.04	16.59581	YES	YES
69	a	413.05	31.27404	YES	YES
70	a	414.66	6.44399	YES	YES
71	a	425.07	30.27192	YES	YES
72	a	426.51	5.73647	YES	YES
73	a	438.99	12.49597	YES	YES
74	a	454.74	17.46750	YES	YES
75	a	456.55	6.10767	YES	YES
76	a	473.12	7.68470	YES	YES
77	a	479.24	9.30669	YES	YES
78	a	490.74	13.42931	YES	YES
79	a	494.73	16.44650	YES	YES
80	a	498.54	19.38703	YES	YES
81	a	506.94	8.17460	YES	YES
82	a	510.47	58.19025	YES	YES
83	a	516.13	163.80397	YES	YES
84	a	527.22	83.36513	YES	YES
85	a	532.91	1.44826	YES	YES
86	a	546.54	15.72167	YES	YES
87	a	586.04	5.27578	YES	YES
88	a	592.35	2.22002	YES	YES
89	a	607.97	0.13543	YES	YES
90	a	609.49	0.81620	YES	YES
91	a	609.75	1.02374	YES	YES
92	a	610.27	0.91507	YES	YES
93	a	611.58	2.66678	YES	YES
94	a	612.01	0.48506	YES	YES
95	a	613.85	4.23349	YES	YES
96	a	655.07	44.91164	YES	YES
97	a	655.52	0.85197	YES	YES
98	a	668.27	47.71862	YES	YES
99	a	671.16	10.83083	YES	YES
100	a	673.69	18.49011	YES	YES
101	a	678.91	8.15383	YES	YES
102	a	680.47	10.24893	YES	YES
103	a	685.59	8.28908	YES	YES
104	a	690.52	39.87297	YES	YES
105	a	690.71	17.62480	YES	YES
106	a	693.69	18.59569	YES	YES
107	a	694.08	39.91368	YES	YES
108	a	698.91	32.82209	YES	YES
109	a	700.18	70.17205	YES	YES
110	a	705.00	8.19726	YES	YES
111	a	711.12	16.80136	YES	YES
112	a	737.03	10.91102	YES	YES
113	a	739.23	8.83273	YES	YES
114	a	743.24	5.10526	YES	YES
115	a	745.25	6.38487	YES	YES
116	a	746.82	1.78879	YES	YES
117	a	747.24	1.06280	YES	YES
118	a	757.04	17.60772	YES	YES
119	a	768.35	1.49125	YES	YES
120	a	828.98	0.60612	YES	YES
121	a	830.27	0.55855	YES	YES
122	a	831.71	0.64161	YES	YES
123	a	835.76	1.79375	YES	YES
124	a	837.01	5.00743	YES	YES
125	a	837.65	1.64544	YES	YES
126	a	843.71	1.59882	YES	YES
127	a	854.37	0.29479	YES	YES
128	a	904.41	0.18026	YES	YES
129	a	905.37	2.29935	YES	YES
130	a	908.42	0.35063	YES	YES
131	a	909.16	0.18831	YES	YES
132	a	910.13	0.91205	YES	YES
133	a	914.72	0.14647	YES	YES
134	a	920.59	1.56181	YES	YES
135	a	928.20	0.95403	YES	YES
136	a	939.53	17.61456	YES	YES
137	a	955.25	0.32521	YES	YES
138	a	956.05	0.37042	YES	YES
139	a	958.35	0.03661	YES	YES
140	a	960.15	0.01000	YES	YES
141	a	960.67	0.48509	YES	YES
142	a	964.63	0.95214	YES	YES
143	a	975.03	0.14911	YES	YES
144	a	977.74	0.11670	YES	YES
145	a	978.73	0.14826	YES	YES
146	a	981.74	1.09129	YES	YES
147	a	981.88	0.40390	YES	YES
148	a	982.41	0.91360	YES	YES
149	a	982.68	1.60020	YES	YES
150	a	983.14	4.77269	YES	YES
151	a	983.59	1.07773	YES	YES
152	a	983.90	2.42480	YES	YES
153	a	984.16	0.56932	YES	YES
154	a	984.89	0.10346	YES	YES
155	a	986.08	4.82368	YES	YES
156	a	986.28	1.45291	YES	YES
157	a	987.33	0.53912	YES	YES
158	a	988.09	1.73069	YES	YES
159	a	1015.16	9.06490	YES	YES
160	a	1021.85	0.77145	YES	YES
161	a	1022.53	1.14082	YES	YES
162	a	1022.89	0.99485	YES	YES
163	a	1024.03	8.25704	YES	YES
164	a	1024.54	3.24786	YES	YES
165	a	1024.89	1.33206	YES	YES

166	a	1025.71	8.59565	YES	YES
167	a	1026.10	0.19728	YES	YES
168	a	1026.47	1.84770	YES	YES
169	a	1068.46	16.31509	YES	YES
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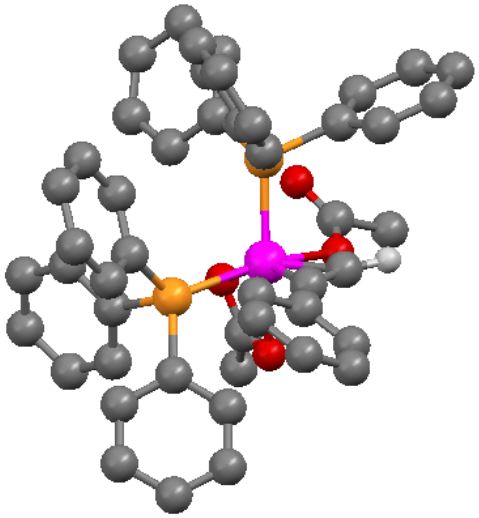
171	a	1070.83	4.88375	YES	YES
172	a	1071.96	4.44838	YES	YES
173	a	1072.26	15.34300	YES	YES
174	a	1073.88	6.47631	YES	YES
175	a	1074.76	11.92248	YES	YES
176	a	1076.47	3.52225	YES	YES
177	a	1076.98	6.46814	YES	YES
178	a	1079.11	17.01162	YES	YES
179	a	1079.90	3.55836	YES	YES
180	a	1081.77	8.31531	YES	YES
181	a	1081.97	14.48298	YES	YES
182	a	1139.61	0.05962	YES	YES
183	a	1141.74	0.15753	YES	YES
184	a	1141.78	0.42786	YES	YES
185	a	1141.98	0.28312	YES	YES
186	a	1142.55	0.26246	YES	YES
187	a	1142.88	1.24003	YES	YES
188	a	1143.32	0.19495	YES	YES
189	a	1158.31	2.27678	YES	YES
190	a	1165.61	2.49940	YES	YES
191	a	1167.22	5.06922	YES	YES
192	a	1172.13	2.63426	YES	YES
193	a	1173.60	7.24435	YES	YES
194	a	1176.69	3.55543	YES	YES
195	a	1177.20	4.00023	YES	YES
196	a	1187.84	0.07407	YES	YES
197	a	1287.31	6.61918	YES	YES
198	a	1290.74	10.86192	YES	YES

* zero point VIBRATIONAL energy : 0.7450417 Hartree *

Cis 2_afbx



bp86-SVP SCF energy: -2931.4159695400
pbe-TZVPP SCF energy: -2930.963741435

XYZ Coordinates
97

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C	-2.79019	1.68652	-1.34023
H	-1.56442	-1.11029	-2.99928
C	-4.85474	3.63459	-1.13513
C	-4.54400	3.05843	-2.38152
C	-3.52792	2.10070	-2.48649
C	-3.11388	2.27732	-0.09525
C	-4.13462	3.23574	0.00336
H	-5.65232	4.39145	-1.05438
H	-5.09946	3.36116	-3.28520
H	-3.28258	1.65783	-3.46533
H	-2.57012	1.96773	0.80757
H	-4.36773	3.67572	0.98752
C	2.54480	0.45350	-2.17808
C	3.85338	0.58745	-2.91436
H	3.94656	-0.26347	-3.62564
H	4.70589	0.53550	-2.20682
H	3.87966	1.53103	-3.49648
C	1.51096	-2.67625	-2.51512
C	1.77645	-3.37618	-3.85449
H	2.72360	-3.95039	-3.79427
H	1.80974	-2.65732	-4.69955
H	0.94648	-4.09182	-4.05119
C	2.43495	1.89498	0.87928
C	3.32724	2.53288	-0.01330
H	2.95798	2.91636	-0.97680
C	4.68069	2.70164	0.31781
H	5.35433	3.20695	-0.39430
C	5.17320	2.23674	1.54929
H	6.23528	2.37312	1.81193
C	4.29612	1.60529	2.44454
H	4.66220	1.24525	3.42036
C	2.93947	1.43536	2.11307
H	2.27654	0.95517	2.84677
C	-0.21900	1.86856	2.01203
C	-0.14500	0.78961	2.92020
H	0.35464	-0.14644	2.62627
C	-0.70609	0.88747	4.20437
H	-0.62806	0.03267	4.89459
C	-1.37556	2.05773	4.59596
H	-1.82124	2.13308	5.60158
C	-1.48501	3.12564	3.69006
H	-2.02122	4.04514	3.97857
C	-0.91129	3.03472	2.41053
H	-1.01924	3.88159	1.71703
C	0.41144	3.36346	-0.44224
C	0.84072	4.53318	0.23240
H	1.29411	4.46144	1.23435
C	0.71650	5.79358	-0.37176
H	1.05272	6.69324	0.17030
C	0.17793	5.90554	-1.66643
H	0.08422	6.89552	-2.14340
C	-0.22390	4.74928	-2.35215
H	-0.63022	4.82212	-3.37408
C	-0.10553	3.48537	-1.74637
H	-0.39299	2.58422	-2.30426
C	-1.71466	-1.68378	1.57175
C	-1.69670	-2.27022	2.85760
H	-0.83262	-2.86567	3.18595
C	-2.76928	-2.09248	3.74853
H	-2.72737	-2.56363	4.74519
C	-3.88342	-1.32169	3.37861
H	-4.72491	-1.18480	4.07792
C	-3.90898	-0.72144	2.10953
H	-4.76748	-0.10226	1.80143
C	-2.83421	-0.89816	1.22168
H	-2.87002	-0.41035	0.23737
C	-1.15777	-3.39107	-0.63251
C	-2.49865	-3.27286	-1.06332
H	-3.07873	-2.36487	-0.84185
C	-3.12439	-4.31307	-1.77030
H	-4.17228	-4.19511	-2.09347
C	-2.42386	-5.49657	-2.05477
H	-2.91594	-6.31712	-2.60333
C	-1.09012	-5.62311	-1.63329
H	-0.52459	-6.54466	-1.85217
C	-0.45749	-4.58003	-0.93433
H	0.60022	-4.67825	-0.65459
C	0.97136	-2.76282	1.31263
C	0.79990	-4.03016	1.91709
H	-0.12937	-4.60101	1.76210
C	1.81667	-4.58487	2.71310
H	1.66850	-5.57728	3.17118
C	3.01589	-3.88232	2.92007
H	3.81432	-4.32017	3.54238
C	3.19629	-2.62768	2.31491
H	4.14162	-2.07619	2.44829
C	2.18556	-2.07477	1.51092
H	2.36221	-1.12024	0.99398
O	2.47484	-0.28560	-1.12711
O	1.48310	1.02437	-2.59234
O	1.98684	-3.11339	-1.46379
O	0.71368	-1.64256	-2.64547
P	0.63584	1.69475	0.36288
P	-0.35806	-1.96313	0.29131
Ru	0.32322	-0.21525	-1.11466

Vibrational Frequencies

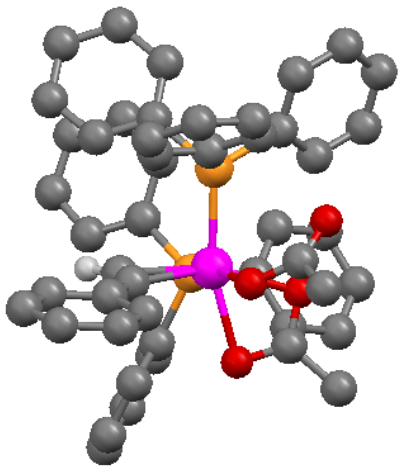
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.74	0.00682	YES	YES
8	a	17.31	0.01525	YES	YES
9	a	23.73	0.01805	YES	YES
10	a	28.10	0.27510	YES	YES
11	a	37.50	0.03431	YES	YES
12	a	43.81	0.04527	YES	YES
13	a	46.80	0.30411	YES	YES
14	a	48.23	0.31648	YES	YES
15	a	51.56	0.09812	YES	YES
16	a	53.23	0.48572	YES	YES

17	a	55.20	0.52068	YES	YES
18	a	59.07	0.84364	YES	YES
19	a	63.77	0.10437	YES	YES
20	a	67.63	0.05759	YES	YES
21	a	70.03	0.39975	YES	YES
22	a	73.81	2.04708	YES	YES
23	a	76.10	0.52378	YES	YES
24	a	79.85	0.04041	YES	YES
25	a	82.16	1.19258	YES	YES
26	a	86.10	0.52178	YES	YES
27	a	86.84	0.34086	YES	YES
28	a	90.59	0.88831	YES	YES
29	a	92.60	0.90234	YES	YES
30	a	99.93	0.38761	YES	YES
31	a	104.46	0.96670	YES	YES
32	a	110.42	1.99560	YES	YES
33	a	117.99	0.60070	YES	YES
34	a	122.68	2.90795	YES	YES
35	a	124.87	0.36546	YES	YES
36	a	127.98	0.57566	YES	YES
37	a	141.30	1.99668	YES	YES
38	a	156.85	3.52800	YES	YES
39	a	162.64	0.79604	YES	YES
40	a	175.68	3.00642	YES	YES
41	a	178.97	4.74982	YES	YES
42	a	189.10	0.25444	YES	YES
43	a	200.41	1.98021	YES	YES
44	a	201.58	3.79133	YES	YES
45	a	206.08	1.77994	YES	YES
46	a	211.18	1.28622	YES	YES
47	a	216.33	3.67518	YES	YES
48	a	220.30	2.60114	YES	YES
49	a	229.18	1.15349	YES	YES
50	a	232.49	4.25044	YES	YES
51	a	252.50	2.21369	YES	YES
52	a	253.43	0.25175	YES	YES
53	a	255.38	0.47598	YES	YES
54	a	258.32	1.43011	YES	YES
55	a	261.22	0.93633	YES	YES
56	a	269.05	2.50223	YES	YES
57	a	270.41	0.66060	YES	YES
58	a	281.07	4.06282	YES	YES
59	a	292.66	11.97492	YES	YES
60	a	325.34	12.76420	YES	YES
61	a	341.91	7.63400	YES	YES
62	a	396.41	0.05540	YES	YES
63	a	401.36	0.71434	YES	YES
64	a	404.18	3.22008	YES	YES
65	a	405.04	19.60654	YES	YES
66	a	406.81	3.82196	YES	YES
67	a	410.37	8.12249	YES	YES
68	a	412.39	2.69504	YES	YES
69	a	415.91	1.88374	YES	YES
70	a	420.08	9.24000	YES	YES
71	a	426.23	20.76456	YES	YES
72	a	429.68	7.86100	YES	YES
73	a	457.70	15.56410	YES	YES
74	a	458.77	29.95774	YES	YES
75	a	468.96	7.70929	YES	YES
76	a	470.82	3.32656	YES	YES
77	a	482.11	7.76359	YES	YES
78	a	488.55	2.72321	YES	YES
79	a	490.66	28.10329	YES	YES
80	a	505.45	8.26011	YES	YES
81	a	507.54	69.49787	YES	YES
82	a	512.23	49.86269	YES	YES
83	a	517.51	120.92797	YES	YES
84	a	523.90	23.46415	YES	YES
85	a	531.15	32.23392	YES	YES
86	a	549.09	7.79254	YES	YES
87	a	589.70	4.06701	YES	YES
88	a	598.02	2.58136	YES	YES
89	a	608.63	0.14761	YES	YES
90	a	609.72	1.09974	YES	YES
91	a	609.82	0.09041	YES	YES
92	a	609.99	0.62367	YES	YES
93	a	611.87	0.91990	YES	YES
94	a	612.36	1.24203	YES	YES
95	a	613.70	0.37281	YES	YES
96	a	653.86	11.66498	YES	YES
97	a	668.57	9.99358	YES	YES
98	a	669.08	4.31758	YES	YES
99	a	671.31	66.38171	YES	YES
100	a	671.94	10.59035	YES	YES
101	a	676.36	11.90086	YES	YES
102	a	686.10	10.90912	YES	YES
103	a	690.39	18.92784	YES	YES
104	a	692.50	33.04276	YES	YES
105	a	695.12	47.14641	YES	YES
106	a	696.90	47.67853	YES	YES
107	a	701.44	26.98394	YES	YES
108	a	701.90	50.28489	YES	YES
109	a	707.68	4.12170	YES	YES
110	a	709.52	20.81754	YES	YES
111	a	711.59	14.46527	YES	YES
112	a	735.25	7.03200	YES	YES
113	a	737.96	5.74421	YES	YES
114	a	740.04	8.35942	YES	YES
115	a	741.89	4.51376	YES	YES
116	a	745.37	9.64695	YES	YES
117	a	748.29	2.22320	YES	YES
118	a	754.33	11.85250	YES	YES
119	a	772.37	0.88011	YES	YES
120	a	817.15	5.37401	YES	YES
121	a	825.91	0.68509	YES	YES
122	a	827.53	1.13522	YES	YES
123	a	829.82	0.57087	YES	YES
124	a	836.43	0.29074	YES	YES
125	a	839.43	0.85148	YES	YES
126	a	845.43	0.48262	YES	YES
127	a	847.01	0.53448	YES	YES
128	a	898.44	4.06440	YES	YES
129	a	901.53	1.52097	YES	YES
130	a	905.88	0.59804	YES	YES
131	a	911.79	0.69519	YES	YES
132	a	915.61	0.94203	YES	YES
133	a	916.34	2.31998	YES	YES
134	a	919.83	0.34889	YES	YES
135	a	924.82	0.02788	YES	YES
136	a	940.79	22.71908	YES	YES
137	a	952.24	1.87228	YES	YES
138	a	953.33	0.49025	YES	YES
139	a	956.28	0.55611	YES	YES
140	a	960.65	0.26708	YES	YES
141	a	961.92	0.25371	YES	YES
142	a	967.86	0.17310	YES	YES
143	a	969.14	0.54123	YES	YES
144	a	974.73	0.43111	YES	YES
145	a	978.38	0.27925	YES	YES
146	a	980.20	0.38500	YES	YES
147	a	981.50	0.38603	YES	YES
148	a	982.08	3.06933	YES	YES
149	a	982.32	0.14862	YES	YES
150	a	983.12	1.13845	YES	YES
151	a	983.44	2.74807	YES	YES
152	a	983.52	2.81529	YES	YES
153	a	984.47	1.15074	YES	YES
154	a	984.53	1.92553	YES	YES
155	a	984.84	4.42464	YES	YES
156	a	985.33	0.83383	YES	YES
157	a	987.53	0.53283	YES	YES
158	a	987.88	0.34973	YES	YES
159	a	988.70	1.27875	YES	YES
160	a	1016.53	9.78670	YES	YES
161	a	1022.68	8.34093	YES	YES
162	a	1023.52	0.24230	YES	YES
163	a	1023.66	0.99799	YES	YES
164	a	1024.27	0.51290	YES	YES

165	a	1024.60	2.13973	YES	YES
166	a	1025.87	1.62431	YES	YES
167	a	1026.32	0.36837	YES	YES
168	a	1026.60	3.04135	YES	YES
169	a	1064.47	14.14578	YES	YES
170	a	1066.04	13.70939	YES	YES
171	a	1070.29	25.84137	YES	YES
172	a	1071.62	7.20570	YES	YES
173	a	1072.23	12.49815	YES	YES
174	a	1073.41	5.61825	YES	YES
175	a	1074.28	6.32752	YES	YES
176	a	1074.79	5.78446	YES	YES
177	a	1076.03	2.79585	YES	YES
178	a	1078.39	10.41260	YES	YES
179	a	1081.26	0.32125	YES	YES
180	a	1081.67	1.02485	YES	YES
181	a	1083.22	15.61630	YES	YES
182	a	1138.10	0.29407	YES	YES
183	a	1140.57	0.01950	YES	YES
184	a	1140.82	0.16669	YES	YES
185	a	1141.46	0.20775	YES	YES
186	a	1141.83	0.60517	YES	YES
187	a	1142.05	0.68431	YES	YES
188	a	1142.18	0.34941	YES	YES
189	a	1158.47	3.70881	YES	YES
190	a	1167.45	6.94411	YES	YES
191	a	1168.77	2.22338	YES	YES
192	a	1170.48	2.33601	YES	YES
193	a	1171.61	2.80828	YES	YES
194	a	1175.81	2.15409	YES	YES
195	a	1177.84	3.28159	YES	YES
196	a	1184.08	1.53162	YES	YES
197	a	1288.78	8.56947	YES	YES
198	a	1289.14	31.19597	YES	YES

* zero point VIBRATIONAL energy : 0.7457356 Hartree *

Cis 2_afby



bp86-SVP SCF energy: -2931.4249930650
pbe-TZVPP SCF energy: -2930.973509485

XYZ Coordinates
97

C	-0.72195	-1.13436	-2.06064
C	-1.31577	-0.07959	-1.62931
C	-0.79497	-2.30356	-2.91552
H	-2.20848	0.55289	-1.62595
C	-1.06366	-4.51513	-4.67221
C	-2.18128	-3.71278	-4.37192
C	-2.05108	-2.62108	-3.50509
C	0.32131	-3.11960	-3.22513
C	0.18168	-4.21059	-4.09602
H	-1.16619	-5.37470	-5.35575
H	-3.16368	-3.94152	-4.81843
H	-2.92653	-1.99158	-3.27440
H	1.28546	-2.86836	-2.76114
H	1.06118	-4.83479	-4.32797
C	2.78189	1.05560	-1.40119
C	4.17834	1.47481	-1.79035
H	4.79009	0.55865	-1.94741
H	4.65107	2.06230	-0.97699
H	4.16485	2.04931	-2.73888
C	2.87153	-2.07428	-0.35278
C	3.86431	-3.01787	-1.04308
H	4.80299	-3.06766	-0.45447
H	4.07839	-2.70398	-2.08601
H	3.42033	-4.03832	-1.07978
C	0.84735	3.31609	0.58135
C	1.94290	3.84486	-0.14036
H	2.07623	3.58487	-1.20205
C	2.84601	4.73005	0.46594
H	3.68882	5.13266	-0.12006
C	2.67391	5.10758	1.80911
H	3.38211	5.80502	2.28625
C	1.58499	4.59763	2.53274
H	1.42511	4.89696	3.58186
C	0.67917	3.70851	1.92524
H	-0.17516	3.34563	2.51372
C	-1.92504	2.35523	0.53891
C	-2.06668	1.95181	1.88547
H	-1.22771	1.47064	2.41207
C	-3.27814	2.14392	2.56791
H	-3.36005	1.83436	3.62184
C	-4.38346	2.70268	1.90598
H	-5.33669	2.84458	2.44157
C	-4.26980	3.06278	0.55416
H	-5.13465	3.48677	0.01724
C	-3.04972	2.89676	-0.12390
H	-2.97743	3.20461	-1.17814
C	-0.53984	3.11944	-1.88644
C	-0.79359	4.50891	-1.78542
H	-0.82824	4.99377	-0.79610
C	-1.00377	5.28389	-2.93599
H	-1.20229	6.36406	-2.83718
C	-0.95712	4.68503	-4.20775
H	-1.11833	5.29393	-5.11311
C	-0.69658	3.31025	-4.31725
H	-0.64590	2.83199	-5.30935
C	-0.48655	2.52975	-3.16528
H	-0.26637	1.45827	-3.26568
C	-1.87558	-1.23528	1.78611
C	-2.22180	-1.21011	3.15683
H	-1.43930	-1.13645	3.92568
C	-3.56416	-1.26452	3.56942
H	-3.79835	-1.24964	4.64723
C	-4.59836	-1.33742	2.62279
H	-5.65150	-1.38432	2.94672
C	-4.27322	-1.34379	1.25711
H	-5.07092	-1.38947	0.49715
C	-2.93061	-1.29212	0.84625
H	-2.70464	-1.29031	-0.22944
C	0.05472	-3.16049	0.99032
C	-0.92893	-3.84809	0.24628
H	-1.76684	-3.30379	-0.21176
C	-0.86360	-5.23999	0.07369
H	-1.64244	-5.74864	-0.51791
C	0.18505	-5.97519	0.64905
H	0.23493	-7.06933	0.51906
C	1.17331	-5.30141	1.38526
H	2.00817	-5.86302	1.83718
C	1.11619	-3.90636	1.55057
H	1.92497	-3.39200	2.08610
C	0.84582	-0.92736	2.76112
C	0.82554	-1.79623	3.87751
H	0.27540	-2.74941	3.83240
C	1.51223	-1.46018	5.05668
H	1.49033	-2.15282	5.91486
C	2.22468	-0.25170	5.14103
H	2.76566	0.00924	6.06608
C	2.25414	0.61291	4.03453
H	2.82579	1.55462	4.07862
C	1.57557	0.27535	2.85153
H	1.65409	0.93296	1.97373
O	2.50846	0.81281	-0.16867
O	1.86836	0.90000	-2.27639
O	2.96587	-1.82114	0.85127
O	1.94042	-1.64059	-1.17068
P	-0.28998	2.13041	-0.31778
P	-0.07919	-1.29656	1.19190
Ru	0.59808	-0.07699	-0.69146

Vibrational Frequencies

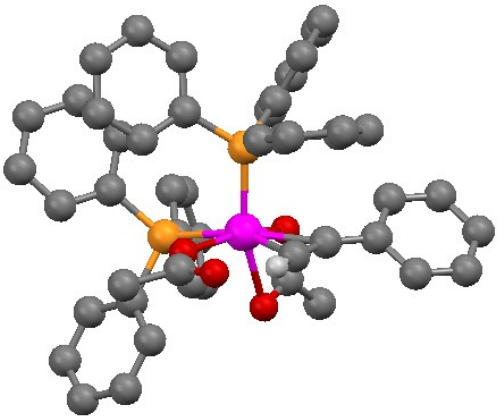
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.60	0.06890	YES	YES
8	a	15.24	0.03383	YES	YES
9	a	21.96	0.15648	YES	YES
10	a	22.61	0.12426	YES	YES
11	a	31.60	0.03855	YES	YES
12	a	35.15	0.05187	YES	YES
13	a	43.01	0.11435	YES	YES
14	a	45.20	0.14000	YES	YES
15	a	48.76	0.16403	YES	YES
16	a	53.29	0.54712	YES	YES
17	a	53.90	0.00917	YES	YES
18	a	55.53	0.12647	YES	YES

19	a	60.91	0.72123	YES	YES
20	a	64.47	0.11717	YES	YES
21	a	66.56	0.58456	YES	YES
22	a	74.63	0.77435	YES	YES
23	a	75.59	1.47294	YES	YES
24	a	81.22	0.91055	YES	YES
25	a	83.90	0.49063	YES	YES
26	a	87.19	0.22584	YES	YES
27	a	92.06	1.03758	YES	YES
28	a	97.10	1.14964	YES	YES
29	a	103.00	2.43367	YES	YES
30	a	104.19	0.36467	YES	YES
31	a	107.25	0.34324	YES	YES
32	a	115.05	2.96814	YES	YES
33	a	117.96	0.81320	YES	YES
34	a	122.24	0.79293	YES	YES
35	a	127.81	1.02525	YES	YES
36	a	132.77	0.55182	YES	YES
37	a	143.30	0.33801	YES	YES
38	a	159.54	3.92470	YES	YES
39	a	175.25	2.78568	YES	YES
40	a	178.40	1.58084	YES	YES
41	a	192.00	0.80327	YES	YES
42	a	198.65	2.89020	YES	YES
43	a	201.47	2.34953	YES	YES
44	a	205.39	1.73246	YES	YES
45	a	207.34	1.00364	YES	YES
46	a	214.18	3.04724	YES	YES
47	a	219.02	3.07104	YES	YES
48	a	225.20	3.38121	YES	YES
49	a	228.28	1.89904	YES	YES
50	a	233.25	6.19793	YES	YES
51	a	251.89	1.25239	YES	YES
52	a	254.10	1.99258	YES	YES
53	a	254.93	0.02594	YES	YES
54	a	257.84	0.98957	YES	YES
55	a	260.27	3.93007	YES	YES
56	a	267.07	0.56894	YES	YES
57	a	275.17	0.14233	YES	YES
58	a	281.80	7.15446	YES	YES
59	a	298.46	6.18674	YES	YES
60	a	317.83	10.87089	YES	YES
61	a	366.15	5.53809	YES	YES
62	a	397.13	0.27183	YES	YES
63	a	398.85	0.88465	YES	YES
64	a	403.01	0.27105	YES	YES
65	a	403.59	0.97050	YES	YES
66	a	404.47	9.34585	YES	YES
67	a	407.83	8.19186	YES	YES
68	a	410.77	37.04623	YES	YES
69	a	415.09	6.84104	YES	YES
70	a	417.60	0.14898	YES	YES
71	a	426.09	15.00892	YES	YES
72	a	430.07	10.22528	YES	YES
73	a	457.83	31.44463	YES	YES
74	a	459.97	10.93082	YES	YES
75	a	465.20	6.86552	YES	YES
76	a	474.64	4.22472	YES	YES
77	a	482.38	8.45647	YES	YES
78	a	485.78	8.02760	YES	YES
79	a	491.25	61.85417	YES	YES
80	a	495.91	6.72500	YES	YES
81	a	504.86	28.43009	YES	YES
82	a	512.00	49.94785	YES	YES
83	a	518.07	139.78618	YES	YES
84	a	528.57	40.54100	YES	YES
85	a	535.18	16.68450	YES	YES
86	a	565.67	17.20832	YES	YES
87	a	591.72	5.38936	YES	YES
88	a	598.38	1.73769	YES	YES
89	a	608.49	0.12072	YES	YES
90	a	609.17	0.74813	YES	YES
91	a	609.59	1.17497	YES	YES
92	a	609.83	0.17697	YES	YES
93	a	611.70	0.02557	YES	YES
94	a	613.88	0.74932	YES	YES
95	a	614.95	5.53097	YES	YES
96	a	646.12	30.52408	YES	YES
97	a	658.73	12.36833	YES	YES
98	a	666.29	9.76299	YES	YES
99	a	670.32	47.01153	YES	YES
100	a	670.33	14.98864	YES	YES
101	a	671.11	29.37698	YES	YES
102	a	680.20	9.49990	YES	YES
103	a	686.27	13.85145	YES	YES
104	a	688.94	21.97572	YES	YES
105	a	691.90	36.97872	YES	YES
106	a	693.02	39.00154	YES	YES
107	a	697.10	40.39438	YES	YES
108	a	698.12	34.04967	YES	YES
109	a	702.18	24.74614	YES	YES
110	a	705.82	21.41492	YES	YES
111	a	707.56	7.28418	YES	YES
112	a	734.29	5.88240	YES	YES
113	a	736.20	5.84399	YES	YES
114	a	738.99	8.17152	YES	YES
115	a	742.11	5.33624	YES	YES
116	a	745.69	7.18435	YES	YES
117	a	747.36	2.60457	YES	YES
118	a	760.73	16.20742	YES	YES
119	a	781.68	1.68961	YES	YES
120	a	823.19	1.21367	YES	YES
121	a	832.12	0.64043	YES	YES
122	a	833.47	0.48100	YES	YES
123	a	834.49	0.79406	YES	YES
124	a	835.95	0.65628	YES	YES
125	a	838.66	0.55140	YES	YES
126	a	842.95	0.19228	YES	YES
127	a	890.59	15.04181	YES	YES
128	a	898.51	2.12437	YES	YES
129	a	907.74	0.80232	YES	YES
130	a	909.75	0.11874	YES	YES
131	a	912.80	1.64574	YES	YES
132	a	913.02	1.12752	YES	YES
133	a	915.10	1.83758	YES	YES
134	a	915.12	2.16256	YES	YES
135	a	917.45	0.34861	YES	YES
136	a	939.26	21.25815	YES	YES
137	a	949.87	1.79408	YES	YES
138	a	957.47	0.12029	YES	YES
139	a	959.39	0.79503	YES	YES
140	a	959.99	0.26765	YES	YES
141	a	960.84	0.08195	YES	YES
142	a	961.26	0.37666	YES	YES
143	a	966.13	0.43138	YES	YES
144	a	977.34	0.61192	YES	YES
145	a	980.02	0.65701	YES	YES
146	a	980.24	2.89187	YES	YES
147	a	981.94	1.83384	YES	YES
148	a	982.39	1.39193	YES	YES
149	a	982.92	1.17651	YES	YES
150	a	983.45	0.68210	YES	YES
151	a	983.75	0.67735	YES	YES
152	a	984.08	1.72130	YES	YES
153	a	984.22	0.16131	YES	YES
154	a	985.00	2.12618	YES	YES
155	a	985.49	6.83322	YES	YES
156	a	985.95	0.45906	YES	YES
157	a	986.58	0.29527	YES	YES
158	a	987.01	1.89786	YES	YES
159	a	989.52	0.76048	YES	YES
160	a	1016.90	7.38343	YES	YES
161	a	1023.61	0.74785	YES	YES
162	a	1023.82	1.05501	YES	YES
163	a	1024.01	1.54509	YES	YES
164	a	1024.87	0.46650	YES	YES
165	a	1025.57	10.42603	YES	YES
166	a	1026.29	1.40924	YES	YES

167	a	1026.60	6.85789	YES	YES
168	a	1026.87	0.37002	YES	YES
169	a	1062.39	12.64455	YES	YES
170	a	1069.14	18.87051	YES	YES
171	a	1070.02	7.05063	YES	YES
172	a	1070.86	29.25345	YES	YES
173	a	1071.34	16.86567	YES	YES
174	a	1074.31	3.70772	YES	YES
175	a	1074.83	7.25658	YES	YES
176	a	1075.23	5.71513	YES	YES
177	a	1078.21	0.72982	YES	YES
178	a	1079.76	14.17285	YES	YES
179	a	1080.44	11.02806	YES	YES
180	a	1082.12	3.53296	YES	YES
181	a	1082.56	2.59515	YES	YES
182	a	1138.52	0.44926	YES	YES
183	a	1140.35	0.13375	YES	YES
184	a	1140.81	0.29794	YES	YES
185	a	1141.66	0.56513	YES	YES
186	a	1142.80	0.34684	YES	YES
187	a	1142.83	0.73752	YES	YES
188	a	1143.62	0.53554	YES	YES
189	a	1154.65	7.29218	YES	YES
190	a	1168.93	3.25862	YES	YES
191	a	1169.18	1.32756	YES	YES
192	a	1170.66	3.92627	YES	YES
193	a	1172.45	10.46121	YES	YES
194	a	1175.88	3.59301	YES	YES
195	a	1177.14	1.54336	YES	YES
196	a	1186.45	0.08262	YES	YES
197	a	1284.09	147.00544	YES	YES
198	a	1288.01	0.51010	YES	YES

* zero point VIBRATIONAL energy : 0.7457619 Hartree *

Cis 2_pfax



bp86-SVP SCF energy: -2931.4262894350
pbe-TZVPP SCF energy: -2930.975269306

XYZ Coordinates
97

C	1.49976	-2.18606	-1.52258
C	0.78706	-1.68621	-2.44603
C	2.45430	-3.12898	-0.98560
H	0.18246	-1.53248	-3.35390
C	4.32478	-5.05047	-0.05173
C	3.45363	-4.41105	0.84782
C	2.53069	-3.45767	0.39256
C	3.34132	-3.78215	-1.88541
C	4.26195	-4.73112	-1.42114
H	5.05252	-5.79482	0.31243
H	3.49360	-4.65473	1.92274
H	1.86278	-2.94961	1.10243
H	3.29440	-3.52814	-2.95627
H	4.94040	-5.22596	-2.13641
C	3.11881	-0.02898	-0.21573
C	4.56754	-0.11237	0.19262
H	4.94913	-1.11461	-0.09403
H	4.67178	-0.00383	1.29152
H	5.16569	0.65910	-0.33257
C	-1.10907	0.60130	-3.47502
C	-1.80380	1.85658	-4.02239
H	-2.11018	1.68614	-5.07401
H	-1.13079	2.73885	-3.95984
H	-2.70705	2.09135	-3.41571
C	1.63470	2.43671	1.46586
C	2.96719	2.77109	1.12788
H	3.26521	2.83477	0.07016
C	3.91753	3.04369	2.12522
H	4.94695	3.31077	1.83375
C	3.55878	2.98825	3.48241
H	4.30348	3.20913	4.26514
C	2.23888	2.65976	3.82997
H	1.93663	2.62490	4.88993
C	1.28653	2.38585	2.83252
H	0.25623	2.15883	3.14037
C	-1.17839	2.71122	0.69876
C	-1.80113	2.08049	1.80152
H	-1.36577	1.16765	2.23700
C	-2.99611	2.58289	2.34007
H	-3.45255	2.08267	3.20947
C	-3.61856	3.69865	1.75574
H	-4.56048	4.09082	2.17295
C	-3.04576	4.29266	0.61959
H	-3.54029	5.15010	0.13341
C	-1.83582	3.80538	0.09478
H	-1.40370	4.28646	-0.79472
C	0.99726	3.35569	-1.13719
C	1.09579	4.70169	-0.70897
H	0.82549	4.97477	0.32421
C	1.54657	5.70080	-1.58585
H	1.61264	6.74462	-1.23506
C	1.91825	5.36886	-2.90101
H	2.27472	6.15254	-3.59040
C	1.84404	4.03294	-3.32657
H	2.14789	3.75920	-4.35035
C	1.38731	3.02977	-2.45158
H	1.34239	1.98568	-2.78635
C	-2.85031	-0.55761	0.28517
C	-3.76127	-1.01146	1.26461
H	-3.46794	-1.79254	1.98222
C	-5.05586	-0.47125	1.34070
H	-5.75335	-0.83884	2.11204
C	-5.46283	0.52598	0.43766
H	-6.48214	0.94361	0.49415
C	-4.55814	0.99295	-0.52924
H	-4.85929	1.78611	-1.23323
C	-3.25892	0.46203	-0.60050
H	-2.53507	0.84670	-1.33480
C	-1.68023	-2.85708	-0.92826
C	-2.69959	-2.74879	-1.89776
H	-3.23685	-1.79830	-2.03465
C	-3.03625	-3.84686	-2.70720
H	-3.83191	-3.73815	-3.46259
C	-2.36358	-5.07033	-2.55817
H	-2.63051	-5.93208	-3.19245
C	-1.34059	-5.18540	-1.60135
H	-0.79495	-6.13623	-1.48217
C	-0.99496	-4.08577	-0.79932
H	-0.17653	-4.19392	-0.07004
C	-0.83374	-2.04357	1.75444
C	-1.45669	-3.21961	2.23584
H	-2.13656	-3.79164	1.58500
C	-1.21112	-3.67726	3.54149
H	-1.70425	-4.59792	3.89711
C	-0.34124	-2.96960	4.38875
H	-0.14725	-3.33173	5.41213
C	0.28653	-1.80420	3.91893
H	0.98320	-1.24747	4.56732
C	0.04526	-1.34515	2.61196
H	0.57746	-0.45589	2.24272
O	2.20870	-0.50767	0.56184
O	2.75834	0.44801	-1.33826
O	-1.06768	-0.43367	-4.15318
O	-0.63218	0.78952	-2.26529
P	0.44250	2.04765	0.07102
P	-1.16943	-1.35144	0.05520
Ru	0.62549	-0.23520	-0.86816

Vibrational Frequencies

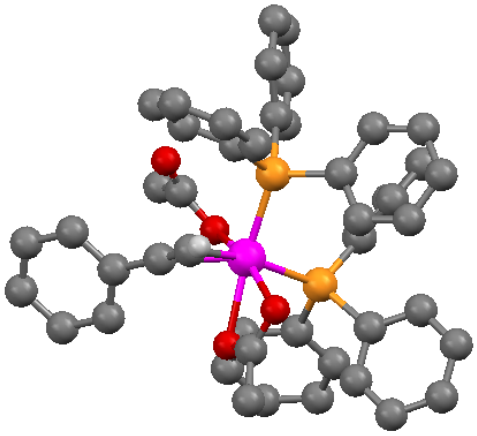
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.53	0.30490	YES	YES
8	a	19.61	0.37782	YES	YES
9	a	23.54	0.12353	YES	YES
10	a	29.90	0.09543	YES	YES
11	a	33.79	0.81798	YES	YES
12	a	35.95	0.02127	YES	YES
13	a	38.99	0.22632	YES	YES
14	a	43.44	0.52577	YES	YES
15	a	46.20	0.15977	YES	YES
16	a	52.09	0.26708	YES	YES
17	a	54.60	0.40575	YES	YES
18	a	57.29	0.19002	YES	YES
19	a	57.86	0.10386	YES	YES

20	a	59.91	0.00814	YES	YES
21	a	63.99	0.16903	YES	YES
22	a	65.31	0.24380	YES	YES
23	a	69.95	0.41555	YES	YES
24	a	71.19	0.12680	YES	YES
25	a	73.60	0.18175	YES	YES
26	a	77.25	0.43923	YES	YES
27	a	80.55	0.12010	YES	YES
28	a	87.60	0.68380	YES	YES
29	a	93.48	0.15213	YES	YES
30	a	96.00	0.42714	YES	YES
31	a	98.36	0.76463	YES	YES
32	a	107.35	0.12119	YES	YES
33	a	108.90	0.72887	YES	YES
34	a	115.00	0.47260	YES	YES
35	a	127.99	0.41052	YES	YES
36	a	137.27	1.25422	YES	YES
37	a	145.84	0.83107	YES	YES
38	a	157.91	1.44001	YES	YES
39	a	167.94	3.20009	YES	YES
40	a	185.14	0.93817	YES	YES
41	a	193.78	2.01305	YES	YES
42	a	197.52	2.95616	YES	YES
43	a	200.28	0.34339	YES	YES
44	a	204.05	5.56828	YES	YES
45	a	206.45	7.58525	YES	YES
46	a	209.10	1.48723	YES	YES
47	a	210.98	2.68217	YES	YES
48	a	219.86	1.48234	YES	YES
49	a	227.03	5.24236	YES	YES
50	a	231.45	0.81069	YES	YES
51	a	237.30	5.20673	YES	YES
52	a	248.26	0.56723	YES	YES
53	a	249.33	1.23736	YES	YES
54	a	254.51	0.30478	YES	YES
55	a	259.79	1.19824	YES	YES
56	a	263.47	1.20004	YES	YES
57	a	268.41	1.06421	YES	YES
58	a	269.75	1.17183	YES	YES
59	a	291.03	18.38701	YES	YES
60	a	323.30	11.03352	YES	YES
61	a	370.67	2.95281	YES	YES
62	a	397.80	1.47683	YES	YES
63	a	399.31	0.13953	YES	YES
64	a	399.86	11.74151	YES	YES
65	a	401.34	3.08230	YES	YES
66	a	403.98	1.77772	YES	YES
67	a	405.99	3.29348	YES	YES
68	a	413.52	2.54281	YES	YES
69	a	415.46	1.50928	YES	YES
70	a	417.54	14.95914	YES	YES
71	a	420.69	6.95808	YES	YES
72	a	426.25	19.12582	YES	YES
73	a	436.82	7.03312	YES	YES
74	a	453.38	23.49971	YES	YES
75	a	459.16	17.24397	YES	YES
76	a	474.06	10.72165	YES	YES
77	a	475.83	0.93518	YES	YES
78	a	482.59	10.73700	YES	YES
79	a	495.42	20.11047	YES	YES
80	a	505.19	4.87789	YES	YES
81	a	507.97	26.69828	YES	YES
82	a	514.31	44.37264	YES	YES
83	a	518.02	141.21719	YES	YES
84	a	524.80	61.25615	YES	YES
85	a	531.64	23.72861	YES	YES
86	a	541.48	6.44542	YES	YES
87	a	585.89	3.27202	YES	YES
88	a	599.66	1.17758	YES	YES
89	a	608.76	0.32613	YES	YES
90	a	609.20	0.74858	YES	YES
91	a	610.05	0.87006	YES	YES
92	a	610.15	0.24409	YES	YES
93	a	612.20	0.72983	YES	YES
94	a	612.75	1.20382	YES	YES
95	a	612.97	0.82707	YES	YES
96	a	636.93	15.94950	YES	YES
97	a	669.31	11.87936	YES	YES
98	a	670.09	37.24171	YES	YES
99	a	672.33	21.27185	YES	YES
100	a	678.00	9.13230	YES	YES
101	a	679.80	11.57270	YES	YES
102	a	686.47	12.59090	YES	YES
103	a	687.79	15.42650	YES	YES
104	a	692.04	26.19574	YES	YES
105	a	696.08	34.21044	YES	YES
106	a	697.62	43.23047	YES	YES
107	a	697.74	39.47318	YES	YES
108	a	701.53	35.42040	YES	YES
109	a	706.11	20.64003	YES	YES
110	a	707.89	11.42451	YES	YES
111	a	734.40	8.49141	YES	YES
112	a	737.37	4.55762	YES	YES
113	a	741.61	1.80999	YES	YES
114	a	743.78	6.63674	YES	YES
115	a	746.52	8.15282	YES	YES
116	a	748.26	4.66311	YES	YES
117	a	754.58	15.63075	YES	YES
118	a	757.07	21.38807	YES	YES
119	a	787.20	9.99729	YES	YES
120	a	827.99	19.17577	YES	YES
121	a	829.00	3.69687	YES	YES
122	a	831.27	1.17430	YES	YES
123	a	833.90	0.48045	YES	YES
124	a	834.47	0.30496	YES	YES
125	a	840.70	0.58371	YES	YES
126	a	842.86	0.98640	YES	YES
127	a	847.25	0.16069	YES	YES
128	a	902.68	2.00935	YES	YES
129	a	903.97	0.40396	YES	YES
130	a	907.91	0.21945	YES	YES
131	a	910.91	1.25290	YES	YES
132	a	915.95	0.14615	YES	YES
133	a	917.57	1.31819	YES	YES
134	a	919.45	0.39810	YES	YES
135	a	923.64	0.72208	YES	YES
136	a	943.54	15.38224	YES	YES
137	a	955.32	0.07265	YES	YES
138	a	956.80	0.36518	YES	YES
139	a	958.04	0.10647	YES	YES
140	a	959.41	0.29800	YES	YES
141	a	963.87	0.08017	YES	YES
142	a	965.82	0.13315	YES	YES
143	a	971.45	0.29146	YES	YES
144	a	976.83	0.10767	YES	YES
145	a	981.13	1.08968	YES	YES
146	a	981.47	1.74845	YES	YES
147	a	981.90	0.50276	YES	YES
148	a	982.21	2.44803	YES	YES
149	a	982.29	1.25256	YES	YES
150	a	983.01	1.09793	YES	YES
151	a	983.49	0.38967	YES	YES
152	a	984.50	0.73809	YES	YES
153	a	984.90	0.48281	YES	YES
154	a	985.38	0.52835	YES	YES
155	a	986.66	0.62594	YES	YES
156	a	986.95	3.91786	YES	YES
157	a	989.23	1.21075	YES	YES
158	a	990.52	8.22998	YES	YES
159	a	997.26	1.30400	YES	YES
160	a	1016.04	5.47636	YES	YES
161	a	1023.64	2.37859	YES	YES
162	a	1023.73	5.22643	YES	YES
163	a	1024.05	5.88968	YES	YES
164	a	1024.35	2.56089	YES	YES
165	a	1024.59	5.46693	YES	YES
166	a	1024.74	1.01286	YES	YES
167	a	1025.92	0.75859	YES	YES

168	a	1026.77	1.43247	YES	YES
169	a	1067.51	12.52888	YES	YES
170	a	1070.37	15.88763	YES	YES
171	a	1071.10	1.82179	YES	YES
172	a	1072.36	5.74291	YES	YES
173	a	1073.25	22.23276	YES	YES
174	a	1073.52	9.09343	YES	YES
175	a	1074.64	6.78048	YES	YES
176	a	1075.95	14.58881	YES	YES
177	a	1076.22	4.49099	YES	YES
178	a	1078.83	1.26525	YES	YES
179	a	1079.80	16.65927	YES	YES
180	a	1080.56	10.99893	YES	YES
181	a	1083.13	0.68731	YES	YES
182	a	1138.57	0.04766	YES	YES
183	a	1140.10	0.09703	YES	YES
184	a	1141.59	0.48562	YES	YES
185	a	1142.02	0.69773	YES	YES
186	a	1142.04	1.11272	YES	YES
187	a	1142.13	0.15833	YES	YES
188	a	1143.13	0.46725	YES	YES
189	a	1157.25	0.59246	YES	YES
190	a	1167.47	1.40147	YES	YES
191	a	1168.58	8.09354	YES	YES
192	a	1170.19	2.89860	YES	YES
193	a	1170.85	1.80299	YES	YES
194	a	1176.15	5.17452	YES	YES
195	a	1177.36	3.43115	YES	YES
196	a	1187.53	1.40857	YES	YES
197	a	1282.25	220.80454	YES	YES
198	a	1288.09	2.40253	YES	YES

* zero point VIBRATIONAL energy : 0.7453421 Hartree *

Cis 2_pfay



bp86-SVP SCF energy: -2931.4330741580
pbe-TZVPP SCF energy: -2930.983132997

XYZ Coordinates
97

C	2.16434	1.82867	-1.17712
C	1.14519	1.88590	-1.91889
C	3.46435	2.06156	-0.59927
H	0.58558	2.22922	-2.78829
C	6.04357	2.58269	0.43991
C	5.73375	1.31199	-0.07828
C	4.45652	1.04704	-0.59317
C	3.78235	3.33745	-0.06592
C	5.06372	3.59207	0.44275
H	7.04993	2.78703	0.84240
H	6.49867	0.51736	-0.08551
H	4.20337	0.05918	-1.00731
H	3.00856	4.11839	-0.05217
H	5.29902	4.58967	0.84987
C	1.48412	-0.98188	-2.76280
C	1.99367	-1.48527	-4.09164
H	2.45667	-0.63497	-4.64107
H	1.16053	-1.88300	-4.70604
H	2.77343	-2.26010	-3.94378
C	1.60548	1.59425	1.93099
C	2.40460	1.43844	3.22658
H	2.07904	2.20528	3.95901
H	3.48122	1.61429	3.00312
H	2.30321	0.42156	3.65920
C	-0.65167	-3.19155	-1.03592
C	0.27061	-3.74114	-1.95800
H	1.34015	-3.49478	-1.87224
C	-0.15371	-4.62462	-2.96276
H	0.58669	-5.04674	-3.66288
C	-1.50948	-4.98013	-3.06825
H	-1.84247	-5.67899	-3.85359
C	-2.43201	-4.44615	-2.15538
H	-3.49724	-4.72486	-2.21528
C	-2.00827	-3.55948	-1.14892
H	-2.75426	-3.17617	-0.43902
C	-1.14902	-2.24259	1.69765
C	-2.50403	-1.84809	1.60441
H	-2.88283	-1.37194	0.68783
C	-3.38118	-2.02035	2.68706
H	-4.43418	-1.71092	2.58409
C	-2.91527	-2.56042	3.89734
H	-3.60223	-2.68989	4.75005
C	-1.56179	-2.91595	4.01704
H	-1.17737	-3.32395	4.96688
C	-0.68585	-2.76208	2.92791
H	0.36916	-3.05124	3.04287
C	1.50718	-2.94785	0.81809
C	1.42997	-4.35302	0.97023
H	0.49117	-4.88419	0.74328
C	2.54275	-5.08569	1.41195
H	2.46535	-6.18015	1.52388
C	3.74919	-4.42586	1.70763
H	4.62523	-5.00144	2.05100
C	3.82975	-3.03163	1.56474
H	4.77041	-2.50454	1.79573
C	2.71703	-2.29241	1.12318
H	2.77561	-1.19805	1.03274
C	-1.75831	1.92276	1.60738
C	-2.52804	3.08045	1.86431
H	-2.81431	3.75001	1.03807
C	-2.92897	3.39824	3.17328
H	-3.52606	4.30811	3.35290
C	-2.56534	2.56738	4.24612
H	-2.87590	2.81984	5.27390
C	-1.79491	1.41877	4.00026
H	-1.49315	0.76309	4.83347
C	-1.39395	1.09939	2.69232
H	-0.76669	0.21439	2.51816
C	-1.34724	3.12747	-0.98526
C	-0.53649	4.18677	-0.51322
H	0.11812	4.01073	0.35508
C	-0.56408	5.43561	-1.15462
H	0.06687	6.25526	-0.77139
C	-1.38130	5.64442	-2.28074
H	-1.39609	6.62620	-2.78327
C	-2.17821	4.59277	-2.76067
H	-2.82507	4.74253	-3.64135
C	-2.16505	3.34194	-2.11522
H	-2.80408	2.53283	-2.50055
C	-2.83331	0.68342	-0.78955
C	-4.09676	0.91694	-0.19951
H	-4.17536	1.53226	0.70982
C	-5.26076	0.36215	-0.75757
H	-6.23727	0.55390	-0.28167
C	-5.18370	-0.42931	-1.91736
H	-6.09901	-0.86087	-2.35643
C	-3.93255	-0.66657	-2.51026
H	-3.85725	-1.28887	-3.41729
C	-2.76304	-0.12062	-1.94981
H	-1.78847	-0.32439	-2.42018
O	0.29996	-0.49737	-2.66742
O	2.22448	-0.98061	-1.72353
O	1.21174	2.70521	1.55850
O	1.43320	0.46201	1.29259
P	0.00304	-1.99905	0.24943
P	-1.25771	1.46314	-0.13162
Ru	0.63250	0.21097	-0.62610

Vibrational Frequencies

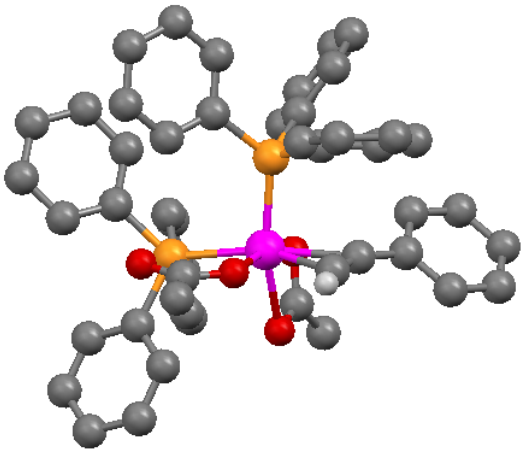
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.52	0.00767	YES	YES
8	a	15.44	0.08867	YES	YES
9	a	23.00	0.00216	YES	YES
10	a	26.83	0.03721	YES	YES
11	a	33.29	0.01007	YES	YES
12	a	35.04	0.03012	YES	YES
13	a	35.72	0.02800	YES	YES
14	a	42.19	0.46332	YES	YES
15	a	46.09	0.06535	YES	YES
16	a	51.85	0.11654	YES	YES
17	a	53.53	0.05109	YES	YES
18	a	56.96	0.56014	YES	YES
19	a	60.45	0.25298	YES	YES

20	a	61.94	0.21447	YES	YES
21	a	64.21	0.16377	YES	YES
22	a	64.43	0.00801	YES	YES
23	a	69.13	0.06624	YES	YES
24	a	71.48	0.42321	YES	YES
25	a	76.99	0.88720	YES	YES
26	a	80.51	0.14324	YES	YES
27	a	82.87	0.45184	YES	YES
28	a	87.20	1.52278	YES	YES
29	a	94.85	1.80303	YES	YES
30	a	95.82	0.36450	YES	YES
31	a	97.89	1.32584	YES	YES
32	a	100.10	1.12477	YES	YES
33	a	105.01	1.25443	YES	YES
34	a	115.16	4.30587	YES	YES
35	a	116.69	0.13244	YES	YES
36	a	124.07	1.59063	YES	YES
37	a	134.91	2.90329	YES	YES
38	a	141.95	1.47800	YES	YES
39	a	157.25	6.85768	YES	YES
40	a	176.21	1.31062	YES	YES
41	a	183.72	6.36905	YES	YES
42	a	196.82	0.61538	YES	YES
43	a	198.66	1.19209	YES	YES
44	a	203.13	4.41085	YES	YES
45	a	205.51	0.17809	YES	YES
46	a	209.92	2.65635	YES	YES
47	a	215.46	1.77775	YES	YES
48	a	223.42	1.72571	YES	YES
49	a	227.43	2.19079	YES	YES
50	a	234.71	2.73967	YES	YES
51	a	247.29	1.07313	YES	YES
52	a	249.31	0.39570	YES	YES
53	a	250.84	0.02106	YES	YES
54	a	254.05	1.36575	YES	YES
55	a	258.58	4.47018	YES	YES
56	a	263.70	0.31609	YES	YES
57	a	266.74	0.04378	YES	YES
58	a	278.76	0.96806	YES	YES
59	a	291.06	23.92291	YES	YES
60	a	316.24	14.05345	YES	YES
61	a	336.69	13.24441	YES	YES
62	a	393.97	6.57593	YES	YES
63	a	396.86	0.82148	YES	YES
64	a	398.46	0.30428	YES	YES
65	a	400.45	1.16166	YES	YES
66	a	401.19	0.22021	YES	YES
67	a	401.65	0.94093	YES	YES
68	a	406.25	0.38571	YES	YES
69	a	410.29	2.37025	YES	YES
70	a	412.20	13.39391	YES	YES
71	a	423.70	10.53122	YES	YES
72	a	425.46	20.72057	YES	YES
73	a	437.54	18.73485	YES	YES
74	a	446.59	12.79471	YES	YES
75	a	452.88	20.31554	YES	YES
76	a	467.09	7.47732	YES	YES
77	a	473.22	14.24032	YES	YES
78	a	482.12	21.76762	YES	YES
79	a	498.37	26.02883	YES	YES
80	a	501.81	3.37733	YES	YES
81	a	504.63	16.27129	YES	YES
82	a	508.85	28.36081	YES	YES
83	a	511.37	47.10206	YES	YES
84	a	518.20	139.74116	YES	YES
85	a	525.78	51.54377	YES	YES
86	a	532.26	17.00892	YES	YES
87	a	594.04	1.52045	YES	YES
88	a	595.66	7.16740	YES	YES
89	a	609.61	0.33063	YES	YES
90	a	609.65	0.33232	YES	YES
91	a	609.91	2.08726	YES	YES
92	a	610.41	0.55080	YES	YES
93	a	611.03	1.46106	YES	YES
94	a	612.39	0.61591	YES	YES
95	a	613.02	1.01935	YES	YES
96	a	661.83	59.81531	YES	YES
97	a	663.07	22.27557	YES	YES
98	a	669.62	5.29327	YES	YES
99	a	670.17	2.64205	YES	YES
100	a	672.32	21.04347	YES	YES
101	a	678.50	12.19210	YES	YES
102	a	680.24	5.54080	YES	YES
103	a	683.72	8.88089	YES	YES
104	a	684.51	13.49613	YES	YES
105	a	689.78	35.63933	YES	YES
106	a	695.62	30.15889	YES	YES
107	a	698.43	45.23690	YES	YES
108	a	700.64	13.70595	YES	YES
109	a	701.18	36.58446	YES	YES
110	a	701.93	44.67290	YES	YES
111	a	705.37	15.61271	YES	YES
112	a	737.19	7.61241	YES	YES
113	a	742.07	5.25312	YES	YES
114	a	744.80	5.74686	YES	YES
115	a	745.36	4.93685	YES	YES
116	a	746.86	7.89327	YES	YES
117	a	749.12	8.22637	YES	YES
118	a	750.62	5.58249	YES	YES
119	a	756.76	9.18553	YES	YES
120	a	797.16	4.28785	YES	YES
121	a	830.26	0.26608	YES	YES
122	a	833.28	0.59186	YES	YES
123	a	835.75	0.35413	YES	YES
124	a	838.41	0.88649	YES	YES
125	a	839.77	1.64993	YES	YES
126	a	844.88	1.06754	YES	YES
127	a	852.57	1.43316	YES	YES
128	a	907.31	0.58074	YES	YES
129	a	910.24	1.98346	YES	YES
130	a	911.06	0.60088	YES	YES
131	a	911.91	0.49398	YES	YES
132	a	913.93	1.55999	YES	YES
133	a	919.06	0.80659	YES	YES
134	a	922.86	2.88812	YES	YES
135	a	927.74	0.31544	YES	YES
136	a	942.85	19.68451	YES	YES
137	a	958.62	0.25983	YES	YES
138	a	959.19	0.43871	YES	YES
139	a	960.08	0.53823	YES	YES
140	a	961.76	0.75853	YES	YES
141	a	962.42	2.05432	YES	YES
142	a	969.74	0.67702	YES	YES
143	a	977.15	0.61271	YES	YES
144	a	978.97	0.10626	YES	YES
145	a	981.69	2.43564	YES	YES
146	a	981.83	0.25770	YES	YES
147	a	982.06	0.41284	YES	YES
148	a	982.45	0.43460	YES	YES
149	a	983.33	1.45414	YES	YES
150	a	983.42	1.43944	YES	YES
151	a	984.01	0.91725	YES	YES
152	a	984.09	2.84945	YES	YES
153	a	984.24	0.09546	YES	YES
154	a	985.41	1.64549	YES	YES
155	a	986.88	6.11716	YES	YES
156	a	986.98	0.66514	YES	YES
157	a	987.98	1.77393	YES	YES
158	a	995.83	3.14508	YES	YES
159	a	996.02	0.00499	YES	YES
160	a	1018.91	7.94457	YES	YES
161	a	1022.62	10.15870	YES	YES
162	a	1024.05	1.73219	YES	YES
163	a	1024.36	1.86591	YES	YES
164	a	1024.74	0.95604	YES	YES
165	a	1024.96	2.09052	YES	YES
166	a	1025.38	3.78730	YES	YES
167	a	1025.64	4.03100	YES	YES

168	a	1026.36	0.61350	YES	YES
169	a	1069.18	4.89447	YES	YES
170	a	1069.77	27.49486	YES	YES
171	a	1070.49	3.18516	YES	YES
172	a	1072.15	15.88453	YES	YES
173	a	1072.17	25.28266	YES	YES
174	a	1074.59	0.92711	YES	YES
175	a	1075.45	6.15760	YES	YES
176	a	1076.98	7.44718	YES	YES
177	a	1077.95	2.65624	YES	YES
178	a	1078.40	0.28834	YES	YES
179	a	1079.57	16.86475	YES	YES
180	a	1079.97	9.68604	YES	YES
181	a	1081.92	0.48823	YES	YES
182	a	1139.84	0.18133	YES	YES
183	a	1140.94	0.36918	YES	YES
184	a	1141.19	0.51041	YES	YES
185	a	1141.75	0.12476	YES	YES
186	a	1142.11	0.45588	YES	YES
187	a	1142.49	0.16508	YES	YES
188	a	1142.79	1.00019	YES	YES
189	a	1158.13	8.01253	YES	YES
190	a	1169.98	9.58896	YES	YES
191	a	1170.44	0.76128	YES	YES
192	a	1171.39	2.86260	YES	YES
193	a	1175.22	3.96566	YES	YES
194	a	1176.82	4.72554	YES	YES
195	a	1177.52	8.44451	YES	YES
196	a	1183.10	1.53261	YES	YES
197	a	1290.64	52.36099	YES	YES
198	a	1291.75	12.91628	YES	YES

* zero point VIBRATIONAL energy : 0.7453570 Hartree *

Cis 2_pfbx



bp86-SVP SCF energy: -2931.4220773590
pbe-TZVPP SCF energy: -2930.969477011

XYZ Coordinates
97

C	1.49398	-2.24595	-1.31256
C	0.82026	-1.76236	-2.26939
C	2.43571	-3.15147	-0.69900
H	0.34127	-1.70685	-3.24586
C	4.28628	-5.01801	0.36931
C	3.37798	-4.35512	1.21329
C	2.46402	-3.42725	0.69199
C	3.36296	-3.82483	-1.54269
C	4.27331	-4.74809	-1.01192
H	5.00554	-5.74247	0.78609
H	3.38136	-4.55891	2.29694
H	1.76605	-2.90113	1.35800
H	3.35492	-3.60836	-2.62292
H	4.98274	-5.26086	-1.68308
C	3.01681	0.00521	-0.11698
C	4.46623	-0.07661	0.28439
H	4.84910	-1.08745	0.01720
H	4.57654	0.05895	1.37867
H	5.06419	0.67927	-0.26336
C	-1.25971	1.35772	-2.81449
C	-1.83826	1.39652	-4.23125
H	-2.10371	2.43783	-4.50359
H	-2.76264	0.77703	-4.26423
H	-1.12535	0.97351	-4.96908
C	1.55142	2.40751	1.47199
C	2.87350	2.77385	1.12453
H	3.15217	2.88317	0.06576
C	3.84336	3.02214	2.11021
H	4.86215	3.31493	1.80498
C	3.51888	2.90936	3.47191
H	4.27716	3.11206	4.24661
C	2.21109	2.54942	3.83269
H	1.93048	2.47154	4.89666
C	1.24118	2.30219	2.84531
H	0.22181	2.05494	3.17161
C	-1.24874	2.77349	0.85653
C	-1.83379	2.08918	1.94528
H	-1.42465	1.12372	2.28079
C	-2.96871	2.60091	2.59710
H	-3.40242	2.04815	3.44632
C	-3.55869	3.79316	2.14978
H	-4.45121	4.19674	2.65641
C	-3.01835	4.45257	1.03201
H	-3.49252	5.37175	0.64784
C	-1.87738	3.94721	0.38742
H	-1.49196	4.45393	-0.50801
C	0.92958	3.41477	-1.07023
C	1.04967	4.74943	-0.62164
H	0.74114	5.02118	0.40075
C	1.57914	5.74182	-1.46355
H	1.65666	6.77995	-1.09949
C	2.01916	5.40987	-2.75637
H	2.44156	6.18716	-3.41501
C	1.92768	4.07958	-3.19868
H	2.28277	3.80438	-4.20574
C	1.38421	3.08855	-2.36362
H	1.32345	2.04869	-2.71570
C	-2.96851	-0.61804	0.44783
C	-3.85595	-1.23406	1.36022
H	-3.53034	-2.09457	1.96353
C	-5.16750	-0.75710	1.51673
H	-5.84184	-1.25190	2.23594
C	-5.61811	0.33888	0.76035
H	-6.65004	0.70958	0.88050
C	-4.73902	0.96370	-0.13692
H	-5.06609	1.83914	-0.72156
C	-3.42118	0.49542	-0.28741
H	-2.73826	1.04195	-0.95445
C	-1.79013	-2.81999	-0.90310
C	-2.85298	-2.68371	-1.82278
H	-3.42038	-1.74133	-1.87148
C	-3.20297	-3.74244	-2.67861
H	-4.03810	-3.61416	-3.38724
C	-2.50117	-4.95807	-2.62511
H	-2.77994	-5.79107	-3.29185
C	-1.43910	-5.10375	-1.71610
H	-0.87457	-6.04988	-1.66830
C	-1.07967	-4.04163	-0.87000
H	-0.23392	-4.17505	-0.17734
C	-0.87131	-2.08897	1.79186
C	-1.39859	-3.32455	2.23596
H	-2.04049	-3.92423	1.57189
C	-1.10753	-3.80724	3.52370
H	-1.52644	-4.77412	3.84924
C	-0.28962	-3.06366	4.39144
H	-0.06220	-3.44338	5.40153
C	0.24326	-1.83777	3.95900
H	0.89800	-1.24987	4.62331
C	-0.04123	-1.35638	2.66949
H	0.42309	-0.41861	2.32931
O	2.10121	-0.42588	0.68044
O	2.65697	0.42796	-1.26381
O	-1.50436	2.27684	-2.01134
O	-0.56078	0.29333	-2.56916
P	0.29994	2.08936	0.08073
P	-1.26852	-1.34680	0.12559
Ru	0.54868	-0.23248	-0.80184

Vibrational Frequencies

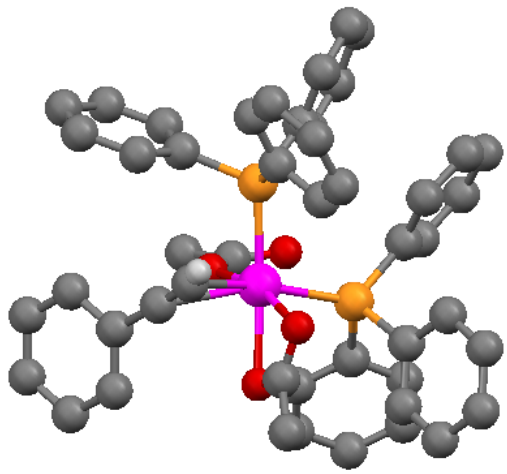
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.49	0.00544	YES	YES
8	a	20.34	0.03603	YES	YES
9	a	25.69	0.08321	YES	YES
10	a	28.45	0.02560	YES	YES
11	a	35.62	0.03005	YES	YES
12	a	41.33	0.05302	YES	YES
13	a	43.01	0.01249	YES	YES
14	a	48.34	0.30108	YES	YES
15	a	51.89	0.47390	YES	YES
16	a	54.06	0.37008	YES	YES
17	a	55.97	0.11279	YES	YES
18	a	59.21	0.11610	YES	YES
19	a	59.72	0.28433	YES	YES

20	a	64.82	0.17579	YES	YES
21	a	65.41	0.18930	YES	YES
22	a	73.00	0.47772	YES	YES
23	a	74.95	0.10518	YES	YES
24	a	79.59	0.49858	YES	YES
25	a	81.19	0.47423	YES	YES
26	a	86.92	1.13038	YES	YES
27	a	89.51	1.03360	YES	YES
28	a	92.67	0.57138	YES	YES
29	a	96.54	1.70662	YES	YES
30	a	108.69	2.02110	YES	YES
31	a	113.99	0.31410	YES	YES
32	a	118.01	0.21972	YES	YES
33	a	123.14	1.09913	YES	YES
34	a	128.72	0.41046	YES	YES
35	a	136.98	1.03296	YES	YES
36	a	137.78	1.16463	YES	YES
37	a	142.61	2.27295	YES	YES
38	a	148.26	2.10386	YES	YES
39	a	159.38	5.54828	YES	YES
40	a	164.67	6.36355	YES	YES
41	a	174.74	4.37542	YES	YES
42	a	186.49	5.07382	YES	YES
43	a	194.90	1.13959	YES	YES
44	a	201.64	0.09612	YES	YES
45	a	205.91	4.13425	YES	YES
46	a	209.73	3.01454	YES	YES
47	a	217.99	1.07649	YES	YES
48	a	222.44	0.86325	YES	YES
49	a	227.50	5.96889	YES	YES
50	a	230.75	2.43226	YES	YES
51	a	242.60	1.92667	YES	YES
52	a	247.70	0.24687	YES	YES
53	a	250.29	1.06051	YES	YES
54	a	256.44	1.45636	YES	YES
55	a	258.90	2.06608	YES	YES
56	a	263.96	0.82564	YES	YES
57	a	266.03	0.91930	YES	YES
58	a	270.55	0.39130	YES	YES
59	a	294.58	15.52861	YES	YES
60	a	327.58	11.18685	YES	YES
61	a	366.42	3.96728	YES	YES
62	a	390.99	31.56138	YES	YES
63	a	399.48	1.27452	YES	YES
64	a	400.22	0.13933	YES	YES
65	a	401.33	0.13776	YES	YES
66	a	404.65	0.46489	YES	YES
67	a	406.72	1.09226	YES	YES
68	a	414.94	3.66354	YES	YES
69	a	416.95	19.86908	YES	YES
70	a	419.13	4.52052	YES	YES
71	a	420.49	13.59432	YES	YES
72	a	428.24	20.50004	YES	YES
73	a	440.46	5.46838	YES	YES
74	a	451.88	30.63622	YES	YES
75	a	466.24	26.01112	YES	YES
76	a	473.83	0.43002	YES	YES
77	a	476.67	12.03936	YES	YES
78	a	482.29	9.80028	YES	YES
79	a	495.15	12.73891	YES	YES
80	a	501.63	13.40951	YES	YES
81	a	507.59	13.87966	YES	YES
82	a	512.92	63.77461	YES	YES
83	a	514.39	37.92442	YES	YES
84	a	518.89	114.93520	YES	YES
85	a	528.07	43.78200	YES	YES
86	a	536.75	2.79302	YES	YES
87	a	597.89	7.06595	YES	YES
88	a	599.25	3.62593	YES	YES
89	a	608.72	0.60657	YES	YES
90	a	609.36	1.00554	YES	YES
91	a	610.33	0.95518	YES	YES
92	a	610.56	0.08179	YES	YES
93	a	612.16	1.34437	YES	YES
94	a	612.49	1.49867	YES	YES
95	a	612.84	0.39795	YES	YES
96	a	656.75	11.32216	YES	YES
97	a	662.68	6.64585	YES	YES
98	a	670.64	25.48772	YES	YES
99	a	671.66	36.22689	YES	YES
100	a	675.23	8.82185	YES	YES
101	a	677.04	13.01310	YES	YES
102	a	682.31	13.69715	YES	YES
103	a	685.38	12.28946	YES	YES
104	a	689.78	12.80434	YES	YES
105	a	692.64	32.25614	YES	YES
106	a	697.47	36.80047	YES	YES
107	a	699.85	38.75803	YES	YES
108	a	700.97	60.73781	YES	YES
109	a	701.06	13.85365	YES	YES
110	a	708.21	5.07285	YES	YES
111	a	709.05	22.07726	YES	YES
112	a	735.24	9.00533	YES	YES
113	a	739.38	4.96663	YES	YES
114	a	741.80	1.72313	YES	YES
115	a	743.39	6.33153	YES	YES
116	a	746.44	7.86255	YES	YES
117	a	749.12	5.91519	YES	YES
118	a	755.58	17.13907	YES	YES
119	a	758.76	1.71471	YES	YES
120	a	775.96	1.28076	YES	YES
121	a	830.05	0.19270	YES	YES
122	a	832.17	0.41406	YES	YES
123	a	834.55	0.95334	YES	YES
124	a	838.02	0.05292	YES	YES
125	a	841.59	0.36405	YES	YES
126	a	842.39	0.46979	YES	YES
127	a	848.24	0.27134	YES	YES
128	a	903.30	0.53638	YES	YES
129	a	905.86	1.65132	YES	YES
130	a	908.77	1.15186	YES	YES
131	a	910.59	0.46233	YES	YES
132	a	917.65	0.13901	YES	YES
133	a	919.29	0.63724	YES	YES
134	a	922.45	0.04683	YES	YES
135	a	928.94	4.30927	YES	YES
136	a	944.11	15.44141	YES	YES
137	a	956.26	0.49869	YES	YES
138	a	956.72	0.05312	YES	YES
139	a	957.98	0.38527	YES	YES
140	a	960.71	0.10234	YES	YES
141	a	964.53	0.02053	YES	YES
142	a	967.69	0.08313	YES	YES
143	a	970.92	0.16810	YES	YES
144	a	978.68	0.11322	YES	YES
145	a	979.32	0.42769	YES	YES
146	a	980.27	0.96476	YES	YES
147	a	980.96	2.07735	YES	YES
148	a	981.93	0.69316	YES	YES
149	a	982.22	0.33342	YES	YES
150	a	982.93	0.83502	YES	YES
151	a	983.64	0.29543	YES	YES
152	a	983.85	1.03083	YES	YES
153	a	984.19	1.48930	YES	YES
154	a	984.99	0.92088	YES	YES
155	a	986.15	0.96673	YES	YES
156	a	988.07	3.35256	YES	YES
157	a	989.13	1.02180	YES	YES
158	a	994.52	2.28603	YES	YES
159	a	1002.42	0.21471	YES	YES
160	a	1023.03	4.25724	YES	YES
161	a	1023.26	6.03786	YES	YES
162	a	1023.81	1.26195	YES	YES
163	a	1023.94	5.85936	YES	YES
164	a	1024.36	1.35876	YES	YES
165	a	1024.69	7.53122	YES	YES
166	a	1025.75	1.05960	YES	YES
167	a	1025.81	3.67723	YES	YES

168	a	1026.63	1.43078	YES	YES
169	a	1062.82	15.37013	YES	YES
170	a	1066.70	16.20396	YES	YES
171	a	1071.31	2.18945	YES	YES
172	a	1072.42	6.76540	YES	YES
173	a	1073.81	5.46572	YES	YES
174	a	1074.33	15.72580	YES	YES
175	a	1075.17	0.37679	YES	YES
176	a	1077.35	12.37861	YES	YES
177	a	1077.97	4.69673	YES	YES
178	a	1079.35	9.49706	YES	YES
179	a	1080.42	11.71913	YES	YES
180	a	1081.02	2.86050	YES	YES
181	a	1082.94	1.06945	YES	YES
182	a	1139.96	0.07156	YES	YES
183	a	1140.52	0.17026	YES	YES
184	a	1141.29	0.00034	YES	YES
185	a	1141.48	0.57121	YES	YES
186	a	1141.98	0.14019	YES	YES
187	a	1142.14	0.37165	YES	YES
188	a	1142.54	0.95932	YES	YES
189	a	1160.61	1.04030	YES	YES
190	a	1166.48	6.33432	YES	YES
191	a	1169.02	1.87318	YES	YES
192	a	1171.31	2.79415	YES	YES
193	a	1172.47	1.25379	YES	YES
194	a	1175.62	2.26697	YES	YES
195	a	1178.50	1.29933	YES	YES
196	a	1186.42	0.52158	YES	YES
197	a	1288.86	0.51490	YES	YES
198	a	1290.29	4.74125	YES	YES

* zero point VIBRATIONAL energy : 0.7458877 Hartree *

Cis 2_pfby



bp86-SVP SCF energy: -2931.4251872430
pbe-TZVPP SCF energy: -2930.974348152

XYZ Coordinates
97

C	1.28981	-1.87073	-2.15442
C	2.00188	-1.76589	-1.12108
C	0.61589	-2.16110	-3.38281
H	2.90399	-1.98875	-0.54831
C	-0.67515	-2.77062	-5.82263
C	0.15795	-1.64062	-5.72818
C	0.79731	-1.33067	-4.52029
C	-0.23418	-3.29314	-3.48342
C	-0.86959	-3.59138	-4.69662
H	-1.17613	-3.01066	-6.77533
H	0.30919	-0.99134	-6.60673
H	1.43651	-0.43963	-4.42959
H	-0.38763	-3.92887	-2.59807
H	-1.52558	-4.47540	-4.76418
C	2.62438	1.11400	-1.56965
C	3.89617	1.67928	-2.14993
H	4.48831	0.84739	-2.59415
H	4.50534	2.15844	-1.35720
H	3.66754	2.40820	-2.95318
C	-2.38861	-0.35353	-1.32497
C	-3.46215	-1.06285	-2.15201
H	-4.31789	-0.37863	-2.32295
H	-3.83244	-1.94815	-1.58733
H	-3.05258	-1.42831	-3.11613
C	1.14777	3.19605	0.37580
C	1.66837	3.91413	-0.72750
H	1.22307	3.78611	-1.72535
C	2.74214	4.80782	-0.57433
H	3.11565	5.35993	-1.45323
C	3.32830	5.00628	0.68620
H	4.16501	5.71380	0.80957
C	2.82743	4.29678	1.78921
H	3.26787	4.44290	2.78983
C	1.75420	3.40208	1.63401
H	1.38215	2.88255	2.52705
C	-1.32010	2.26563	1.59102
C	-0.81753	1.89890	2.85973
H	0.13839	1.35919	2.94312
C	-1.54158	2.17355	4.03143
H	-1.12339	1.88432	5.00919
C	-2.80218	2.78630	3.95151
H	-3.37392	3.00274	4.86931
C	-3.34295	3.09009	2.69063
H	-4.34952	3.53429	2.61222
C	-2.61289	2.82762	1.51933
H	-3.06415	3.03989	0.53995
C	-1.11126	2.93622	-1.28583
C	-1.50041	4.27832	-1.07404
H	-1.34307	4.75310	-0.09196
C	-2.07485	5.02912	-2.11311
H	-2.37932	6.07281	-1.92665
C	-2.24983	4.45605	-3.38433
H	-2.69691	5.04625	-4.20184
C	-1.84285	3.13036	-3.60813
H	-1.96510	2.67335	-4.60424
C	-1.27896	2.37402	-2.56666
H	-0.95827	1.33893	-2.75337
C	-1.10154	-1.31567	2.53461
C	-0.87873	-1.73837	3.86492
H	0.10385	-2.12702	4.17196
C	-1.90711	-1.66988	4.82039
H	-1.71099	-2.00653	5.85251
C	-3.17531	-1.18243	4.46357
H	-3.98357	-1.13555	5.21267
C	-3.39762	-0.73914	3.15016
H	-4.37830	-0.32869	2.85901
C	-2.36833	-0.79295	2.19445
H	-2.55235	-0.38486	1.18734
C	-0.27492	-3.29130	0.65611
C	-1.63779	-3.64051	0.53263
H	-2.41902	-2.92327	0.82655
C	-2.02022	-4.90493	0.05356
H	-3.09190	-5.15196	-0.02825
C	-1.04723	-5.85145	-0.30772
H	-1.34702	-6.84733	-0.67441
C	0.31257	-5.51733	-0.19263
H	1.08968	-6.24857	-0.47153
C	0.69420	-4.24848	0.27556
H	1.76597	-4.01459	0.35206
C	1.72823	-1.81547	2.23181
C	2.02422	-3.02466	2.90363
H	1.35354	-3.89266	2.80309
C	3.16851	-3.13229	3.71255
H	3.38505	-4.08428	4.22567
C	4.03006	-2.03303	3.87013
H	4.92882	-2.11949	4.50359
C	3.74008	-0.82540	3.21385
H	4.41059	0.04267	3.32637
C	2.60033	-0.71728	2.39836
H	2.40199	0.22328	1.86213
O	2.60006	0.66993	-0.36648
O	1.56140	1.00276	-2.27117
O	-2.69284	0.58855	-0.56892
O	-1.19800	-0.85091	-1.48226
P	-0.27692	1.97734	0.07802
P	0.19525	-1.55797	1.20031
Ru	0.60046	-0.16657	-0.62489

Vibrational Frequencies

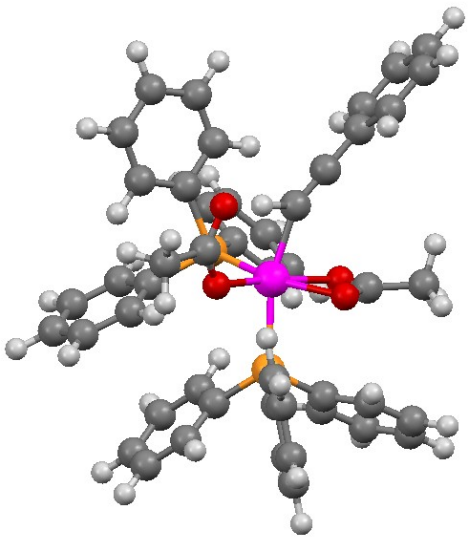
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.68	0.04920	YES	YES
8	a	18.63	0.01841	YES	YES
9	a	26.79	0.04478	YES	YES
10	a	27.37	0.04097	YES	YES
11	a	32.50	0.04084	YES	YES
12	a	35.14	0.00188	YES	YES
13	a	40.60	0.31784	YES	YES
14	a	42.44	0.10517	YES	YES
15	a	46.30	0.17145	YES	YES
16	a	50.56	0.26567	YES	YES
17	a	52.09	0.40392	YES	YES

18	a	55.88	0.14668	YES	YES
19	a	59.48	0.38325	YES	YES
20	a	59.94	0.48094	YES	YES
21	a	61.25	0.03946	YES	YES
22	a	64.60	0.24586	YES	YES
23	a	69.23	0.48428	YES	YES
24	a	71.74	0.24541	YES	YES
25	a	80.04	1.12759	YES	YES
26	a	83.16	0.19677	YES	YES
27	a	89.68	1.61364	YES	YES
28	a	91.91	0.76095	YES	YES
29	a	98.10	0.61209	YES	YES
30	a	100.03	0.58379	YES	YES
31	a	103.20	1.45424	YES	YES
32	a	109.51	0.50481	YES	YES
33	a	113.37	0.90344	YES	YES
34	a	118.56	4.74623	YES	YES
35	a	131.47	0.66836	YES	YES
36	a	135.56	0.40721	YES	YES
37	a	142.15	3.78813	YES	YES
38	a	152.31	5.13392	YES	YES
39	a	158.69	8.40470	YES	YES
40	a	171.85	2.67111	YES	YES
41	a	181.87	2.96928	YES	YES
42	a	188.31	4.86910	YES	YES
43	a	197.67	1.28489	YES	YES
44	a	202.27	1.50452	YES	YES
45	a	206.80	1.56202	YES	YES
46	a	211.68	6.39311	YES	YES
47	a	213.84	0.07680	YES	YES
48	a	219.13	1.48890	YES	YES
49	a	226.09	7.09086	YES	YES
50	a	236.45	0.94387	YES	YES
51	a	246.77	0.10309	YES	YES
52	a	251.36	1.07535	YES	YES
53	a	256.21	1.05477	YES	YES
54	a	259.30	2.83795	YES	YES
55	a	261.41	0.50782	YES	YES
56	a	264.26	0.29954	YES	YES
57	a	269.32	0.75133	YES	YES
58	a	275.82	1.66981	YES	YES
59	a	300.21	15.81130	YES	YES
60	a	315.17	10.06259	YES	YES
61	a	325.46	13.18199	YES	YES
62	a	386.57	32.33217	YES	YES
63	a	396.46	0.45379	YES	YES
64	a	398.16	3.50108	YES	YES
65	a	399.49	0.60031	YES	YES
66	a	404.16	1.37957	YES	YES
67	a	404.88	0.53634	YES	YES
68	a	408.01	8.63652	YES	YES
69	a	413.74	1.65515	YES	YES
70	a	416.93	5.12047	YES	YES
71	a	419.44	8.01105	YES	YES
72	a	428.71	31.79429	YES	YES
73	a	433.96	3.99903	YES	YES
74	a	455.04	24.29689	YES	YES
75	a	463.75	4.61329	YES	YES
76	a	467.25	53.17508	YES	YES
77	a	471.86	3.29357	YES	YES
78	a	478.54	11.74934	YES	YES
79	a	492.15	26.73642	YES	YES
80	a	504.35	11.99336	YES	YES
81	a	508.73	18.45219	YES	YES
82	a	513.26	61.52880	YES	YES
83	a	514.66	2.70289	YES	YES
84	a	518.49	137.36904	YES	YES
85	a	525.60	56.56099	YES	YES
86	a	530.22	9.46570	YES	YES
87	a	592.96	8.07874	YES	YES
88	a	597.13	3.33580	YES	YES
89	a	608.52	0.25072	YES	YES
90	a	609.25	0.59740	YES	YES
91	a	610.04	1.21022	YES	YES
92	a	610.35	0.74092	YES	YES
93	a	612.19	0.86682	YES	YES
94	a	613.11	0.15992	YES	YES
95	a	613.31	0.64068	YES	YES
96	a	662.80	2.80163	YES	YES
97	a	663.36	9.59154	YES	YES
98	a	665.65	66.12574	YES	YES
99	a	669.20	14.92046	YES	YES
100	a	675.39	6.06717	YES	YES
101	a	676.23	17.53691	YES	YES
102	a	683.69	11.77427	YES	YES
103	a	687.57	29.99685	YES	YES
104	a	689.84	13.10152	YES	YES
105	a	690.11	22.00788	YES	YES
106	a	693.89	31.07624	YES	YES
107	a	698.69	33.60335	YES	YES
108	a	700.30	58.65093	YES	YES
109	a	704.19	23.41826	YES	YES
110	a	707.98	4.50646	YES	YES
111	a	708.09	24.72691	YES	YES
112	a	732.74	7.78158	YES	YES
113	a	737.35	6.05143	YES	YES
114	a	739.09	3.03867	YES	YES
115	a	742.88	3.38572	YES	YES
116	a	744.76	10.36114	YES	YES
117	a	746.08	3.86181	YES	YES
118	a	749.00	6.91583	YES	YES
119	a	756.93	16.41980	YES	YES
120	a	780.16	5.43631	YES	YES
121	a	827.31	0.41736	YES	YES
122	a	832.66	0.40476	YES	YES
123	a	833.01	2.06844	YES	YES
124	a	836.89	0.64972	YES	YES
125	a	844.36	0.38720	YES	YES
126	a	844.83	0.28751	YES	YES
127	a	849.04	0.83432	YES	YES
128	a	900.26	0.24782	YES	YES
129	a	909.18	1.17996	YES	YES
130	a	909.74	0.80069	YES	YES
131	a	913.58	0.84350	YES	YES
132	a	919.40	1.17579	YES	YES
133	a	921.12	0.21514	YES	YES
134	a	925.36	0.34517	YES	YES
135	a	926.56	1.49274	YES	YES
136	a	943.69	18.86560	YES	YES
137	a	953.97	0.34362	YES	YES
138	a	955.95	0.84256	YES	YES
139	a	959.10	0.68685	YES	YES
140	a	960.22	0.54449	YES	YES
141	a	966.99	0.14009	YES	YES
142	a	967.78	0.03763	YES	YES
143	a	972.14	0.25712	YES	YES
144	a	977.20	0.38423	YES	YES
145	a	979.29	0.07525	YES	YES
146	a	979.35	0.10309	YES	YES
147	a	980.04	0.49092	YES	YES
148	a	980.35	0.19978	YES	YES
149	a	981.15	2.67311	YES	YES
150	a	982.70	1.13575	YES	YES
151	a	983.27	1.22078	YES	YES
152	a	983.32	1.75450	YES	YES
153	a	984.02	0.82340	YES	YES
154	a	984.18	1.05933	YES	YES
155	a	986.17	1.63163	YES	YES
156	a	988.05	0.35930	YES	YES
157	a	988.57	0.94094	YES	YES
158	a	992.86	2.99247	YES	YES
159	a	998.55	0.04019	YES	YES
160	a	1021.27	5.83575	YES	YES
161	a	1022.32	11.06528	YES	YES
162	a	1023.67	1.62886	YES	YES
163	a	1023.75	1.10632	YES	YES
164	a	1024.20	2.17744	YES	YES
165	a	1024.43	1.13165	YES	YES

166	a	1024.98	4.21299	YES	YES
167	a	1026.58	0.19945	YES	YES
168	a	1026.97	0.70780	YES	YES
169	a	1063.19	13.10729	YES	YES
170	a	1067.09	15.60524	YES	YES
171	a	1071.25	4.35630	YES	YES
172	a	1072.08	10.84793	YES	YES
173	a	1072.52	12.87861	YES	YES
174	a	1072.98	0.65130	YES	YES
175	a	1075.01	0.98419	YES	YES
176	a	1077.45	0.40391	YES	YES
177	a	1078.39	16.62504	YES	YES
178	a	1078.73	19.44756	YES	YES
179	a	1081.54	2.15416	YES	YES
180	a	1082.10	9.92288	YES	YES
181	a	1084.51	0.96700	YES	YES
182	a	1140.14	0.07741	YES	YES
183	a	1140.50	0.31319	YES	YES
184	a	1141.27	0.31642	YES	YES
185	a	1141.66	0.43586	YES	YES
186	a	1142.02	0.36821	YES	YES
187	a	1142.33	0.76961	YES	YES
188	a	1142.75	0.35881	YES	YES
189	a	1158.73	2.77052	YES	YES
190	a	1166.98	3.04311	YES	YES
191	a	1168.03	3.42139	YES	YES
192	a	1171.33	5.30179	YES	YES
193	a	1173.16	2.39230	YES	YES
194	a	1178.33	2.61644	YES	YES
195	a	1180.81	2.67952	YES	YES
196	a	1189.47	2.05549	YES	YES
197	a	1287.51	1.72339	YES	YES
198	a	1288.97	3.21004	YES	YES

* zero point VIBRATIONAL energy : 0.7453777 Hartree *

Cis TS_{34}_pf



bp86-SVP SCF energy: -2931.4234792150
pbe-TZVPP SCF energy: -2930.966886426

XYZ Coordinates
97

C	2.14645	-2.56747	-1.61679
C	1.31539	-1.62558	-1.56831
C	3.07400	-3.64382	-1.64175
H	0.56439	-1.29258	-2.60531
C	4.93751	-5.78760	-1.66816
C	3.97653	-5.69832	-0.64426
C	3.05088	-4.64754	-0.63042
C	4.05979	-3.74370	-2.66557
C	4.97104	-4.80722	-2.67740
H	5.66155	-6.61919	-1.67783
H	3.94769	-6.45896	0.15403
H	2.30555	-4.57371	0.17761
H	4.08870	-2.97359	-3.45277
H	5.72268	-4.87101	-3.48212
C	3.01875	0.31381	-0.18547
C	4.50103	0.22824	0.07460
H	4.88009	-0.72912	-0.34814
H	4.70526	0.23019	1.16450
H	5.03396	1.06355	-0.42286
C	-0.86528	0.18929	-3.43239
C	-1.81777	0.85318	-4.41694
H	-2.84088	0.44213	-4.26200
H	-1.51329	0.62370	-5.45824
H	-1.85842	1.94933	-4.25378
C	1.54187	2.60494	1.66768
C	2.82979	3.02795	1.26388
H	3.04545	3.18251	0.19572
C	3.83861	3.26711	2.21146
H	4.83249	3.60331	1.87141
C	3.58392	3.08807	3.58142
H	4.37459	3.28099	4.32545
C	2.30836	2.67062	3.99339
H	2.08761	2.53750	5.06578
C	1.29746	2.43093	3.04606
H	0.30254	2.12936	3.40456
C	-1.32359	2.78241	1.18034
C	-1.84349	1.98133	2.22296
H	-1.34737	1.03585	2.49535
C	-3.00745	2.35794	2.91047
H	-3.38610	1.72106	3.72649
C	-3.69671	3.52585	2.54492
H	-4.61476	3.81970	3.08046
C	-3.21891	4.30338	1.47838
H	-3.76351	5.21032	1.16579
C	-2.04282	3.93705	0.80155
H	-1.68872	4.56185	-0.03219
C	0.61714	3.69636	-0.78940
C	0.79355	4.99780	-0.26031
H	0.70967	5.16918	0.82550
C	1.08616	6.07914	-1.10567
H	1.21946	7.08657	-0.67702
C	1.21776	5.87599	-2.49165
H	1.45431	6.72457	-3.15532
C	1.05604	4.58670	-3.02231
H	1.17013	4.41545	-4.10573
C	0.75709	3.50172	-2.17758
H	0.63265	2.49246	-2.59244
C	-2.89950	-0.40526	0.39046
C	-3.82113	-0.91189	1.33209
H	-3.53182	-1.72959	2.00998
C	-5.11673	-0.37656	1.42337
H	-5.82316	-0.78466	2.16594
C	-5.51203	0.67068	0.57397
H	-6.53014	1.08883	0.64503
C	-4.59882	1.18583	-0.36060
H	-4.89477	2.01443	-1.02524
C	-3.29963	0.65654	-0.45000
H	-2.58196	1.06498	-1.18033
C	-1.70242	-2.61225	-0.93982
C	-2.80109	-2.52560	-1.82183
H	-3.42147	-1.61626	-1.84178
C	-3.12524	-3.59651	-2.67251
H	-3.98766	-3.50716	-3.35392
C	-2.36004	-4.77354	-2.65182
H	-2.61538	-5.61443	-3.31801
C	-1.26516	-4.87177	-1.77589
H	-0.65394	-5.78918	-1.75220
C	-0.93560	-3.79929	-0.93204
H	-0.07236	-3.88977	-0.25617
C	-0.84598	-1.97995	1.76602
C	-1.49196	-3.16809	2.18219
H	-2.20774	-3.67257	1.51337
C	-1.21726	-3.72752	3.44145
H	-1.72923	-4.65476	3.74953
C	-0.29073	-3.11306	4.30195
H	-0.07296	-3.55565	5.28846
C	0.36686	-1.94216	3.89096
H	1.11224	-1.46380	4.54771
C	0.09558	-1.38092	2.63065
H	0.65194	-0.49125	2.29666
O	2.18765	-0.26375	0.60384
O	2.55396	0.91014	-1.21749
O	-0.29861	-0.88258	-3.77531
O	-0.73482	0.77399	-2.29097
P	0.25722	2.25782	0.34318
P	-1.20529	-1.16053	0.13131
Ru	0.53038	0.09711	-0.72184

Vibrational Frequencies

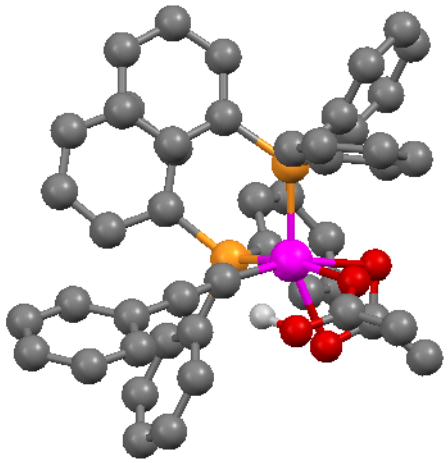
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-438.33	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	9.37	0.03540	YES	YES
9	a	16.17	0.06235	YES	YES
10	a	20.32	0.00601	YES	YES
11	a	21.44	0.05826	YES	YES
12	a	28.16	0.06739	YES	YES

13	a	36.97	0.02753	YES	YES
14	a	38.31	0.19757	YES	YES
15	a	39.29	0.19520	YES	YES
16	a	42.23	0.05632	YES	YES
17	a	45.64	0.11955	YES	YES
18	a	51.88	0.15004	YES	YES
19	a	52.37	0.32369	YES	YES
20	a	54.70	0.05130	YES	YES
21	a	60.16	0.17013	YES	YES
22	a	62.56	0.24252	YES	YES
23	a	65.86	0.12111	YES	YES
24	a	66.37	0.40784	YES	YES
25	a	71.22	0.20569	YES	YES
26	a	72.68	0.15607	YES	YES
27	a	79.26	0.50848	YES	YES
28	a	83.87	1.93167	YES	YES
29	a	93.25	1.29816	YES	YES
30	a	94.85	0.53207	YES	YES
31	a	99.53	0.95345	YES	YES
32	a	100.32	2.47441	YES	YES
33	a	106.44	0.47730	YES	YES
34	a	108.80	0.60388	YES	YES
35	a	111.36	0.74602	YES	YES
36	a	114.34	2.64667	YES	YES
37	a	120.16	0.59503	YES	YES
38	a	135.93	3.36588	YES	YES
39	a	160.06	28.23912	YES	YES
40	a	164.11	0.53465	YES	YES
41	a	182.57	2.43028	YES	YES
42	a	188.18	0.37042	YES	YES
43	a	197.61	1.01485	YES	YES
44	a	203.43	0.60544	YES	YES
45	a	206.56	1.67160	YES	YES
46	a	210.13	1.47129	YES	YES
47	a	211.64	0.92012	YES	YES
48	a	222.19	1.54032	YES	YES
49	a	228.85	0.04475	YES	YES
50	a	238.50	10.99548	YES	YES
51	a	245.18	1.82990	YES	YES
52	a	249.47	0.64067	YES	YES
53	a	251.08	0.31657	YES	YES
54	a	256.64	1.77293	YES	YES
55	a	258.32	18.53612	YES	YES
56	a	265.84	0.18151	YES	YES
57	a	267.63	0.25121	YES	YES
58	a	280.02	10.75522	YES	YES
59	a	304.76	15.14717	YES	YES
60	a	330.74	13.62235	YES	YES
61	a	334.34	33.95948	YES	YES
62	a	392.98	52.61515	YES	YES
63	a	397.10	1.27792	YES	YES
64	a	398.52	0.43785	YES	YES
65	a	399.21	1.44156	YES	YES
66	a	401.34	2.33467	YES	YES
67	a	402.43	6.47476	YES	YES
68	a	407.16	46.14235	YES	YES
69	a	411.61	1.14122	YES	YES
70	a	412.64	0.50997	YES	YES
71	a	417.74	11.04282	YES	YES
72	a	422.77	40.22045	YES	YES
73	a	434.44	24.04814	YES	YES
74	a	448.89	22.23472	YES	YES
75	a	456.18	36.64077	YES	YES
76	a	459.09	49.44679	YES	YES
77	a	477.06	11.55928	YES	YES
78	a	480.68	10.17107	YES	YES
79	a	496.53	23.75332	YES	YES
80	a	505.39	27.88246	YES	YES
81	a	506.70	14.17396	YES	YES
82	a	512.91	74.59734	YES	YES
83	a	513.78	49.75672	YES	YES
84	a	517.97	114.19604	YES	YES
85	a	527.98	74.52411	YES	YES
86	a	556.85	2.01489	YES	YES
87	a	592.65	18.35197	YES	YES
88	a	597.47	11.94221	YES	YES
89	a	608.12	0.54753	YES	YES
90	a	608.92	0.27230	YES	YES
91	a	610.39	2.39721	YES	YES
92	a	610.64	1.22865	YES	YES
93	a	611.34	2.86862	YES	YES
94	a	611.81	0.58121	YES	YES
95	a	612.54	1.25119	YES	YES
96	a	625.43	217.70480	YES	YES
97	a	668.81	19.54088	YES	YES
98	a	669.42	30.70761	YES	YES
99	a	672.58	20.14815	YES	YES
100	a	677.55	5.14193	YES	YES
101	a	678.39	18.63844	YES	YES
102	a	685.48	13.85714	YES	YES
103	a	686.78	11.03827	YES	YES
104	a	688.78	28.52101	YES	YES
105	a	694.85	38.07916	YES	YES
106	a	695.57	16.59807	YES	YES
107	a	696.75	30.99702	YES	YES
108	a	700.39	37.85511	YES	YES
109	a	704.26	107.75023	YES	YES
110	a	705.18	26.34833	YES	YES
111	a	707.10	36.76394	YES	YES
112	a	735.01	15.89215	YES	YES
113	a	738.26	4.33266	YES	YES
114	a	741.19	1.48369	YES	YES
115	a	743.92	2.63905	YES	YES
116	a	746.64	7.20307	YES	YES
117	a	748.20	7.89349	YES	YES
118	a	759.00	25.47632	YES	YES
119	a	798.93	135.37398	YES	YES
120	a	826.36	0.16955	YES	YES
121	a	830.07	1.07285	YES	YES
122	a	832.10	0.17371	YES	YES
123	a	835.73	2.20095	YES	YES
124	a	840.49	1.33278	YES	YES
125	a	843.28	1.18124	YES	YES
126	a	846.25	1.69898	YES	YES
127	a	901.42	2.68868	YES	YES
128	a	901.63	0.30639	YES	YES
129	a	907.24	0.34214	YES	YES
130	a	911.89	3.05872	YES	YES
131	a	915.68	0.89499	YES	YES
132	a	916.38	0.80656	YES	YES
133	a	922.41	2.31351	YES	YES
134	a	923.36	15.66183	YES	YES
135	a	942.48	16.73464	YES	YES
136	a	954.22	0.14631	YES	YES
137	a	954.91	0.29590	YES	YES
138	a	956.11	0.13224	YES	YES
139	a	960.96	0.99453	YES	YES
140	a	963.34	0.32354	YES	YES
141	a	964.93	0.13152	YES	YES
142	a	971.07	0.47137	YES	YES
143	a	976.77	0.15463	YES	YES
144	a	977.95	0.23232	YES	YES
145	a	978.34	3.34431	YES	YES
146	a	980.33	0.11048	YES	YES
147	a	980.90	0.62077	YES	YES
148	a	981.76	0.23474	YES	YES
149	a	982.00	0.77418	YES	YES
150	a	982.22	1.38015	YES	YES
151	a	982.97	2.31187	YES	YES
152	a	984.51	1.81747	YES	YES
153	a	984.94	1.92080	YES	YES
154	a	985.28	1.86911	YES	YES
155	a	985.48	0.54770	YES	YES
156	a	988.96	1.15378	YES	YES
157	a	991.27	1.18107	YES	YES
158	a	997.37	6.39358	YES	YES
159	a	1021.80	1.82949	YES	YES
160	a	1022.21	11.16484	YES	YES

161	a	1023.53	2.11950	YES	YES
162	a	1023.58	4.69841	YES	YES
163	a	1023.65	1.62427	YES	YES
164	a	1024.52	0.61782	YES	YES
165	a	1025.12	0.31281	YES	YES
166	a	1025.85	1.08319	YES	YES
167	a	1026.79	1.20909	YES	YES
168	a	1030.69	58.25780	YES	YES
169	a	1067.74	12.47796	YES	YES
170	a	1069.83	2.50642	YES	YES
171	a	1070.20	16.86010	YES	YES
172	a	1071.16	4.49915	YES	YES
173	a	1071.57	23.19279	YES	YES
174	a	1073.66	28.04851	YES	YES
175	a	1074.98	13.13828	YES	YES
176	a	1075.48	1.78913	YES	YES
177	a	1076.13	0.69080	YES	YES
178	a	1078.48	6.72011	YES	YES
179	a	1080.27	19.76185	YES	YES
180	a	1080.68	14.77478	YES	YES
181	a	1082.06	0.71831	YES	YES
182	a	1122.67	508.92522	YES	YES
183	a	1140.49	0.13417	YES	YES
184	a	1141.02	0.14983	YES	YES
185	a	1141.52	0.39070	YES	YES
186	a	1141.72	0.22531	YES	YES
187	a	1141.98	0.20218	YES	YES
188	a	1142.39	0.10659	YES	YES
189	a	1142.67	1.19447	YES	YES
190	a	1158.39	15.78506	YES	YES
191	a	1166.35	9.27574	YES	YES
192	a	1166.62	2.08794	YES	YES
193	a	1169.57	2.48061	YES	YES
194	a	1170.76	3.16965	YES	YES
195	a	1175.95	1.71151	YES	YES
196	a	1177.18	6.77282	YES	YES
197	a	1217.44	41.06883	YES	YES
198	a	1285.14	0.43582	YES	YES

* zero point VIBRATIONAL energy : 0.7406829 Hartree *

Cis 4_*af*



bp86-SVP SCF energy: -2931.4573997760
pbe-TZVPP SCF energy: -2931.015578524

XYZ Coordinates
97

C	0.38594	-2.70995	1.03681
C	0.57195	-1.53450	0.63271
C	0.09468	-4.04290	1.46117
H	1.99269	-1.76556	1.77192
C	-0.51476	-6.70012	2.29589
C	-1.34968	-6.03273	1.38067
C	-1.05380	-4.72686	0.96726
C	0.92860	-4.73464	2.38632
C	0.62455	-6.04081	2.79306
H	-0.75014	-7.72783	2.61862
H	-2.24532	-6.53844	0.98109
H	-1.70916	-4.20864	0.24888
H	1.82341	-4.22827	2.78289
H	1.28851	-6.55341	3.50983
C	3.11839	1.18786	-1.24323
C	4.42481	1.73238	-1.77707
H	5.09644	1.96893	-0.92168
H	4.24909	2.67422	-2.33723
H	4.93148	0.98440	-2.42045
C	3.19557	-0.31132	2.23275
C	4.37602	0.08694	3.08441
H	5.05161	-0.77619	3.25089
H	3.99522	0.42959	4.07288
H	4.91941	0.92931	2.61335
C	-0.08817	1.08640	-3.26899
C	1.18363	1.31946	-3.84448
H	2.04546	0.71865	-3.51426
C	1.35095	2.27254	-4.85981
H	2.35044	2.43174	-5.29768
C	0.24986	3.01468	-5.32352
H	0.38082	3.76352	-6.12229
C	-1.01929	2.78183	-4.77128
H	-1.89594	3.34069	-5.13959
C	-1.18890	1.82333	-3.75424
H	-2.20014	1.64126	-3.36100
C	-1.97176	-0.61358	-1.78515
C	-2.89808	0.38147	-1.39879
H	-2.55096	1.39579	-1.14455
C	-4.27091	0.09520	-1.32374
H	-4.97666	0.88996	-1.03238
C	-4.73802	-1.20092	-1.59839
H	-5.81532	-1.42713	-1.53398
C	-3.82199	-2.20873	-1.94116
H	-4.17498	-3.23370	-2.14357
C	-2.44996	-1.91824	-2.03812
H	-1.74618	-2.71586	-2.31880
C	0.49611	-1.65468	-2.89042
C	0.03447	-1.85585	-4.21297
H	-0.69974	-1.16153	-4.65398
C	0.50146	-2.93656	-4.97625
H	0.12852	-3.08088	-6.00418
C	1.44379	-3.82809	-4.43214
H	1.81457	-4.67622	-5.03212
C	1.91075	-3.63076	-3.12336
H	2.65074	-4.32262	-2.68821
C	1.44121	-2.55061	-2.35381
H	1.80775	-2.40654	-1.32815
C	-2.20906	0.70511	1.69423
C	-3.29049	1.58418	1.92585
H	-3.15463	2.67218	1.83078
C	-4.55681	1.08280	2.27160
H	-5.38875	1.78530	2.44853
C	-4.76284	-0.30180	2.39331
H	-5.75653	-0.69308	2.66887
C	-3.69580	-1.18311	2.15335
H	-3.84436	-2.27250	2.23434
C	-2.42978	-0.68614	1.79974
H	-1.60278	-1.38439	1.59416
C	0.19391	1.46743	3.07631
C	-0.24408	0.63093	4.12416
H	-1.03872	-0.11001	3.94520
C	0.31777	0.74066	5.40923
H	-0.04186	0.08194	6.21716
C	1.32067	1.69012	5.66533
H	1.75041	1.78487	6.67670
C	1.77000	2.52247	4.62337
H	2.55675	3.27207	4.81289
C	1.21901	2.40653	3.33693
H	1.58532	3.05748	2.52728
C	-0.73494	3.10622	0.89650
C	-1.11310	4.07005	1.86211
H	-1.23550	3.77786	2.91752
C	-1.32328	5.40849	1.49132
H	-1.61666	6.14665	2.25668
C	-1.15453	5.80664	0.15285
H	-1.31589	6.85880	-0.13571
C	-0.76526	4.86074	-0.80886
H	-0.61091	5.16230	-1.85761
C	-0.55167	3.52095	-0.43896
H	-0.20869	2.79641	-1.19227
O	2.20085	1.97462	-0.83818
O	2.93008	-0.08087	-1.16937
O	2.84181	-1.57118	2.34235
O	2.61191	0.53163	1.52199
P	-0.16303	-0.20545	-1.90934
P	-0.47812	1.31256	1.33819
Ru	1.06317	0.24778	-0.01594

Vibrational Frequencies

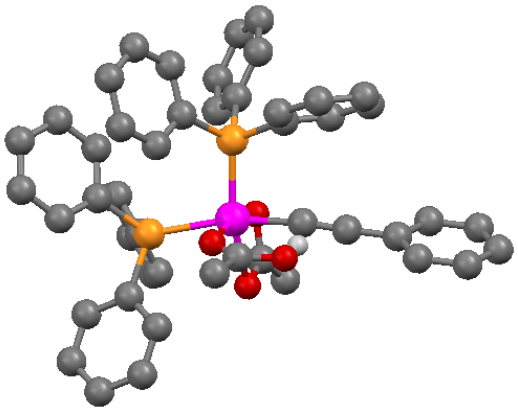
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.35	0.01995	YES	YES
8	a	13.53	0.07949	YES	YES
9	a	17.47	0.02491	YES	YES
10	a	22.11	0.01654	YES	YES
11	a	23.30	0.06095	YES	YES
12	a	25.48	0.14157	YES	YES
13	a	33.43	0.22430	YES	YES
14	a	37.17	0.02641	YES	YES
15	a	39.04	0.02135	YES	YES
16	a	45.10	0.09554	YES	YES
17	a	46.77	0.07634	YES	YES
18	a	48.58	0.13188	YES	YES

19	a	51.34	0.91253	YES	YES
20	a	54.51	0.21073	YES	YES
21	a	56.07	0.15802	YES	YES
22	a	56.61	0.11924	YES	YES
23	a	61.87	0.14501	YES	YES
24	a	63.25	0.22548	YES	YES
25	a	65.47	0.12173	YES	YES
26	a	68.50	0.38543	YES	YES
27	a	73.36	0.69344	YES	YES
28	a	80.62	0.21266	YES	YES
29	a	82.53	0.40414	YES	YES
30	a	87.24	0.99456	YES	YES
31	a	90.08	0.95379	YES	YES
32	a	94.35	0.71284	YES	YES
33	a	99.08	0.75381	YES	YES
34	a	105.75	0.85950	YES	YES
35	a	110.48	2.27995	YES	YES
36	a	119.18	0.23086	YES	YES
37	a	120.10	1.45598	YES	YES
38	a	163.05	1.26027	YES	YES
39	a	170.82	0.39875	YES	YES
40	a	174.15	0.25859	YES	YES
41	a	185.15	0.92462	YES	YES
42	a	190.51	2.41253	YES	YES
43	a	195.06	1.80869	YES	YES
44	a	201.87	1.22819	YES	YES
45	a	204.22	5.53382	YES	YES
46	a	213.37	0.91832	YES	YES
47	a	219.71	4.28168	YES	YES
48	a	227.49	1.04896	YES	YES
49	a	230.99	6.71309	YES	YES
50	a	242.90	0.48369	YES	YES
51	a	245.79	1.60601	YES	YES
52	a	247.23	0.57384	YES	YES
53	a	247.91	0.94828	YES	YES
54	a	253.39	1.21421	YES	YES
55	a	253.56	0.53705	YES	YES
56	a	262.57	1.98750	YES	YES
57	a	268.39	0.18237	YES	YES
58	a	272.48	3.47461	YES	YES
59	a	307.45	4.68982	YES	YES
60	a	322.10	14.87090	YES	YES
61	a	395.42	0.27466	YES	YES
62	a	398.37	0.16714	YES	YES
63	a	399.29	0.38416	YES	YES
64	a	400.27	0.04818	YES	YES
65	a	403.00	0.01890	YES	YES
66	a	408.49	0.50731	YES	YES
67	a	410.36	8.81166	YES	YES
68	a	412.64	11.87316	YES	YES
69	a	420.26	2.65690	YES	YES
70	a	424.14	41.59409	YES	YES
71	a	427.98	12.18977	YES	YES
72	a	435.16	2.15567	YES	YES
73	a	443.13	34.51418	YES	YES
74	a	457.74	13.66809	YES	YES
75	a	463.98	6.33818	YES	YES
76	a	471.65	1.60481	YES	YES
77	a	476.60	9.66548	YES	YES
78	a	491.33	8.37785	YES	YES
79	a	494.31	43.20999	YES	YES
80	a	495.35	7.86084	YES	YES
81	a	507.18	27.36920	YES	YES
82	a	516.07	52.15747	YES	YES
83	a	518.82	182.24221	YES	YES
84	a	531.50	92.56560	YES	YES
85	a	535.21	1.82753	YES	YES
86	a	558.39	20.19937	YES	YES
87	a	580.06	1.23191	YES	YES
88	a	597.70	3.42411	YES	YES
89	a	608.82	0.13010	YES	YES
90	a	609.45	0.46739	YES	YES
91	a	609.84	0.85371	YES	YES
92	a	610.07	0.93045	YES	YES
93	a	611.35	1.89486	YES	YES
94	a	612.07	0.30438	YES	YES
95	a	613.62	0.21247	YES	YES
96	a	632.86	9.45088	YES	YES
97	a	667.17	60.71513	YES	YES
98	a	671.27	18.95885	YES	YES
99	a	672.74	11.74529	YES	YES
100	a	679.98	12.39856	YES	YES
101	a	680.39	7.92739	YES	YES
102	a	686.65	10.61149	YES	YES
103	a	688.02	17.85283	YES	YES
104	a	692.32	31.53590	YES	YES
105	a	694.50	31.96316	YES	YES
106	a	696.75	30.20341	YES	YES
107	a	697.36	44.68471	YES	YES
108	a	702.15	55.16724	YES	YES
109	a	703.05	10.68971	YES	YES
110	a	708.06	10.38297	YES	YES
111	a	736.23	7.00433	YES	YES
112	a	740.91	3.58036	YES	YES
113	a	742.05	3.79166	YES	YES
114	a	743.31	9.80584	YES	YES
115	a	745.56	4.76242	YES	YES
116	a	749.15	3.71102	YES	YES
117	a	755.01	24.33951	YES	YES
118	a	792.54	7.80590	YES	YES
119	a	825.39	0.28939	YES	YES
120	a	832.21	0.29045	YES	YES
121	a	835.39	0.67604	YES	YES
122	a	837.42	0.49538	YES	YES
123	a	838.67	0.73103	YES	YES
124	a	844.67	0.82056	YES	YES
125	a	846.36	0.22420	YES	YES
126	a	886.42	19.65203	YES	YES
127	a	895.58	19.46099	YES	YES
128	a	898.95	8.26081	YES	YES
129	a	906.82	1.25279	YES	YES
130	a	909.78	0.83910	YES	YES
131	a	912.07	0.59675	YES	YES
132	a	912.17	0.45965	YES	YES
133	a	919.16	0.23205	YES	YES
134	a	922.84	0.50750	YES	YES
135	a	935.77	27.80973	YES	YES
136	a	951.20	0.03565	YES	YES
137	a	957.74	0.31319	YES	YES
138	a	958.88	0.11447	YES	YES
139	a	961.56	0.08946	YES	YES
140	a	962.30	0.40322	YES	YES
141	a	967.96	0.33016	YES	YES
142	a	970.69	0.10008	YES	YES
143	a	971.64	0.27625	YES	YES
144	a	978.53	3.17985	YES	YES
145	a	981.82	0.26114	YES	YES
146	a	982.12	2.26157	YES	YES
147	a	982.20	0.70866	YES	YES
148	a	982.34	1.13047	YES	YES
149	a	982.84	1.22225	YES	YES
150	a	983.00	1.87840	YES	YES
151	a	983.51	2.07230	YES	YES
152	a	984.21	1.02631	YES	YES
153	a	984.26	0.45735	YES	YES
154	a	984.45	0.97357	YES	YES
155	a	987.86	0.52740	YES	YES
156	a	988.19	1.58312	YES	YES
157	a	996.78	0.19886	YES	YES
158	a	1002.20	4.32458	YES	YES
159	a	1022.48	0.96237	YES	YES
160	a	1022.98	1.47591	YES	YES
161	a	1023.43	0.35957	YES	YES
162	a	1024.06	8.17808	YES	YES
163	a	1024.51	4.25181	YES	YES
164	a	1025.18	2.10755	YES	YES
165	a	1025.34	5.09615	YES	YES
166	a	1025.67	0.18829	YES	YES

167	a	1030.32	7.82147	YES	YES
168	a	1069.05	20.48156	YES	YES
169	a	1069.16	4.29603	YES	YES
170	a	1070.08	16.03292	YES	YES
171	a	1070.35	16.95801	YES	YES
172	a	1071.69	7.98392	YES	YES
173	a	1073.37	2.35703	YES	YES
174	a	1074.64	26.13607	YES	YES
175	a	1074.71	10.99050	YES	YES
176	a	1075.91	0.70331	YES	YES
177	a	1078.24	0.54429	YES	YES
178	a	1078.86	7.54077	YES	YES
179	a	1079.41	13.62200	YES	YES
180	a	1081.69	11.01179	YES	YES
181	a	1137.51	0.06807	YES	YES
182	a	1140.91	0.31475	YES	YES
183	a	1141.13	0.06805	YES	YES
184	a	1141.20	0.37984	YES	YES
185	a	1141.58	0.03042	YES	YES
186	a	1141.93	0.35700	YES	YES
187	a	1142.40	0.90951	YES	YES
188	a	1159.89	2.27108	YES	YES
189	a	1165.17	2.81527	YES	YES
190	a	1167.99	4.11823	YES	YES
191	a	1168.58	3.12613	YES	YES
192	a	1170.03	5.91023	YES	YES
193	a	1173.96	3.58263	YES	YES
194	a	1174.97	2.53157	YES	YES
195	a	1214.46	22.63731	YES	YES
196	a	1252.36	58.39531	YES	YES
197	a	1287.00	5.15328	YES	YES
198	a	1288.40	5.86575	YES	YES

* zero point VIBRATIONAL energy : 0.7453363 Hartree *

Cis 4_pf



bp86-SVP SCF energy: -2931.4354736580
pbe-TZVPP SCF energy: -2930.991583687

XYZ Coordinates
97

C	1.46415	-3.37720	-0.07599
C	1.04457	-2.19920	-0.13453
C	1.91116	-4.73184	0.00121
H	0.99767	-2.40134	-1.84481
C	2.79850	-7.43152	0.17798
C	2.54449	-6.68936	1.34602
C	2.10773	-5.35987	1.26385
C	2.17214	-5.49735	-1.16997
C	2.60907	-6.82576	-1.07781
H	3.14343	-8.47659	0.24580
H	2.68943	-7.15307	2.33664
H	1.91248	-4.78109	2.18104
H	2.02575	-5.02980	-2.15680
H	2.80487	-7.39733	-2.00089
C	2.63364	-0.29136	1.48452
C	3.74705	-0.53087	2.47158
H	3.92620	-1.62687	2.54563
H	3.46533	-0.15674	3.47720
H	4.68502	-0.05156	2.12497
C	0.56915	-1.00804	-3.12866
C	0.36053	-0.67073	-4.58438
H	-0.71109	-0.83116	-4.84133
H	0.96992	-1.33319	-5.23110
H	0.60519	0.39377	-4.77116
C	1.35989	2.96202	1.53415
C	2.73418	2.82784	1.84416
H	3.41241	2.35055	1.12002
C	3.25018	3.31526	3.05567
H	4.32645	3.20543	3.27004
C	2.40575	3.94664	3.98489
H	2.81163	4.33324	4.93445
C	1.04173	4.09054	3.68543
H	0.36825	4.59823	4.39634
C	0.52307	3.60314	2.47191
H	-0.54469	3.75581	2.25585
C	-0.70801	3.30427	-0.50190
C	-1.88200	3.20692	0.28177
H	-1.93972	2.47844	1.10674
C	-2.99806	4.01522	0.01439
H	-3.89520	3.92868	0.64869
C	-2.97923	4.91072	-1.06794
H	-3.85758	5.54200	-1.28226
C	-1.83999	4.98019	-1.88524
H	-1.81866	5.66407	-2.75044
C	-0.71336	4.18740	-1.60430
H	0.17110	4.26410	-2.25426
C	2.08137	2.90415	-1.20569
C	2.46958	4.26255	-1.12087
H	1.98293	4.92909	-0.38979
C	3.47626	4.77248	-1.95499
H	3.76606	5.83370	-1.87590
C	4.11867	3.93056	-2.88130
H	4.91438	4.32954	-3.53262
C	3.75048	2.57853	-2.96243
H	4.26174	1.90771	-3.67285
C	2.73890	2.06689	-2.12906
H	2.46933	1.00352	-2.17949
C	-2.90693	0.28335	-0.64426
C	-4.21591	0.41085	-0.12812
H	-4.46697	-0.00866	0.85903
C	-5.21231	1.07713	-0.86117
H	-6.22825	1.16779	-0.44083
C	-4.91880	1.62194	-2.12296
H	-5.70216	2.14283	-2.69848
C	-3.61842	1.50716	-2.64090
H	-3.37364	1.94360	-3.62344
C	-2.61784	0.84863	-1.90540
H	-1.59487	0.77758	-2.30668
C	-2.12148	-2.42561	-0.22364
C	-2.86419	-2.68334	-1.39554
H	-3.19452	-1.84972	-2.03510
C	-3.20076	-4.00144	-1.75397
H	-3.78344	-4.18352	-2.67263
C	-2.80596	-5.07713	-0.94288
H	-3.07198	-6.11021	-1.22220
C	-2.06637	-4.82989	0.22737
H	-1.74380	-5.66794	0.86681
C	-1.71884	-3.51696	0.58073
H	-1.12803	-3.33857	1.49259
C	-2.09771	-0.59420	2.02389
C	-3.15446	-1.37159	2.55340
H	-3.67460	-2.10503	1.91651
C	-3.54257	-1.23063	3.89662
H	-4.36703	-1.84713	4.29275
C	-2.88029	-0.31514	4.73268
H	-3.18266	-0.20941	5.78805
C	-1.82147	0.45172	4.21937
H	-1.27955	1.15855	4.86930
C	-1.42931	0.31035	2.87706
H	-0.56866	0.88212	2.49784
O	1.40818	-0.34560	1.86778
O	2.86675	-0.07870	0.24645
O	0.90131	-2.24879	-2.88263
O	0.39178	-0.12942	-2.24947
P	0.75369	2.22422	-0.08169
P	-1.57647	-0.69996	0.23544
Ru	0.65096	-0.24784	-0.11344

Vibrational Frequencies

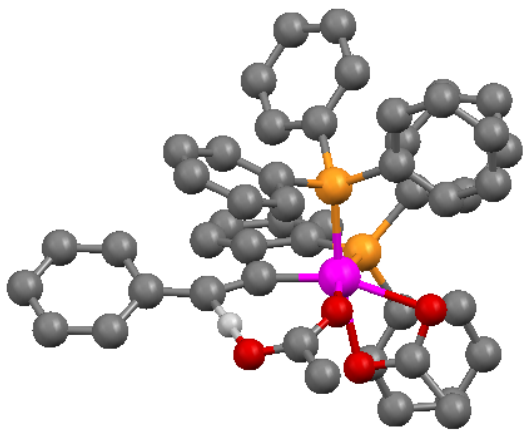
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.80	0.02066	YES	YES
8	a	17.62	0.00582	YES	YES
9	a	19.73	0.01222	YES	YES
10	a	20.27	0.00547	YES	YES
11	a	23.38	0.05643	YES	YES
12	a	30.57	0.31160	YES	YES
13	a	36.14	0.03488	YES	YES
14	a	40.12	0.19188	YES	YES
15	a	42.87	0.04673	YES	YES
16	a	45.25	0.02830	YES	YES
17	a	52.46	0.38810	YES	YES
18	a	53.63	0.09283	YES	YES
19	a	54.46	0.00876	YES	YES
20	a	58.06	0.02889	YES	YES

21	a	59.98	0.47085	YES	YES
22	a	64.48	1.06133	YES	YES
23	a	65.79	0.01066	YES	YES
24	a	69.58	0.74814	YES	YES
25	a	74.47	0.29076	YES	YES
26	a	74.64	0.18570	YES	YES
27	a	78.37	0.39903	YES	YES
28	a	88.83	0.95185	YES	YES
29	a	90.05	0.20211	YES	YES
30	a	92.27	0.53092	YES	YES
31	a	96.59	2.32873	YES	YES
32	a	99.95	0.67033	YES	YES
33	a	104.43	0.93219	YES	YES
34	a	114.64	0.32888	YES	YES
35	a	118.25	0.32415	YES	YES
36	a	119.36	0.21392	YES	YES
37	a	122.97	0.14720	YES	YES
38	a	137.08	3.66257	YES	YES
39	a	170.96	2.38336	YES	YES
40	a	183.27	0.97399	YES	YES
41	a	185.98	0.20753	YES	YES
42	a	192.63	0.36074	YES	YES
43	a	199.96	0.93433	YES	YES
44	a	200.44	2.61123	YES	YES
45	a	203.16	1.05350	YES	YES
46	a	208.81	2.72632	YES	YES
47	a	213.49	2.39417	YES	YES
48	a	219.66	1.34732	YES	YES
49	a	227.05	0.64214	YES	YES
50	a	241.30	3.81226	YES	YES
51	a	245.01	1.62405	YES	YES
52	a	247.98	0.34158	YES	YES
53	a	249.48	0.13032	YES	YES
54	a	253.60	0.98779	YES	YES
55	a	265.75	0.05667	YES	YES
56	a	267.20	1.65169	YES	YES
57	a	273.03	5.59245	YES	YES
58	a	288.87	4.29878	YES	YES
59	a	313.22	12.77936	YES	YES
60	a	332.41	9.46147	YES	YES
61	a	392.82	7.99685	YES	YES
62	a	396.90	0.10362	YES	YES
63	a	398.82	1.14236	YES	YES
64	a	400.92	0.10725	YES	YES
65	a	402.02	0.97273	YES	YES
66	a	402.56	3.35923	YES	YES
67	a	407.12	44.50143	YES	YES
68	a	410.28	0.74375	YES	YES
69	a	411.55	0.27746	YES	YES
70	a	416.98	8.29869	YES	YES
71	a	422.92	17.56168	YES	YES
72	a	434.40	9.96395	YES	YES
73	a	440.95	4.70956	YES	YES
74	a	451.38	9.75457	YES	YES
75	a	460.27	25.03112	YES	YES
76	a	479.10	23.27477	YES	YES
77	a	481.65	2.57484	YES	YES
78	a	489.19	18.76960	YES	YES
79	a	499.22	11.78469	YES	YES
80	a	505.30	17.54304	YES	YES
81	a	510.97	36.66144	YES	YES
82	a	512.05	28.24030	YES	YES
83	a	516.35	157.44904	YES	YES
84	a	525.09	95.72253	YES	YES
85	a	537.43	3.47410	YES	YES
86	a	544.51	1.74416	YES	YES
87	a	585.85	0.47333	YES	YES
88	a	594.81	2.01917	YES	YES
89	a	608.45	0.46640	YES	YES
90	a	609.27	0.26117	YES	YES
91	a	609.90	0.15987	YES	YES
92	a	610.27	1.26322	YES	YES
93	a	611.09	1.46663	YES	YES
94	a	612.27	0.30357	YES	YES
95	a	614.31	0.11028	YES	YES
96	a	643.67	5.43646	YES	YES
97	a	668.63	8.42501	YES	YES
98	a	671.44	22.38741	YES	YES
99	a	672.88	34.51101	YES	YES
100	a	677.49	9.65745	YES	YES
101	a	679.38	10.56346	YES	YES
102	a	684.64	10.12005	YES	YES
103	a	685.01	13.34002	YES	YES
104	a	692.53	29.92198	YES	YES
105	a	697.19	42.60593	YES	YES
106	a	698.57	78.18574	YES	YES
107	a	699.86	7.62003	YES	YES
108	a	700.31	35.03135	YES	YES
109	a	704.09	15.40288	YES	YES
110	a	704.69	4.92597	YES	YES
111	a	735.87	11.13003	YES	YES
112	a	740.05	3.48800	YES	YES
113	a	741.12	1.29550	YES	YES
114	a	743.80	4.07082	YES	YES
115	a	746.64	5.82870	YES	YES
116	a	748.34	6.47224	YES	YES
117	a	756.12	24.46863	YES	YES
118	a	786.74	0.46084	YES	YES
119	a	825.71	0.17051	YES	YES
120	a	833.50	0.52730	YES	YES
121	a	835.85	1.20355	YES	YES
122	a	836.65	0.97949	YES	YES
123	a	839.06	0.19885	YES	YES
124	a	841.36	1.26112	YES	YES
125	a	843.35	0.27201	YES	YES
126	a	894.58	0.07879	YES	YES
127	a	899.10	12.31881	YES	YES
128	a	905.27	0.70446	YES	YES
129	a	908.54	0.91628	YES	YES
130	a	909.12	0.62428	YES	YES
131	a	911.88	39.14952	YES	YES
132	a	912.70	3.67194	YES	YES
133	a	913.68	1.49705	YES	YES
134	a	918.49	1.15636	YES	YES
135	a	942.57	16.46670	YES	YES
136	a	951.22	0.09150	YES	YES
137	a	957.06	0.49190	YES	YES
138	a	957.98	0.40771	YES	YES
139	a	960.11	0.41721	YES	YES
140	a	961.75	0.11306	YES	YES
141	a	962.17	0.44858	YES	YES
142	a	967.58	0.32876	YES	YES
143	a	972.37	0.21025	YES	YES
144	a	979.82	0.93628	YES	YES
145	a	980.84	2.82109	YES	YES
146	a	981.02	1.04874	YES	YES
147	a	981.80	0.75190	YES	YES
148	a	982.11	0.72990	YES	YES
149	a	982.30	0.28517	YES	YES
150	a	982.45	1.20064	YES	YES
151	a	983.37	0.97579	YES	YES
152	a	983.79	0.53409	YES	YES
153	a	983.94	2.88305	YES	YES
154	a	984.76	1.27545	YES	YES
155	a	985.61	0.43560	YES	YES
156	a	986.97	0.79239	YES	YES
157	a	987.89	1.12690	YES	YES
158	a	1003.15	2.71029	YES	YES
159	a	1022.25	13.67403	YES	YES
160	a	1022.58	2.67747	YES	YES
161	a	1023.41	1.39271	YES	YES
162	a	1024.25	1.52282	YES	YES
163	a	1024.75	0.97206	YES	YES
164	a	1025.13	5.64800	YES	YES
165	a	1025.40	0.86405	YES	YES
166	a	1026.20	8.07614	YES	YES
167	a	1026.42	1.07655	YES	YES
168	a	1066.42	11.46381	YES	YES

169	a	1068.03	11.04902	YES	YES
170	a	1069.16	5.21697	YES	YES
171	a	1069.59	18.44869	YES	YES
172	a	1071.46	19.43455	YES	YES
173	a	1073.26	8.61818	YES	YES
174	a	1073.64	11.21118	YES	YES
175	a	1075.72	13.57932	YES	YES
176	a	1076.19	1.13763	YES	YES
177	a	1077.82	0.65628	YES	YES
178	a	1079.60	15.01121	YES	YES
179	a	1079.89	7.09442	YES	YES
180	a	1081.90	3.76835	YES	YES
181	a	1137.78	0.02879	YES	YES
182	a	1140.50	0.19376	YES	YES
183	a	1141.27	0.13003	YES	YES
184	a	1141.81	0.14368	YES	YES
185	a	1142.18	0.71201	YES	YES
186	a	1142.38	0.75265	YES	YES
187	a	1142.68	0.29664	YES	YES
188	a	1159.13	0.56543	YES	YES
189	a	1162.32	2.37063	YES	YES
190	a	1165.83	9.34574	YES	YES
191	a	1169.46	1.33269	YES	YES
192	a	1172.41	7.60608	YES	YES
193	a	1173.33	2.51322	YES	YES
194	a	1176.32	1.54630	YES	YES
195	a	1215.18	38.22902	YES	YES
196	a	1250.25	53.69667	YES	YES
197	a	1283.71	4.04425	YES	YES
198	a	1288.20	4.39966	YES	YES

* zero point VIBRATIONAL energy : 0.7451800 Hartree *

Cis TS_{45}_af



bp86-SVP SCF energy: -2931.4495187980
pbe-TZVPP SCF energy: -2930.996932771

XYZ Coordinates
97

C	-0.28921	0.08204	-3.14753
C	0.06436	0.02636	-1.90869
C	-0.93059	0.72604	-4.27121
H	0.24230	-1.13456	-3.29641
C	-2.18153	1.96865	-6.51005
C	-2.37486	2.47952	-5.21315
C	-1.76348	1.86850	-4.10958
C	-0.75349	0.21875	-5.58746
C	-1.36977	0.83309	-6.68643
H	-2.66423	2.45008	-7.37662
H	-3.01682	3.36356	-5.05822
H	-1.93717	2.26740	-3.09677
H	-0.12046	-0.67135	-5.73287
H	-1.21391	0.41893	-7.69700
C	3.28768	-1.49177	0.03615
C	4.70532	-1.98519	0.20409
H	5.17781	-2.15891	-0.78376
H	4.72568	-2.91138	0.81392
H	5.29368	-1.20488	0.73712
C	0.92320	-3.06273	-2.43829
C	1.37402	-4.50365	-2.64566
H	0.92012	-4.92140	-3.56720
H	1.12595	-5.13062	-1.76535
H	2.47984	-4.51269	-2.77353
C	3.18135	1.55104	0.98612
C	3.91307	1.79725	-0.19838
H	3.39921	1.79415	-1.17294
C	5.29219	2.04943	-0.14424
H	5.84600	2.24191	-1.07793
C	5.96421	2.05227	1.09165
H	7.04829	2.25018	1.13337
C	5.24486	1.80503	2.27188
H	5.76005	1.80963	3.24714
C	3.86014	1.55663	2.22130
H	3.31209	1.37639	3.15859
C	0.74020	1.26237	2.55965
C	1.11399	0.15578	3.35981
H	1.74738	-0.63709	2.92954
C	0.68760	0.06816	4.69474
H	0.99095	-0.79778	5.30618
C	-0.12750	1.07231	5.24636
H	-0.46254	1.00142	6.29470
C	-0.52250	2.15901	4.44986
H	-1.17740	2.94255	4.86557
C	-0.09484	2.25453	3.11400
H	-0.43153	3.10350	2.50060
C	0.92277	2.97776	0.16097
C	0.34200	3.15420	-1.10866
H	0.09234	2.27098	-1.71789
C	0.12006	4.44473	-1.62389
H	-0.32408	4.55715	-2.62654
C	0.47612	5.57495	-0.87192
H	0.30300	6.58699	-1.27431
C	1.07590	5.40969	0.39023
H	1.37886	6.29112	0.97974
C	1.30964	4.12274	0.89826
H	1.81512	4.01085	1.87137
C	-2.28089	0.23970	1.17064
C	-2.91635	0.18197	2.42893
H	-2.79956	-0.70474	3.06916
C	-3.69136	1.26188	2.88706
H	-4.17860	1.19818	3.87433
C	-3.84207	2.41544	2.10001
H	-4.45516	3.25823	2.46048
C	-3.19337	2.49347	0.85547
H	-3.28642	3.39919	0.23420
C	-2.41321	1.41794	0.40005
H	-1.89261	1.49735	-0.56728
C	-2.41874	-1.88866	-0.81351
C	-3.41494	-1.14440	-1.47795
H	-3.58382	-0.08620	-1.22712
C	-4.21973	-1.74507	-2.46206
H	-4.99257	-1.14510	-2.97025
C	-4.04070	-3.09641	-2.79650
H	-4.67153	-3.56612	-3.56930
C	-3.05119	-3.84681	-2.13810
H	-2.90298	-4.91025	-2.39009
C	-2.24657	-3.25011	-1.15485
H	-1.47724	-3.84951	-0.64493
C	-1.33621	-2.49438	1.74496
C	-2.57873	-3.03710	2.15224
H	-3.51744	-2.65898	1.71525
C	-2.62680	-4.07382	3.09701
H	-3.60181	-4.48557	3.40724
C	-1.43515	-4.59529	3.63356
H	-1.47373	-5.41548	4.37005
C	-0.19927	-4.08007	3.21267
H	0.73991	-4.49956	3.61026
C	-0.14542	-3.03384	2.27230
H	0.83003	-2.66010	1.92308
O	2.41947	-1.66937	0.96145
O	2.94854	-0.85131	-1.01702
O	0.67985	-2.38380	-3.48530
O	0.85285	-2.66953	-1.22280
P	1.33792	1.27859	0.80252
P	-1.26724	-1.15008	0.46064
Ru	0.85450	-0.70229	-0.37245

Vibrational Frequencies

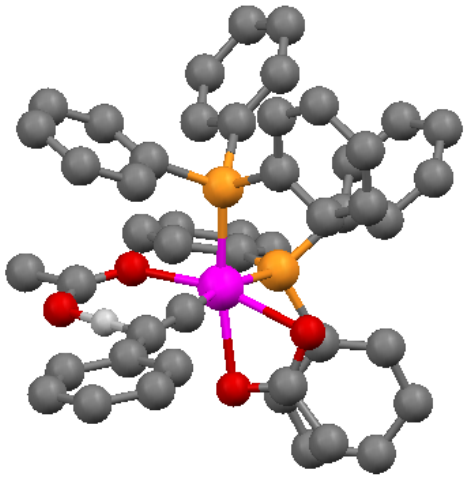
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-648.56	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	4.15	0.00690	YES	YES
9	a	12.80	0.05037	YES	YES
10	a	15.71	0.00385	YES	YES
11	a	23.39	0.02546	YES	YES
12	a	28.61	0.02915	YES	YES
13	a	31.76	0.14812	YES	YES
14	a	36.95	0.03471	YES	YES
15	a	41.53	0.36984	YES	YES
16	a	43.86	0.57576	YES	YES
17	a	47.08	0.13770	YES	YES
18	a	49.91	0.12519	YES	YES
19	a	51.10	0.03571	YES	YES

20	a	55.76	0.49130	YES	YES
21	a	57.79	0.12390	YES	YES
22	a	60.32	0.48801	YES	YES
23	a	61.44	0.35106	YES	YES
24	a	62.90	0.31025	YES	YES
25	a	66.80	0.10457	YES	YES
26	a	70.02	0.02896	YES	YES
27	a	72.25	0.17176	YES	YES
28	a	76.55	0.14878	YES	YES
29	a	79.10	0.86072	YES	YES
30	a	84.30	3.08364	YES	YES
31	a	86.53	1.06167	YES	YES
32	a	87.91	0.12637	YES	YES
33	a	96.72	2.26513	YES	YES
34	a	104.99	0.15682	YES	YES
35	a	106.46	0.53026	YES	YES
36	a	114.94	0.24937	YES	YES
37	a	120.79	8.07701	YES	YES
38	a	134.90	2.36073	YES	YES
39	a	168.38	0.77510	YES	YES
40	a	175.96	1.28094	YES	YES
41	a	182.52	1.60127	YES	YES
42	a	190.17	0.58210	YES	YES
43	a	192.31	2.50821	YES	YES
44	a	200.41	4.23639	YES	YES
45	a	204.50	1.26255	YES	YES
46	a	214.87	0.76289	YES	YES
47	a	218.60	4.54997	YES	YES
48	a	221.61	6.65360	YES	YES
49	a	226.01	1.40048	YES	YES
50	a	244.36	0.73181	YES	YES
51	a	245.28	0.60746	YES	YES
52	a	248.37	1.82722	YES	YES
53	a	249.81	0.21870	YES	YES
54	a	253.40	11.03038	YES	YES
55	a	260.36	0.54693	YES	YES
56	a	267.09	3.39306	YES	YES
57	a	270.51	2.81826	YES	YES
58	a	283.92	12.15044	YES	YES
59	a	291.32	43.35650	YES	YES
60	a	301.44	1.06253	YES	YES
61	a	331.19	25.04232	YES	YES
62	a	393.64	0.03014	YES	YES
63	a	395.37	0.04249	YES	YES
64	a	397.71	0.57446	YES	YES
65	a	400.12	0.34296	YES	YES
66	a	406.33	0.17263	YES	YES
67	a	407.33	0.48228	YES	YES
68	a	411.36	2.77712	YES	YES
69	a	413.64	27.29287	YES	YES
70	a	418.68	8.42821	YES	YES
71	a	427.98	13.96285	YES	YES
72	a	431.82	8.59659	YES	YES
73	a	443.71	20.15232	YES	YES
74	a	448.11	2.34109	YES	YES
75	a	461.81	28.80819	YES	YES
76	a	465.02	10.36294	YES	YES
77	a	475.30	13.33377	YES	YES
78	a	492.00	22.47253	YES	YES
79	a	495.76	44.07838	YES	YES
80	a	505.10	1.14725	YES	YES
81	a	513.64	38.30826	YES	YES
82	a	516.90	37.28962	YES	YES
83	a	518.28	195.05985	YES	YES
84	a	529.94	70.18959	YES	YES
85	a	544.02	29.99127	YES	YES
86	a	572.76	44.99802	YES	YES
87	a	591.30	12.10868	YES	YES
88	a	596.14	5.82925	YES	YES
89	a	608.54	0.54028	YES	YES
90	a	609.01	0.77609	YES	YES
91	a	610.00	1.51333	YES	YES
92	a	610.24	0.25594	YES	YES
93	a	610.98	0.58776	YES	YES
94	a	611.40	1.59772	YES	YES
95	a	612.49	2.95670	YES	YES
96	a	655.89	15.38596	YES	YES
97	a	668.44	57.60010	YES	YES
98	a	672.85	24.28447	YES	YES
99	a	674.22	3.99541	YES	YES
100	a	680.65	2.75902	YES	YES
101	a	682.75	16.10198	YES	YES
102	a	689.03	19.69270	YES	YES
103	a	691.80	5.89818	YES	YES
104	a	692.22	44.35769	YES	YES
105	a	693.16	52.81966	YES	YES
106	a	696.03	10.67638	YES	YES
107	a	696.51	40.21790	YES	YES
108	a	696.90	26.94376	YES	YES
109	a	700.72	17.61756	YES	YES
110	a	705.97	27.91650	YES	YES
111	a	711.21	11.39037	YES	YES
112	a	736.43	6.10966	YES	YES
113	a	739.38	14.24314	YES	YES
114	a	741.74	4.62397	YES	YES
115	a	744.16	4.85066	YES	YES
116	a	747.77	4.89019	YES	YES
117	a	748.47	4.67291	YES	YES
118	a	751.28	25.30725	YES	YES
119	a	814.20	39.98744	YES	YES
120	a	822.73	0.62291	YES	YES
121	a	829.03	0.46145	YES	YES
122	a	833.71	0.54490	YES	YES
123	a	835.12	1.02947	YES	YES
124	a	838.84	0.12098	YES	YES
125	a	846.69	1.21958	YES	YES
126	a	852.80	0.85124	YES	YES
127	a	888.95	2.59434	YES	YES
128	a	901.92	0.21907	YES	YES
129	a	907.11	1.72694	YES	YES
130	a	907.95	0.20216	YES	YES
131	a	912.59	0.82025	YES	YES
132	a	922.26	1.71462	YES	YES
133	a	924.42	12.08828	YES	YES
134	a	930.74	0.81041	YES	YES
135	a	940.60	26.36456	YES	YES
136	a	948.15	0.48380	YES	YES
137	a	953.66	0.24022	YES	YES
138	a	957.75	0.36132	YES	YES
139	a	958.55	0.54976	YES	YES
140	a	962.48	0.27995	YES	YES
141	a	969.61	1.13324	YES	YES
142	a	970.85	0.76292	YES	YES
143	a	975.83	0.41408	YES	YES
144	a	980.44	2.23617	YES	YES
145	a	981.20	0.33010	YES	YES
146	a	981.24	0.24058	YES	YES
147	a	981.75	0.92187	YES	YES
148	a	982.71	1.59023	YES	YES
149	a	982.78	1.17324	YES	YES
150	a	983.15	1.36006	YES	YES
151	a	983.36	2.58029	YES	YES
152	a	983.97	1.30418	YES	YES
153	a	985.33	0.61129	YES	YES
154	a	986.69	1.80285	YES	YES
155	a	990.01	7.06499	YES	YES
156	a	990.71	13.53676	YES	YES
157	a	991.59	2.00117	YES	YES
158	a	998.46	4.70873	YES	YES
159	a	1010.26	0.83574	YES	YES
160	a	1020.83	10.36120	YES	YES
161	a	1022.73	1.03431	YES	YES
162	a	1023.75	0.94136	YES	YES
163	a	1024.03	0.69769	YES	YES
164	a	1024.62	1.07424	YES	YES
165	a	1025.77	1.24572	YES	YES
166	a	1025.96	2.45656	YES	YES
167	a	1026.27	0.37348	YES	YES

168	a	1028.65	15.00916	YES	YES
169	a	1068.45	6.48076	YES	YES
170	a	1070.77	10.69092	YES	YES
171	a	1071.15	8.18519	YES	YES
172	a	1071.93	2.65943	YES	YES
173	a	1073.89	13.94988	YES	YES
174	a	1075.03	0.54362	YES	YES
175	a	1076.10	15.35366	YES	YES
176	a	1077.65	22.89545	YES	YES
177	a	1077.81	6.36112	YES	YES
178	a	1078.89	11.38274	YES	YES
179	a	1080.90	5.53497	YES	YES
180	a	1083.09	10.56857	YES	YES
181	a	1084.03	18.62288	YES	YES
182	a	1137.03	0.17411	YES	YES
183	a	1141.57	0.15791	YES	YES
184	a	1141.89	0.21702	YES	YES
185	a	1142.41	0.09770	YES	YES
186	a	1142.51	0.75808	YES	YES
187	a	1142.88	0.37713	YES	YES
188	a	1143.48	0.32439	YES	YES
189	a	1160.70	1.80174	YES	YES
190	a	1163.51	0.67165	YES	YES
191	a	1167.92	4.61835	YES	YES
192	a	1171.56	2.53793	YES	YES
193	a	1172.41	8.63064	YES	YES
194	a	1175.71	1.36483	YES	YES
195	a	1176.49	6.51427	YES	YES
196	a	1220.86	11.81990	YES	YES
197	a	1271.91	36.86725	YES	YES
198	a	1286.26	3.81990	YES	YES

* zero point VIBRATIONAL energy : 0.7409582 Hartree *

Cis TS_{45}_pf



bp86-SVP SCF energy: -2931.4309519020
pbe-TZVPP SCF energy: -2930.978025056

XYZ Coordinates
97

C	1.01880	-2.65417	-2.42198
C	0.92230	-1.78854	-1.48219
C	1.30882	-3.95779	-2.96930
H	0.47744	-1.66648	-3.16180
C	1.86446	-6.52811	-4.04797
C	2.09916	-6.26363	-2.68541
C	1.82721	-4.99779	-2.14955
C	1.07620	-4.23926	-4.34191
C	1.35238	-5.50856	-4.87047
H	2.08109	-7.52510	-4.46619
H	2.50090	-7.05572	-2.03080
H	2.01354	-4.79266	-1.08277
H	0.67448	-3.44281	-4.98897
H	1.16533	-5.70441	-5.93988
C	3.23934	-0.34856	-0.01387
C	4.69132	-0.52093	0.35054
H	5.30061	-0.64794	-0.56690
H	4.82431	-1.38972	1.02675
H	5.04574	0.39241	0.87862
C	-0.43459	0.36848	-3.42133
C	-1.04996	1.41049	-4.34979
H	-1.27778	0.95932	-5.33549
H	-0.33386	2.24982	-4.49234
H	-1.97646	1.82932	-3.90337
C	2.70827	2.60650	0.97780
C	3.45338	2.96908	-0.16806
H	2.98630	2.92199	-1.16466
C	4.78606	3.39151	-0.04914
H	5.34995	3.67301	-0.95391
C	5.40130	3.44947	1.21486
H	6.44929	3.78021	1.30723
C	4.67087	3.08459	2.35723
H	5.14080	3.12993	3.35413
C	3.33189	2.66606	2.24097
H	2.77245	2.39340	3.14923
C	0.28386	1.98825	2.44724
C	0.71053	0.88215	3.22073
H	1.40166	0.14486	2.78004
C	0.26782	0.72592	4.54405
H	0.61389	-0.13912	5.13391
C	-0.61851	1.65934	5.10964
H	-0.96876	1.53378	6.14786
C	-1.06387	2.74547	4.33947
H	-1.77152	3.47500	4.76731
C	-0.61737	2.91101	3.01646
H	-0.98829	3.76165	2.42501
C	0.30167	3.72101	0.05471
C	0.56784	4.93548	0.73018
H	1.13663	4.92904	1.67448
C	0.12871	6.15713	0.19685
H	0.34068	7.09607	0.73520
C	-0.56526	6.18564	-1.02696
H	-0.90363	7.14730	-1.44788
C	-0.80751	4.98725	-1.71735
H	-1.33058	5.00490	-2.68821
C	-0.37598	3.75908	-1.18178
H	-0.53479	2.81761	-1.73410
C	-2.40934	0.34256	1.04889
C	-3.03804	0.16668	2.29899
H	-2.82800	-0.72703	2.90576
C	-3.93238	1.13518	2.78805
H	-4.41298	0.98223	3.76881
C	-4.21268	2.28937	2.03858
H	-4.92083	3.04266	2.42249
C	-3.57161	2.48564	0.80342
H	-3.76536	3.39671	0.21334
C	-2.67007	1.52437	0.31806
H	-2.15698	1.68976	-0.64255
C	-2.38953	-1.69594	-1.00241
C	-3.47291	-1.01772	-1.60056
H	-3.73428	0.00369	-1.28492
C	-4.25196	-1.64195	-2.59143
H	-5.09784	-1.09506	-3.04081
C	-3.96295	-2.95402	-2.99858
H	-4.57462	-3.44346	-3.77471
C	-2.89055	-3.64130	-2.40459
H	-2.65104	-4.67238	-2.71242
C	-2.11056	-3.01918	-1.41693
H	-1.27867	-3.57680	-0.96130
C	-1.16029	-2.27976	1.51565
C	-2.31255	-3.00991	1.89198
H	-3.28931	-2.77286	1.43881
C	-2.22091	-4.05218	2.82793
H	-3.12687	-4.61374	3.11127
C	-0.97618	-4.38681	3.39176
H	-0.90370	-5.21050	4.12175
C	0.17377	-3.67747	3.00981
H	1.15550	-3.94543	3.43488
C	0.08607	-2.62818	2.07586
H	0.99528	-2.09244	1.76078
O	2.31456	-0.71041	0.81301
O	2.88164	0.17700	-1.11514
O	-0.09950	-0.74054	-3.93861
O	-0.30565	0.73403	-2.19738
P	0.92728	2.09643	0.70966
P	-1.26420	-0.90305	0.26962
Ru	0.74135	-0.14305	-0.56859

Vibrational Frequencies

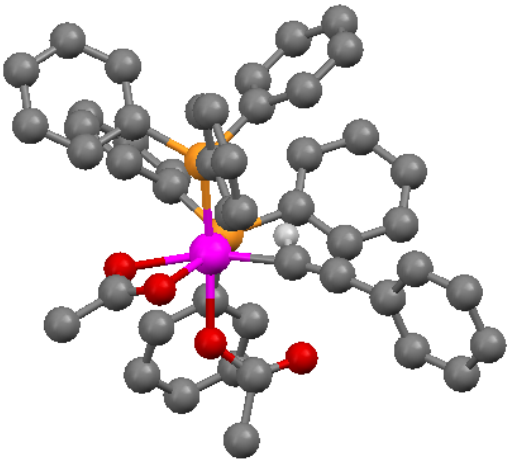
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-727.99	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	13.18	0.02164	YES	YES
9	a	16.83	0.02173	YES	YES
10	a	20.81	0.01386	YES	YES
11	a	22.78	0.02165	YES	YES
12	a	27.33	0.00612	YES	YES
13	a	32.31	0.17660	YES	YES
14	a	36.94	0.03443	YES	YES
15	a	40.46	0.04364	YES	YES
16	a	43.75	0.22161	YES	YES
17	a	47.10	0.68927	YES	YES

18	a	50.16	0.06377	YES	YES
19	a	50.58	0.38172	YES	YES
20	a	57.72	0.04340	YES	YES
21	a	59.01	0.47340	YES	YES
22	a	62.36	0.28475	YES	YES
23	a	65.88	0.10253	YES	YES
24	a	68.70	0.65031	YES	YES
25	a	70.10	0.21448	YES	YES
26	a	70.95	0.07036	YES	YES
27	a	71.70	0.72803	YES	YES
28	a	73.90	0.24968	YES	YES
29	a	80.96	0.69181	YES	YES
30	a	83.14	0.92478	YES	YES
31	a	84.98	1.98776	YES	YES
32	a	86.05	0.10602	YES	YES
33	a	93.55	1.63463	YES	YES
34	a	97.72	0.97771	YES	YES
35	a	103.99	0.94957	YES	YES
36	a	109.97	1.42337	YES	YES
37	a	123.43	0.03572	YES	YES
38	a	128.91	6.54315	YES	YES
39	a	149.48	4.34827	YES	YES
40	a	172.65	4.23681	YES	YES
41	a	184.01	1.79479	YES	YES
42	a	188.38	0.46619	YES	YES
43	a	192.06	1.13477	YES	YES
44	a	194.94	1.01360	YES	YES
45	a	202.01	3.58026	YES	YES
46	a	209.58	1.72730	YES	YES
47	a	211.80	2.84052	YES	YES
48	a	214.99	1.94913	YES	YES
49	a	223.82	0.82092	YES	YES
50	a	245.13	1.25694	YES	YES
51	a	246.22	0.35960	YES	YES
52	a	247.98	0.31785	YES	YES
53	a	249.57	3.49079	YES	YES
54	a	253.06	4.59855	YES	YES
55	a	266.62	2.34456	YES	YES
56	a	266.76	1.02135	YES	YES
57	a	267.31	1.03281	YES	YES
58	a	287.13	6.66107	YES	YES
59	a	304.03	24.18871	YES	YES
60	a	315.18	28.61601	YES	YES
61	a	322.06	15.10015	YES	YES
62	a	395.50	0.66924	YES	YES
63	a	397.94	0.46090	YES	YES
64	a	398.18	1.53188	YES	YES
65	a	400.68	18.01074	YES	YES
66	a	402.37	7.46319	YES	YES
67	a	403.63	0.31437	YES	YES
68	a	407.95	3.62558	YES	YES
69	a	411.18	0.72034	YES	YES
70	a	414.69	3.20712	YES	YES
71	a	419.45	14.86403	YES	YES
72	a	432.53	16.78301	YES	YES
73	a	436.57	14.38150	YES	YES
74	a	450.54	2.11667	YES	YES
75	a	453.52	9.88791	YES	YES
76	a	467.08	21.17487	YES	YES
77	a	476.81	7.92307	YES	YES
78	a	490.18	42.37086	YES	YES
79	a	493.76	28.26537	YES	YES
80	a	502.12	12.03928	YES	YES
81	a	510.87	41.40192	YES	YES
82	a	513.89	139.52125	YES	YES
83	a	523.04	0.26829	YES	YES
84	a	526.95	104.76228	YES	YES
85	a	541.86	33.73646	YES	YES
86	a	575.41	49.86344	YES	YES
87	a	589.88	3.49842	YES	YES
88	a	594.74	4.29898	YES	YES
89	a	605.60	0.72857	YES	YES
90	a	608.34	0.09148	YES	YES
91	a	609.11	0.25180	YES	YES
92	a	609.84	1.92380	YES	YES
93	a	610.14	0.61599	YES	YES
94	a	610.85	1.44987	YES	YES
95	a	611.94	0.97248	YES	YES
96	a	634.53	7.31645	YES	YES
97	a	670.27	45.22788	YES	YES
98	a	671.42	8.49729	YES	YES
99	a	672.63	22.75803	YES	YES
100	a	679.86	3.74385	YES	YES
101	a	680.87	18.16001	YES	YES
102	a	683.73	2.49019	YES	YES
103	a	690.40	3.68805	YES	YES
104	a	690.98	17.57410	YES	YES
105	a	692.97	25.99516	YES	YES
106	a	694.12	40.98905	YES	YES
107	a	694.97	43.44816	YES	YES
108	a	699.52	65.72506	YES	YES
109	a	704.46	7.38958	YES	YES
110	a	707.02	29.45060	YES	YES
111	a	710.31	6.52803	YES	YES
112	a	736.61	6.90344	YES	YES
113	a	738.80	16.00701	YES	YES
114	a	741.64	6.86652	YES	YES
115	a	743.92	2.37495	YES	YES
116	a	746.97	7.88479	YES	YES
117	a	747.82	4.09908	YES	YES
118	a	754.56	23.64912	YES	YES
119	a	808.81	30.51875	YES	YES
120	a	827.21	0.09307	YES	YES
121	a	829.17	0.21084	YES	YES
122	a	833.83	0.21147	YES	YES
123	a	839.53	2.27596	YES	YES
124	a	842.61	0.48730	YES	YES
125	a	848.66	0.33452	YES	YES
126	a	852.04	0.68040	YES	YES
127	a	896.17	1.11124	YES	YES
128	a	903.23	0.56136	YES	YES
129	a	905.28	0.33224	YES	YES
130	a	911.92	2.73940	YES	YES
131	a	914.50	1.93371	YES	YES
132	a	923.97	8.72517	YES	YES
133	a	926.41	0.39399	YES	YES
134	a	930.75	0.21232	YES	YES
135	a	942.81	18.32363	YES	YES
136	a	951.72	1.06373	YES	YES
137	a	953.53	0.32388	YES	YES
138	a	957.77	0.08767	YES	YES
139	a	962.24	0.44758	YES	YES
140	a	965.85	0.70409	YES	YES
141	a	971.02	9.64791	YES	YES
142	a	973.21	0.25543	YES	YES
143	a	976.91	0.82432	YES	YES
144	a	979.61	18.22433	YES	YES
145	a	980.43	2.62006	YES	YES
146	a	980.91	0.87932	YES	YES
147	a	980.99	1.28748	YES	YES
148	a	981.76	1.18396	YES	YES
149	a	981.88	1.21073	YES	YES
150	a	982.56	0.22672	YES	YES
151	a	982.78	2.99921	YES	YES
152	a	983.28	0.33510	YES	YES
153	a	984.21	2.08874	YES	YES
154	a	984.53	1.38219	YES	YES
155	a	985.11	4.88833	YES	YES
156	a	985.97	1.42518	YES	YES
157	a	996.98	0.50702	YES	YES
158	a	1002.63	1.35497	YES	YES
159	a	1003.15	4.02836	YES	YES
160	a	1022.92	6.91801	YES	YES
161	a	1023.18	1.46514	YES	YES
162	a	1023.93	0.43958	YES	YES
163	a	1023.98	1.28438	YES	YES
164	a	1024.45	1.56669	YES	YES
165	a	1025.04	0.98463	YES	YES

166	a	1025.38	4.37004	YES	YES
167	a	1026.03	1.66892	YES	YES
168	a	1027.08	15.88380	YES	YES
169	a	1069.36	7.12819	YES	YES
170	a	1069.67	7.24919	YES	YES
171	a	1070.96	17.62241	YES	YES
172	a	1071.18	4.15297	YES	YES
173	a	1072.49	0.87027	YES	YES
174	a	1074.23	0.31027	YES	YES
175	a	1075.46	1.83914	YES	YES
176	a	1076.99	19.52790	YES	YES
177	a	1078.31	1.16802	YES	YES
178	a	1079.48	11.01353	YES	YES
179	a	1081.08	15.67603	YES	YES
180	a	1082.26	16.02937	YES	YES
181	a	1085.27	13.70397	YES	YES
182	a	1138.13	0.01753	YES	YES
183	a	1139.95	0.54802	YES	YES
184	a	1141.93	0.31007	YES	YES
185	a	1142.14	0.02679	YES	YES
186	a	1142.28	0.34716	YES	YES
187	a	1142.49	0.82410	YES	YES
188	a	1142.66	0.07908	YES	YES
189	a	1159.22	0.22214	YES	YES
190	a	1167.12	1.71761	YES	YES
191	a	1169.53	3.26571	YES	YES
192	a	1170.80	7.79471	YES	YES
193	a	1171.15	9.60088	YES	YES
194	a	1173.79	0.97754	YES	YES
195	a	1177.03	4.54446	YES	YES
196	a	1219.15	12.67247	YES	YES
197	a	1270.91	63.95596	YES	YES
198	a	1293.04	2.33720	YES	YES

* zero point VIBRATIONAL energy : 0.7408635 Hartree *

Cis 3_afam



bp86-SVP SCF energy: -2931.4271080150
pbe-TZVPP SCF energy: -2930.975997597

XYZ Coordinates
97

C	1.47203	-0.02130	-2.85811
C	0.96604	0.18449	-1.73594
C	2.19407	-0.14147	-4.07715
H	0.91310	-0.51156	-0.77288
C	3.69222	-0.35360	-6.47286
C	4.30655	0.11253	-5.29460
C	3.57203	0.22074	-4.10727
C	1.58721	-0.61395	-5.27354
C	2.33221	-0.71517	-6.45604
H	4.27467	-0.43553	-7.40575
H	5.37248	0.39587	-5.30353
H	4.03722	0.58097	-3.17546
H	0.52251	-0.89610	-5.25721
H	1.84818	-1.08124	-7.37710
C	-0.89332	3.23136	0.35116
C	-1.25170	4.65816	0.67478
H	-0.31079	5.22746	0.84526
H	-1.85941	4.71022	1.60144
H	-1.78992	5.12662	-0.17425
C	3.00063	2.02730	-0.15122
C	3.81991	3.32137	-0.22746
H	4.90197	3.08404	-0.26900
H	3.60633	3.97616	0.64349
H	3.53558	3.88390	-1.14482
C	-3.45178	0.23211	0.41546
C	-3.86055	1.58530	0.47585
H	-3.29645	2.34908	-0.08247
C	-5.00328	1.95829	1.19930
H	-5.30768	3.01770	1.22941
C	-5.76335	0.98504	1.87269
H	-6.66267	1.27722	2.43995
C	-5.37582	-0.36280	1.80463
H	-5.97388	-1.13798	2.31225
C	-4.22897	-0.73877	1.08076
H	-3.95553	-1.80341	1.02764
C	-1.88055	-1.97522	-0.75227
C	-1.76316	-2.78036	0.40370
H	-1.70200	-2.31202	1.39988
C	-1.72370	-4.18030	0.29961
H	-1.65248	-4.79216	1.21378
C	-1.76118	-4.79784	-0.96173
H	-1.72193	-5.89671	-1.04338
C	-1.83415	-4.00486	-2.11820
H	-1.84540	-4.47773	-3.11442
C	-1.89967	-2.60479	-2.01643
H	-1.96746	-1.99875	-2.93258
C	-2.58979	0.39555	-2.25997
C	-3.88759	-0.03000	-2.63234
H	-4.48412	-0.65146	-1.94435
C	-4.43107	0.33295	-3.87399
H	-5.44314	-0.00882	-4.14819
C	-3.68892	1.13499	-4.75996
H	-4.11642	1.42640	-5.73407
C	-2.40437	1.56697	-4.39444
H	-1.81669	2.20188	-5.07787
C	-1.85402	1.20062	-3.15183
H	-0.85142	1.55012	-2.87447
C	1.76572	-2.01514	1.28520
C	1.32859	-3.24044	1.83260
H	0.51868	-3.26129	2.57770
C	1.92494	-4.44888	1.43312
H	1.57443	-5.39833	1.87119
C	2.95783	-4.44887	0.48145
H	3.42320	-5.39880	0.16934
C	3.39127	-3.23204	-0.07270
H	4.19954	-3.22016	-0.82263
C	2.80196	-2.01873	0.31931
H	3.15165	-1.05909	-0.10714
C	2.37259	0.52602	2.63470
C	3.64823	-0.02458	2.86427
H	3.91779	-1.00367	2.43953
C	4.59176	0.67740	3.63599
H	5.58768	0.23615	3.80840
C	4.27160	1.93246	4.17725
H	5.01351	2.48083	4.78160
C	3.00129	2.48893	3.94129
H	2.74326	3.47725	4.35704
C	2.05531	1.79359	3.17302
H	1.06581	2.23967	2.98184
C	-0.08331	-0.70143	3.18683
C	0.43184	-1.37138	4.32289
H	1.47341	-1.73208	4.32879
C	-0.36902	-1.56294	5.45884
H	0.04390	-2.09197	6.33394
C	-1.68643	-1.06810	5.48728
H	-2.31189	-1.21240	6.38403
C	-2.19176	-0.37315	4.37774
H	-3.21364	0.03927	4.39511
C	-1.39370	-0.18904	3.23271
H	-1.78349	0.38678	2.38115
O	-0.70915	2.37934	1.30066
O	-0.73795	2.83358	-0.84786
O	3.52588	0.92937	-0.38436
O	1.75152	2.24668	0.16472
P	-1.91731	-0.12550	-0.59285
P	1.02116	-0.37401	1.72384
Ru	0.12155	0.92580	-0.00777

Vibrational Frequencies

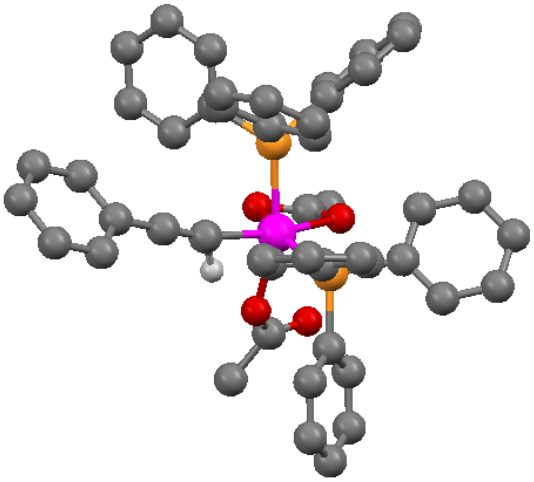
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.83	0.02523	YES	YES
8	a	12.72	0.03664	YES	YES
9	a	19.12	0.11179	YES	YES
10	a	25.20	0.42079	YES	YES
11	a	31.98	0.01837	YES	YES
12	a	37.67	0.13066	YES	YES
13	a	40.38	0.50227	YES	YES
14	a	41.06	0.06329	YES	YES
15	a	45.69	0.26582	YES	YES
16	a	48.09	0.44178	YES	YES
17	a	49.40	0.09727	YES	YES
18	a	52.45	0.07394	YES	YES

19	a	53.98	0.04792	YES	YES
20	a	55.84	0.46455	YES	YES
21	a	57.01	0.45224	YES	YES
22	a	63.95	0.11344	YES	YES
23	a	66.23	0.68250	YES	YES
24	a	68.63	0.19954	YES	YES
25	a	70.23	0.24210	YES	YES
26	a	74.89	1.92821	YES	YES
27	a	81.50	0.83289	YES	YES
28	a	85.42	1.57645	YES	YES
29	a	90.83	1.76065	YES	YES
30	a	93.75	1.17521	YES	YES
31	a	99.07	2.42834	YES	YES
32	a	102.10	0.28212	YES	YES
33	a	107.41	1.19164	YES	YES
34	a	109.99	1.38783	YES	YES
35	a	113.81	0.24900	YES	YES
36	a	114.54	0.08653	YES	YES
37	a	121.60	0.10436	YES	YES
38	a	145.81	8.04990	YES	YES
39	a	155.76	1.24472	YES	YES
40	a	165.50	0.81657	YES	YES
41	a	187.56	1.04268	YES	YES
42	a	190.22	0.36292	YES	YES
43	a	196.54	1.16852	YES	YES
44	a	201.00	4.90302	YES	YES
45	a	211.81	1.47481	YES	YES
46	a	214.48	0.36135	YES	YES
47	a	215.74	1.20517	YES	YES
48	a	218.32	4.43662	YES	YES
49	a	221.72	2.50620	YES	YES
50	a	237.10	6.73052	YES	YES
51	a	245.47	1.88207	YES	YES
52	a	246.65	1.30002	YES	YES
53	a	247.21	1.49368	YES	YES
54	a	251.01	0.79799	YES	YES
55	a	258.18	16.32106	YES	YES
56	a	268.38	1.32702	YES	YES
57	a	269.10	1.03493	YES	YES
58	a	278.08	17.58780	YES	YES
59	a	311.09	6.39065	YES	YES
60	a	333.41	7.69405	YES	YES
61	a	342.87	22.32320	YES	YES
62	a	384.93	18.23885	YES	YES
63	a	394.94	0.77167	YES	YES
64	a	398.25	0.05158	YES	YES
65	a	399.14	0.64375	YES	YES
66	a	401.64	0.02903	YES	YES
67	a	406.55	1.63442	YES	YES
68	a	408.72	1.66028	YES	YES
69	a	411.90	14.19570	YES	YES
70	a	415.55	36.32448	YES	YES
71	a	418.12	23.81183	YES	YES
72	a	425.20	27.65239	YES	YES
73	a	433.59	10.93805	YES	YES
74	a	441.51	12.33129	YES	YES
75	a	458.17	10.28294	YES	YES
76	a	463.76	23.08508	YES	YES
77	a	480.51	7.47638	YES	YES
78	a	492.31	10.27165	YES	YES
79	a	498.15	35.78443	YES	YES
80	a	499.96	4.00112	YES	YES
81	a	504.79	24.77439	YES	YES
82	a	507.72	13.15871	YES	YES
83	a	513.13	70.61152	YES	YES
84	a	516.65	201.92487	YES	YES
85	a	520.93	106.12146	YES	YES
86	a	533.67	13.09168	YES	YES
87	a	553.43	5.39628	YES	YES
88	a	592.75	3.55513	YES	YES
89	a	594.74	1.60380	YES	YES
90	a	608.00	0.43722	YES	YES
91	a	609.26	0.69988	YES	YES
92	a	609.47	0.27300	YES	YES
93	a	610.29	1.92379	YES	YES
94	a	610.77	2.08805	YES	YES
95	a	611.68	0.51013	YES	YES
96	a	612.54	0.02326	YES	YES
97	a	655.96	21.78254	YES	YES
98	a	672.06	13.54106	YES	YES
99	a	673.19	51.77527	YES	YES
100	a	675.24	25.84385	YES	YES
101	a	680.49	7.95567	YES	YES
102	a	682.64	10.77879	YES	YES
103	a	688.56	12.07274	YES	YES
104	a	692.09	28.71591	YES	YES
105	a	693.92	36.20656	YES	YES
106	a	694.78	20.78607	YES	YES
107	a	695.04	29.10433	YES	YES
108	a	698.78	20.18910	YES	YES
109	a	700.02	75.61226	YES	YES
110	a	705.77	7.57570	YES	YES
111	a	711.31	16.48572	YES	YES
112	a	738.27	8.93641	YES	YES
113	a	739.19	8.24060	YES	YES
114	a	742.52	7.87863	YES	YES
115	a	745.70	3.94781	YES	YES
116	a	745.85	1.11943	YES	YES
117	a	746.56	3.38971	YES	YES
118	a	762.18	21.54289	YES	YES
119	a	783.71	11.07332	YES	YES
120	a	830.85	0.71592	YES	YES
121	a	831.56	0.26727	YES	YES
122	a	836.90	0.27623	YES	YES
123	a	837.12	1.71273	YES	YES
124	a	837.84	0.07765	YES	YES
125	a	843.97	1.72928	YES	YES
126	a	857.34	0.92613	YES	YES
127	a	906.63	0.04031	YES	YES
128	a	908.05	0.39716	YES	YES
129	a	909.99	0.26359	YES	YES
130	a	912.80	0.85637	YES	YES
131	a	915.29	0.10871	YES	YES
132	a	915.70	1.36196	YES	YES
133	a	918.21	2.20919	YES	YES
134	a	933.51	0.38378	YES	YES
135	a	942.45	25.64711	YES	YES
136	a	955.35	0.41756	YES	YES
137	a	958.12	0.25121	YES	YES
138	a	959.38	0.07049	YES	YES
139	a	961.76	0.20948	YES	YES
140	a	964.73	0.08186	YES	YES
141	a	965.49	0.64896	YES	YES
142	a	976.64	0.73570	YES	YES
143	a	979.30	0.30268	YES	YES
144	a	980.62	0.29671	YES	YES
145	a	981.19	0.31668	YES	YES
146	a	981.98	1.74067	YES	YES
147	a	982.69	1.40138	YES	YES
148	a	983.07	1.87412	YES	YES
149	a	983.58	1.24384	YES	YES
150	a	984.06	0.53681	YES	YES
151	a	984.69	0.76653	YES	YES
152	a	984.98	3.46254	YES	YES
153	a	985.05	0.16998	YES	YES
154	a	987.30	0.43107	YES	YES
155	a	988.13	3.96265	YES	YES
156	a	988.66	1.06590	YES	YES
157	a	988.74	5.72384	YES	YES
158	a	1017.79	3.81958	YES	YES
159	a	1022.72	1.35684	YES	YES
160	a	1023.20	0.55223	YES	YES
161	a	1023.90	2.88413	YES	YES
162	a	1024.09	1.20306	YES	YES
163	a	1024.16	3.52283	YES	YES
164	a	1024.85	8.65632	YES	YES
165	a	1025.23	3.21759	YES	YES
166	a	1026.74	0.58801	YES	YES

167	a	1027.38	5.89676	YES	YES
168	a	1069.41	26.72285	YES	YES
169	a	1069.70	3.87909	YES	YES
170	a	1070.07	8.80570	YES	YES
171	a	1073.50	2.23072	YES	YES
172	a	1073.86	32.63586	YES	YES
173	a	1074.44	23.01330	YES	YES
174	a	1075.46	25.65265	YES	YES
175	a	1077.07	3.43441	YES	YES
176	a	1077.47	1.35609	YES	YES
177	a	1078.74	1.36410	YES	YES
178	a	1080.28	14.45424	YES	YES
179	a	1082.79	21.04450	YES	YES
180	a	1083.35	11.61773	YES	YES
181	a	1104.29	543.22966	YES	YES
182	a	1139.87	0.49076	YES	YES
183	a	1141.93	0.35982	YES	YES
184	a	1141.96	0.49929	YES	YES
185	a	1142.44	0.12697	YES	YES
186	a	1142.93	0.14578	YES	YES
187	a	1143.15	0.26770	YES	YES
188	a	1144.47	0.64225	YES	YES
189	a	1158.91	7.18789	YES	YES
190	a	1167.32	2.01378	YES	YES
191	a	1169.37	3.49226	YES	YES
192	a	1171.05	10.01226	YES	YES
193	a	1172.83	6.88631	YES	YES
194	a	1173.85	0.88435	YES	YES
195	a	1180.74	6.60486	YES	YES
196	a	1222.12	16.76919	YES	YES
197	a	1289.90	3.33546	YES	YES
198	a	1290.84	4.49857	YES	YES

* zero point VIBRATIONAL energy : 0.7436358 Hartree *

Cis 3_afbx



bp86-SVP SCF energy: -2931.4148277940
pbe-TZVPP SCF energy: -2930.963027787

XYZ Coordinates
97

C	-1.99498	1.12261	-2.00215
C	-1.00606	1.15776	-1.22512
C	-3.12267	1.06529	-2.86236
H	-0.22288	2.00801	-1.16714
C	-5.38038	0.95696	-4.57999
C	-5.54511	1.24996	-3.21308
C	-4.43498	1.31078	-2.36201
C	-2.97408	0.76974	-4.24923
C	-4.09030	0.72188	-5.09280
H	-6.25709	0.91547	-5.24709
H	-6.55286	1.43911	-2.80720
H	-4.56062	1.54969	-1.29389
H	-1.96413	0.59054	-4.65101
H	-3.95528	0.49780	-6.16407
C	0.88847	2.16096	2.55490
C	1.38706	2.90389	3.76025
H	2.18358	3.59196	3.40168
H	1.83084	2.20146	4.49529
H	0.57216	3.49856	4.22157
C	2.15679	3.64354	-0.02893
C	2.27024	4.88781	-0.91934
H	2.92926	5.63946	-0.43962
H	1.26392	5.32880	-1.09297
H	2.68116	4.60769	-1.91377
C	-0.95902	-1.04227	2.98264
C	-0.88427	-0.08940	4.02639
H	-1.03712	0.97801	3.80207
C	-0.65473	-0.49034	5.35094
H	-0.60352	0.26978	6.14824
C	-0.49973	-1.85295	5.66209
H	-0.32101	-2.16865	6.70337
C	-0.58962	-2.80822	4.63757
H	-0.49136	-3.88187	4.86964
C	-0.81840	-2.40740	3.30774
H	-0.90963	-3.17951	2.52905
C	-1.83904	-1.85090	0.29502
C	-0.96751	-2.94825	0.10491
H	0.05813	-2.91978	0.50518
C	-1.38648	-4.08393	-0.60671
H	-0.69324	-4.93110	-0.73228
C	-2.67139	-4.12863	-1.17313
H	-2.99832	-5.01747	-1.73777
C	-3.52919	-3.02592	-1.03042
H	-4.53171	-3.03859	-1.48914
C	-3.11930	-1.89751	-0.29935
H	-3.80901	-1.04751	-0.19109
C	-2.85991	0.52756	1.62547
C	-3.88193	-0.14921	2.33244
H	-3.73766	-1.19775	2.64119
C	-5.08374	0.50143	2.65069
H	-5.87073	-0.04275	3.19904
C	-5.27745	1.84445	2.28004
H	-6.21788	2.35993	2.53765
C	-4.26291	2.52729	1.59065
H	-4.39868	3.58450	1.30843
C	-3.06067	1.87362	1.26148
H	-2.26874	2.42137	0.73366
C	1.29962	-1.79865	-1.90161
C	1.95923	-3.04790	-1.92875
H	2.77410	-3.25968	-1.21956
C	1.58562	-4.03271	-2.85931
H	2.11381	-5.00118	-2.86664
C	0.54988	-3.78622	-3.77636
H	0.25868	-4.56013	-4.50608
C	-0.11644	-2.54961	-3.75116
H	-0.94004	-2.34897	-4.45606
C	0.25310	-1.56437	-2.82025
H	-0.28621	-0.60531	-2.79424
C	3.06148	0.47592	-1.82396
C	3.13196	0.30277	-3.22087
H	2.44513	-0.39000	-3.73125
C	4.08801	1.00572	-3.97790
H	4.13118	0.85856	-5.07006
C	4.98600	1.88022	-3.34620
H	5.73909	2.42592	-3.93911
C	4.91869	2.05757	-1.95171
H	5.61201	2.74867	-1.44416
C	3.95931	1.36827	-1.19489
H	3.90395	1.54020	-0.10743
C	2.96241	-1.31103	0.42889
C	4.29201	-1.63418	0.06951
H	4.69075	-1.32072	-0.90791
C	5.11586	-2.35288	0.95122
H	6.15063	-2.59317	0.65521
C	4.62675	-2.75844	2.20535
H	5.27670	-3.31724	2.89939
C	3.30996	-2.43716	2.57266
H	2.91739	-2.73461	3.55886
C	2.48570	-1.71489	1.69286
H	1.47061	-1.43896	2.01122
O	1.48302	1.09455	2.14904
O	-0.12607	2.56241	1.88293
O	2.75695	3.56376	1.04722
O	1.39945	2.71588	-0.56929
P	-1.26052	-0.37230	1.25875
P	1.82784	-0.42385	-0.75523
Ru	0.38258	1.04133	0.34019

Vibrational Frequencies

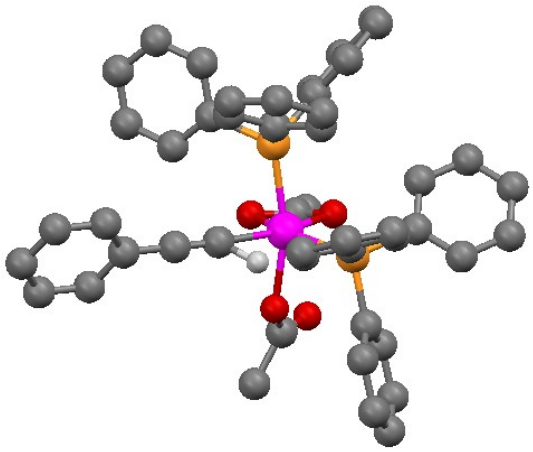
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.42	0.12597	YES	YES
8	a	14.71	0.01238	YES	YES
9	a	20.63	0.02727	YES	YES
10	a	21.56	0.00591	YES	YES
11	a	32.01	0.26424	YES	YES
12	a	34.23	0.26840	YES	YES
13	a	36.67	0.09736	YES	YES
14	a	38.45	0.14912	YES	YES
15	a	42.08	0.20672	YES	YES
16	a	46.66	0.25207	YES	YES
17	a	49.10	1.63087	YES	YES
18	a	50.86	0.35050	YES	YES

19	a	54.58	0.59378	YES	YES
20	a	55.88	0.06148	YES	YES
21	a	58.77	0.14534	YES	YES
22	a	63.13	0.13233	YES	YES
23	a	66.08	0.46138	YES	YES
24	a	71.63	0.32839	YES	YES
25	a	73.71	0.84731	YES	YES
26	a	74.58	0.55964	YES	YES
27	a	82.40	0.67825	YES	YES
28	a	87.90	1.11202	YES	YES
29	a	90.43	0.81707	YES	YES
30	a	91.58	0.62174	YES	YES
31	a	93.76	0.42531	YES	YES
32	a	100.50	0.94193	YES	YES
33	a	107.97	1.80674	YES	YES
34	a	113.34	0.82669	YES	YES
35	a	117.38	1.12278	YES	YES
36	a	117.88	0.67288	YES	YES
37	a	130.72	0.52708	YES	YES
38	a	141.23	8.84423	YES	YES
39	a	159.10	0.87969	YES	YES
40	a	165.08	4.72745	YES	YES
41	a	177.95	0.18607	YES	YES
42	a	190.45	2.33648	YES	YES
43	a	193.58	1.07265	YES	YES
44	a	198.69	0.80804	YES	YES
45	a	206.60	4.55546	YES	YES
46	a	209.06	2.94083	YES	YES
47	a	216.70	3.26626	YES	YES
48	a	226.09	8.95452	YES	YES
49	a	230.11	10.77537	YES	YES
50	a	235.60	4.22139	YES	YES
51	a	243.19	15.53094	YES	YES
52	a	246.98	0.57682	YES	YES
53	a	248.14	2.22947	YES	YES
54	a	250.45	4.82740	YES	YES
55	a	253.79	0.69117	YES	YES
56	a	257.48	17.49941	YES	YES
57	a	265.65	1.57586	YES	YES
58	a	269.28	2.63925	YES	YES
59	a	284.81	9.02736	YES	YES
60	a	334.00	9.70290	YES	YES
61	a	360.60	7.40884	YES	YES
62	a	369.09	19.18654	YES	YES
63	a	393.44	0.58283	YES	YES
64	a	399.76	0.16745	YES	YES
65	a	400.67	0.83187	YES	YES
66	a	400.83	0.38953	YES	YES
67	a	402.94	47.86963	YES	YES
68	a	407.48	0.39771	YES	YES
69	a	408.70	6.31307	YES	YES
70	a	412.97	3.30572	YES	YES
71	a	418.38	33.55659	YES	YES
72	a	424.90	8.69998	YES	YES
73	a	428.12	18.63158	YES	YES
74	a	432.55	21.73827	YES	YES
75	a	450.72	4.67949	YES	YES
76	a	461.09	15.66178	YES	YES
77	a	482.42	3.44209	YES	YES
78	a	487.58	6.65631	YES	YES
79	a	488.60	9.44055	YES	YES
80	a	498.84	14.93083	YES	YES
81	a	503.13	16.20846	YES	YES
82	a	506.90	8.16367	YES	YES
83	a	509.12	48.99692	YES	YES
84	a	513.50	46.90480	YES	YES
85	a	516.25	173.01791	YES	YES
86	a	529.52	48.81038	YES	YES
87	a	557.86	16.21379	YES	YES
88	a	571.51	8.50755	YES	YES
89	a	585.95	4.53628	YES	YES
90	a	608.47	0.16651	YES	YES
91	a	608.85	0.53309	YES	YES
92	a	609.56	0.73966	YES	YES
93	a	610.07	0.14427	YES	YES
94	a	611.21	1.69467	YES	YES
95	a	611.72	0.32136	YES	YES
96	a	612.31	0.08433	YES	YES
97	a	637.53	9.35690	YES	YES
98	a	670.88	10.54618	YES	YES
99	a	674.22	13.95266	YES	YES
100	a	677.90	51.50270	YES	YES
101	a	679.28	10.85831	YES	YES
102	a	682.48	8.73759	YES	YES
103	a	687.08	11.30701	YES	YES
104	a	688.21	22.31865	YES	YES
105	a	690.60	31.78953	YES	YES
106	a	694.07	35.38445	YES	YES
107	a	694.43	31.93662	YES	YES
108	a	700.02	38.82813	YES	YES
109	a	700.72	35.29096	YES	YES
110	a	700.92	33.43099	YES	YES
111	a	706.45	7.00143	YES	YES
112	a	735.21	6.55645	YES	YES
113	a	741.04	7.30198	YES	YES
114	a	741.51	8.02284	YES	YES
115	a	743.17	7.37337	YES	YES
116	a	746.23	4.26240	YES	YES
117	a	747.47	4.63769	YES	YES
118	a	762.61	25.91570	YES	YES
119	a	773.11	0.50089	YES	YES
120	a	830.02	0.29792	YES	YES
121	a	832.64	0.54826	YES	YES
122	a	835.54	0.95108	YES	YES
123	a	836.18	0.54485	YES	YES
124	a	838.20	2.36684	YES	YES
125	a	840.60	0.84007	YES	YES
126	a	843.03	0.79976	YES	YES
127	a	906.31	6.12927	YES	YES
128	a	906.83	0.52245	YES	YES
129	a	908.34	0.30642	YES	YES
130	a	909.85	1.38777	YES	YES
131	a	911.47	3.32276	YES	YES
132	a	913.92	1.99189	YES	YES
133	a	914.51	2.95233	YES	YES
134	a	916.87	0.17231	YES	YES
135	a	942.52	11.94054	YES	YES
136	a	955.90	0.19860	YES	YES
137	a	958.47	0.98787	YES	YES
138	a	960.01	1.04084	YES	YES
139	a	961.23	0.34610	YES	YES
140	a	961.30	1.42417	YES	YES
141	a	964.16	0.42270	YES	YES
142	a	965.59	0.31787	YES	YES
143	a	978.51	11.08928	YES	YES
144	a	980.96	0.98430	YES	YES
145	a	981.11	0.66519	YES	YES
146	a	982.15	1.84738	YES	YES
147	a	982.52	0.45526	YES	YES
148	a	983.08	0.32940	YES	YES
149	a	983.38	0.81639	YES	YES
150	a	983.66	1.34025	YES	YES
151	a	984.12	5.63734	YES	YES
152	a	984.70	1.25510	YES	YES
153	a	985.14	10.54598	YES	YES
154	a	985.64	5.67797	YES	YES
155	a	986.19	0.48876	YES	YES
156	a	986.64	1.85591	YES	YES
157	a	986.87	1.87497	YES	YES
158	a	988.06	1.97326	YES	YES
159	a	1014.70	107.69414	YES	YES
160	a	1016.92	12.36047	YES	YES
161	a	1022.76	45.14356	YES	YES
162	a	1023.06	39.21584	YES	YES
163	a	1023.59	2.40203	YES	YES
164	a	1024.00	3.25562	YES	YES
165	a	1024.35	1.43287	YES	YES
166	a	1025.37	5.57344	YES	YES

167	a	1025.97	13.16078	YES	YES
168	a	1026.92	432.85408	YES	YES
169	a	1068.27	27.54882	YES	YES
170	a	1070.24	11.21345	YES	YES
171	a	1071.53	3.16182	YES	YES
172	a	1072.07	16.24137	YES	YES
173	a	1073.19	18.53963	YES	YES
174	a	1073.93	14.21495	YES	YES
175	a	1075.41	2.00135	YES	YES
176	a	1076.79	8.03868	YES	YES
177	a	1077.66	8.03861	YES	YES
178	a	1078.95	2.36117	YES	YES
179	a	1079.43	0.07049	YES	YES
180	a	1080.74	9.52227	YES	YES
181	a	1081.99	12.12989	YES	YES
182	a	1140.65	0.10789	YES	YES
183	a	1141.10	0.20660	YES	YES
184	a	1141.89	0.30449	YES	YES
185	a	1142.08	0.13726	YES	YES
186	a	1142.37	0.41294	YES	YES
187	a	1142.49	0.60110	YES	YES
188	a	1143.23	0.47190	YES	YES
189	a	1158.42	0.79087	YES	YES
190	a	1166.40	3.03600	YES	YES
191	a	1167.45	8.24174	YES	YES
192	a	1168.58	1.73363	YES	YES
193	a	1173.29	1.88368	YES	YES
194	a	1174.56	2.51498	YES	YES
195	a	1175.57	1.31134	YES	YES
196	a	1208.86	3.17695	YES	YES
197	a	1282.16	394.88982	YES	YES
198	a	1286.98	0.17466	YES	YES

* zero point VIBRATIONAL energy : 0.7430033 Hartree *

Cis 3_afby



bp86-SVP SCF energy: -2931.4179705050
pbe-TZVPP SCF energy: -2930.968169239

XYZ Coordinates
97

C	-2.46945	0.06143	-2.08941
C	-1.42752	0.29282	-1.43869
C	-3.67965	-0.11806	-2.81465
H	-0.30970	-0.06419	-1.65236
C	-6.09184	-0.46179	-4.27135
C	-5.31629	0.69922	-4.45075
C	-4.12489	0.87353	-3.73530
C	-4.47476	-1.28753	-2.64658
C	-5.66453	-1.45230	-3.36740
H	-7.02878	-0.59474	-4.83711
H	-5.64524	1.47824	-5.15866
H	-3.51432	1.77960	-3.87391
H	-4.13677	-2.06264	-1.94066
H	-6.26808	-2.36410	-3.22373
C	0.38862	3.14181	0.99783
C	0.69068	4.48099	1.60354
H	1.19373	5.07857	0.81286
H	1.38376	4.37288	2.46288
H	-0.24402	4.99349	1.91090
C	1.16973	3.25011	-2.11652
C	1.03111	3.77094	-3.55452
H	1.52153	4.76121	-3.64727
H	-0.04512	3.86399	-3.82021
H	1.48511	3.05390	-4.27190
C	-0.47098	0.14861	3.26731
C	-0.47144	1.48519	3.73179
H	-0.83030	2.29128	3.07313
C	-0.06877	1.79222	5.03991
H	-0.08060	2.84077	5.38062
C	0.33631	0.76841	5.91461
H	0.65002	1.00888	6.94407
C	0.32163	-0.56355	5.47110
H	0.61585	-1.37849	6.15360
C	-0.07976	-0.87300	4.15815
H	-0.10226	-1.92736	3.84425
C	-1.31209	-1.94707	1.37671
C	-0.23012	-2.83539	1.57289
H	0.77565	-2.44513	1.79572
C	-0.41561	-4.22455	1.48257
H	0.43914	-4.89882	1.65351
C	-1.67823	-4.74939	1.15956
H	-1.82326	-5.84000	1.08542
C	-2.75068	-3.87447	0.92055
H	-3.74303	-4.27429	0.65298
C	-2.57193	-2.48462	1.03103
H	-3.42550	-1.81297	0.85375
C	-2.79018	0.52333	1.73745
C	-3.53704	0.05332	2.84431
H	-3.09546	-0.68198	3.53722
C	-4.84084	0.51572	3.07642
H	-5.40813	0.13598	3.94270
C	-5.41620	1.46429	2.21134
H	-6.43913	1.83319	2.39586
C	-4.67821	1.94251	1.11808
H	-5.11663	2.69080	0.43750
C	-3.37189	1.47655	0.87882
H	-2.80225	1.86847	0.02670
C	1.66766	-2.31510	-1.00400
C	2.56933	-3.30957	-0.56405
H	3.42246	-3.03766	0.07642
C	2.38878	-4.65303	-0.93438
H	3.10393	-5.41474	-0.58107
C	1.30823	-5.02388	-1.75231
H	1.16921	-6.07792	-2.04509
C	0.40236	-4.04334	-2.18970
H	-0.45448	-4.32134	-2.82482
C	0.57669	-2.70100	-1.81442
H	-0.15750	-1.95776	-2.16223
C	2.95798	0.02614	-2.09335
C	3.13470	-0.77594	-3.23850
H	2.65021	-1.76208	-3.30823
C	3.93981	-0.32628	-4.30213
H	4.06925	-0.96407	-5.19230
C	4.57527	0.92303	-4.22725
H	5.20728	1.27398	-5.06011
C	4.39779	1.72826	-3.08634
H	4.88003	2.71762	-3.02322
C	3.59102	1.28812	-2.02671
H	3.43807	1.94451	-1.15472
C	3.22961	-0.51148	0.70476
C	4.58177	-0.79108	0.39340
H	4.88285	-0.97165	-0.65049
C	5.55102	-0.83326	1.40858
H	6.60025	-1.05341	1.14999
C	5.18815	-0.58495	2.74425
H	5.95246	-0.60985	3.53896
C	3.85187	-0.29023	3.05754
H	3.55628	-0.07444	4.09709
C	2.87842	-0.25090	2.04407
H	1.84342	0.01469	2.29828
O	1.24037	2.17779	1.06422
O	-0.71839	2.89707	0.40592
O	1.69380	3.94310	-1.23543
O	0.69418	2.03705	-1.98973
P	-1.04535	-0.11357	1.50260
P	1.93673	-0.50781	-0.63162
Ru	0.14060	0.95127	-0.25088

Vibrational Frequencies

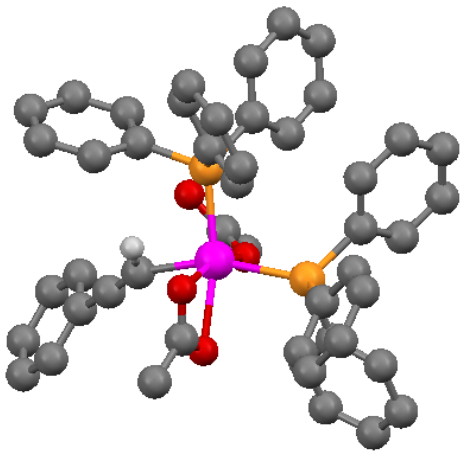
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.38	0.30683	YES	YES
8	a	14.87	0.18223	YES	YES
9	a	16.04	0.08640	YES	YES
10	a	19.28	0.06549	YES	YES
11	a	24.55	0.07922	YES	YES
12	a	32.32	0.29700	YES	YES
13	a	33.84	0.10568	YES	YES
14	a	36.56	0.14315	YES	YES
15	a	42.52	0.04453	YES	YES
16	a	43.87	2.08611	YES	YES
17	a	45.99	0.11533	YES	YES
18	a	49.00	0.20034	YES	YES
19	a	54.25	0.10536	YES	YES

20	a	54.95	0.05290	YES	YES
21	a	57.41	0.14076	YES	YES
22	a	60.97	0.04413	YES	YES
23	a	64.12	1.00600	YES	YES
24	a	66.81	0.81473	YES	YES
25	a	73.33	0.62956	YES	YES
26	a	74.35	0.02400	YES	YES
27	a	78.70	0.25998	YES	YES
28	a	84.65	0.89638	YES	YES
29	a	88.11	0.20546	YES	YES
30	a	91.10	0.83588	YES	YES
31	a	93.82	0.10518	YES	YES
32	a	98.84	0.95162	YES	YES
33	a	109.01	2.25918	YES	YES
34	a	112.86	0.89743	YES	YES
35	a	115.57	0.71707	YES	YES
36	a	117.39	0.06485	YES	YES
37	a	138.76	2.34497	YES	YES
38	a	150.54	5.63920	YES	YES
39	a	162.28	1.00829	YES	YES
40	a	164.36	2.48478	YES	YES
41	a	177.70	1.26729	YES	YES
42	a	192.36	1.30228	YES	YES
43	a	198.01	1.63007	YES	YES
44	a	198.26	2.11150	YES	YES
45	a	209.59	4.37268	YES	YES
46	a	213.30	1.17806	YES	YES
47	a	218.58	1.44632	YES	YES
48	a	227.66	0.75599	YES	YES
49	a	230.33	9.01639	YES	YES
50	a	237.38	3.30016	YES	YES
51	a	247.16	0.62968	YES	YES
52	a	248.22	0.08755	YES	YES
53	a	249.45	2.96430	YES	YES
54	a	251.92	5.97313	YES	YES
55	a	257.72	10.26371	YES	YES
56	a	265.16	2.05505	YES	YES
57	a	269.56	0.50800	YES	YES
58	a	282.08	8.96424	YES	YES
59	a	306.65	5.18112	YES	YES
60	a	340.85	3.82220	YES	YES
61	a	360.51	17.19154	YES	YES
62	a	391.77	2.23508	YES	YES
63	a	397.71	0.16551	YES	YES
64	a	398.83	0.34353	YES	YES
65	a	400.44	2.66922	YES	YES
66	a	402.88	0.45237	YES	YES
67	a	404.58	0.86495	YES	YES
68	a	411.57	7.86774	YES	YES
69	a	412.94	25.82253	YES	YES
70	a	418.35	66.54860	YES	YES
71	a	422.51	20.20882	YES	YES
72	a	427.13	0.68276	YES	YES
73	a	438.72	11.75765	YES	YES
74	a	443.28	29.25230	YES	YES
75	a	458.58	7.75703	YES	YES
76	a	486.09	2.73636	YES	YES
77	a	487.51	25.33641	YES	YES
78	a	490.45	2.34307	YES	YES
79	a	498.70	39.41181	YES	YES
80	a	502.19	30.18810	YES	YES
81	a	505.12	5.11169	YES	YES
82	a	508.20	26.94471	YES	YES
83	a	514.22	173.65085	YES	YES
84	a	516.74	111.99256	YES	YES
85	a	526.45	74.31624	YES	YES
86	a	533.23	4.86730	YES	YES
87	a	556.00	12.08088	YES	YES
88	a	561.95	4.04509	YES	YES
89	a	585.74	2.86844	YES	YES
90	a	608.39	0.31619	YES	YES
91	a	608.78	0.32511	YES	YES
92	a	609.22	1.18572	YES	YES
93	a	609.90	0.33005	YES	YES
94	a	610.50	1.53732	YES	YES
95	a	611.57	0.45737	YES	YES
96	a	612.77	0.09224	YES	YES
97	a	645.08	8.93074	YES	YES
98	a	670.93	9.82540	YES	YES
99	a	674.77	16.73721	YES	YES
100	a	678.87	6.35581	YES	YES
101	a	679.77	57.11709	YES	YES
102	a	683.26	7.83183	YES	YES
103	a	687.98	13.46402	YES	YES
104	a	688.70	15.18942	YES	YES
105	a	690.00	36.23107	YES	YES
106	a	692.98	43.42008	YES	YES
107	a	696.55	33.74782	YES	YES
108	a	696.99	26.70831	YES	YES
109	a	698.06	22.78502	YES	YES
110	a	698.88	48.47104	YES	YES
111	a	706.05	9.89408	YES	YES
112	a	737.52	10.26357	YES	YES
113	a	740.42	5.03080	YES	YES
114	a	741.18	6.91510	YES	YES
115	a	743.29	4.87507	YES	YES
116	a	745.70	4.07521	YES	YES
117	a	747.39	5.47526	YES	YES
118	a	760.52	23.32632	YES	YES
119	a	780.62	8.96591	YES	YES
120	a	828.94	0.04545	YES	YES
121	a	831.98	1.04812	YES	YES
122	a	832.31	0.14535	YES	YES
123	a	833.74	1.01424	YES	YES
124	a	834.85	1.75717	YES	YES
125	a	837.29	0.11103	YES	YES
126	a	842.57	0.97466	YES	YES
127	a	904.74	0.52139	YES	YES
128	a	905.59	0.10995	YES	YES
129	a	906.24	1.67676	YES	YES
130	a	907.74	0.37555	YES	YES
131	a	911.13	0.45342	YES	YES
132	a	911.77	0.82382	YES	YES
133	a	913.51	0.36168	YES	YES
134	a	914.97	0.20731	YES	YES
135	a	943.73	17.59380	YES	YES
136	a	956.63	0.09749	YES	YES
137	a	957.01	0.44407	YES	YES
138	a	957.64	0.18348	YES	YES
139	a	957.90	0.04002	YES	YES
140	a	958.88	0.28981	YES	YES
141	a	961.90	0.09765	YES	YES
142	a	964.28	0.16320	YES	YES
143	a	979.75	0.06589	YES	YES
144	a	980.35	0.87757	YES	YES
145	a	981.17	0.07169	YES	YES
146	a	981.34	1.15308	YES	YES
147	a	982.11	1.46810	YES	YES
148	a	982.20	1.43131	YES	YES
149	a	982.93	0.44890	YES	YES
150	a	983.44	2.96105	YES	YES
151	a	983.86	1.44874	YES	YES
152	a	984.18	0.82582	YES	YES
153	a	985.79	7.92699	YES	YES
154	a	985.91	0.07106	YES	YES
155	a	986.56	1.38419	YES	YES
156	a	986.77	1.06930	YES	YES
157	a	987.66	2.84076	YES	YES
158	a	988.23	0.85092	YES	YES
159	a	1013.13	16.81058	YES	YES
160	a	1015.92	5.11448	YES	YES
161	a	1022.96	1.58582	YES	YES
162	a	1023.21	0.45356	YES	YES
163	a	1023.47	0.83502	YES	YES
164	a	1024.14	2.14621	YES	YES
165	a	1024.28	2.25834	YES	YES
166	a	1025.06	0.66886	YES	YES
167	a	1025.69	0.90417	YES	YES

168	a	1068.75	21.44623	YES	YES
169	a	1070.07	16.27073	YES	YES
170	a	1070.31	3.92568	YES	YES
171	a	1071.10	5.17819	YES	YES
172	a	1072.18	21.04611	YES	YES
173	a	1073.55	18.32534	YES	YES
174	a	1075.45	14.04550	YES	YES
175	a	1076.72	3.60541	YES	YES
176	a	1078.22	0.17370	YES	YES
177	a	1078.60	6.08243	YES	YES
178	a	1079.65	3.77315	YES	YES
179	a	1081.13	14.76572	YES	YES
180	a	1082.57	7.33796	YES	YES
181	a	1141.23	0.05829	YES	YES
182	a	1141.27	0.13404	YES	YES
183	a	1141.97	0.40867	YES	YES
184	a	1142.21	0.19853	YES	YES
185	a	1142.80	0.45091	YES	YES
186	a	1143.02	0.11693	YES	YES
187	a	1143.72	0.43376	YES	YES
188	a	1156.38	10.59671	YES	YES
189	a	1164.28	3.80905	YES	YES
190	a	1167.84	3.69734	YES	YES
191	a	1171.01	5.11291	YES	YES
192	a	1172.15	4.14321	YES	YES
193	a	1172.94	3.64624	YES	YES
194	a	1173.78	1.41995	YES	YES
195	a	1200.66	119.75812	YES	YES
196	a	1258.39	321.22281	YES	YES
197	a	1286.13	6.95630	YES	YES
198	a	1287.51	0.97136	YES	YES

* zero point VIBRATIONAL energy : 0.7434893 Hartree *

Cis 3_pfay



bp86-SVP SCF energy: -2931.4121714070
pbe-TZVPP SCF energy: -2930.959478585

XYZ Coordinates
97

C	1.16797	-3.51438	0.74584
C	0.60913	-2.40668	0.89144
C	1.74290	-4.75942	0.38490
H	-0.22121	-1.98101	1.51863
C	2.84273	-7.24934	-0.38572
C	1.80244	-6.67419	-1.14112
C	1.25117	-5.44329	-0.76574
C	2.79728	-5.34921	1.13720
C	3.33661	-6.58293	0.75184
H	3.27154	-8.21994	-0.68592
H	1.41789	-7.19369	-2.03480
H	0.44487	-4.96936	-1.34911
H	3.18099	-4.82153	2.02472
H	4.15256	-7.03207	1.34224
C	1.74284	-0.09361	2.70505
C	2.41057	-0.12965	4.05956
H	2.20304	-1.11209	4.54003
H	1.99538	0.66178	4.71791
H	3.50853	-0.01575	3.95762
C	0.53205	-1.87813	-2.13827
C	1.43905	-2.23316	-3.32246
H	0.83805	-2.70063	-4.12966
H	2.19554	-2.97704	-2.98409
H	1.98293	-1.34658	-3.70934
C	1.27463	3.16328	1.09344
C	2.25834	2.98040	2.09461
H	2.92194	2.10344	2.04823
C	2.42480	3.92411	3.11967
H	3.20328	3.76381	3.88401
C	1.61446	5.07236	3.16603
H	1.74767	5.81527	3.96997
C	0.64500	5.27109	2.17045
H	0.01620	6.17721	2.18084
C	0.47637	4.32627	1.14118
H	-0.27364	4.52139	0.36010
C	0.24494	2.70756	-1.60677
C	-1.10212	3.10546	-1.44120
H	-1.64372	2.86872	-0.51144
C	-1.77707	3.79564	-2.46007
H	-2.82451	4.10152	-2.30548
C	-1.13095	4.06665	-3.67747
H	-1.66405	4.60026	-4.48183
C	0.19265	3.63787	-3.86908
H	0.70472	3.82937	-4.82705
C	0.87912	2.96825	-2.84126
H	1.91858	2.64660	-3.00596
C	2.90103	1.81928	-0.80720
C	3.59514	3.04708	-0.92779
H	3.09268	3.99494	-0.67526
C	4.92808	3.07298	-1.36696
H	5.45404	4.03828	-1.45617
C	5.58907	1.87252	-1.68360
H	6.63874	1.89122	-2.02171
C	4.90579	0.65177	-1.56374
H	5.41687	-0.29477	-1.80597
C	3.56770	0.61976	-1.13052
H	3.02681	-0.33353	-1.05671
C	-2.65834	0.12700	-1.49050
C	-4.05500	0.29305	-1.62980
H	-4.71720	0.22165	-0.75476
C	-4.62403	0.54859	-2.88806
H	-5.71672	0.67016	-2.97672
C	-3.80594	0.64212	-4.02795
H	-4.25380	0.83693	-5.01694
C	-2.41683	0.48796	-3.89712
H	-1.76373	0.56615	-4.78166
C	-1.84637	0.23823	-2.63735
H	-0.75701	0.14206	-2.53460
C	-2.65608	-1.91847	0.58368
C	-3.09075	-2.81922	-0.40910
H	-2.98951	-2.55523	-1.47126
C	-3.62326	-4.06785	-0.04455
H	-3.96075	-4.76301	-0.83123
C	-3.71388	-4.43686	1.30813
H	-4.12858	-5.41946	1.58894
C	-3.26747	-3.54919	2.30264
H	-3.33078	-3.82976	3.36734
C	-2.74190	-2.29701	1.94365
H	-2.40673	-1.60365	2.73414
C	-2.78592	0.82650	1.35857
C	-4.13688	0.59839	1.71553
H	-4.67256	-0.28142	1.32559
C	-4.80332	1.46198	2.60019
H	-5.85615	1.26447	2.86295
C	-4.12960	2.56241	3.15867
H	-4.65295	3.23715	3.85664
C	-2.77975	2.77959	2.83995
H	-2.22706	3.61911	3.29289
C	-2.11436	1.91408	1.95370
H	-1.04412	2.06638	1.75099
O	0.47951	0.12646	2.61836
O	2.39777	-0.31315	1.63265
O	-0.49169	-2.52868	-1.90217
O	0.97605	-0.85208	-1.44983
P	1.12864	1.83694	-0.22280
P	-1.86981	-0.28413	0.15366
Ru	0.41621	-0.31083	0.50519

Vibrational Frequencies

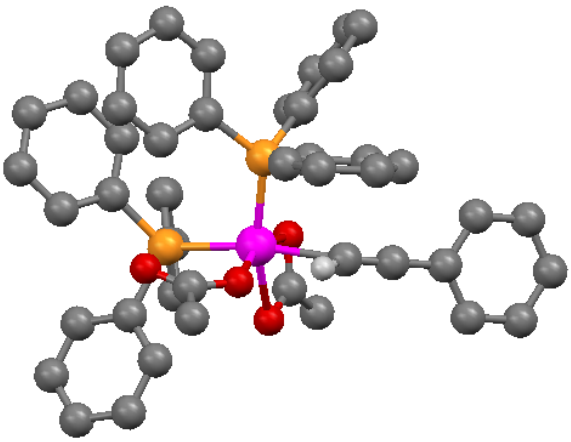
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.09	0.11743	YES	YES
8	a	9.68	0.10217	YES	YES
9	a	12.25	0.01817	YES	YES
10	a	22.00	0.14052	YES	YES
11	a	28.83	0.16933	YES	YES
12	a	30.92	0.31282	YES	YES
13	a	39.03	0.23964	YES	YES
14	a	44.01	0.14944	YES	YES
15	a	46.13	0.04536	YES	YES
16	a	47.87	0.43140	YES	YES
17	a	51.18	0.16538	YES	YES
18	a	54.95	0.31302	YES	YES

19	a	57.92	0.46051	YES	YES
20	a	59.29	0.36952	YES	YES
21	a	63.51	0.57846	YES	YES
22	a	64.70	0.66699	YES	YES
23	a	67.18	1.58325	YES	YES
24	a	70.81	0.03772	YES	YES
25	a	75.01	1.34670	YES	YES
26	a	77.04	1.21134	YES	YES
27	a	78.77	1.23185	YES	YES
28	a	85.42	0.31103	YES	YES
29	a	90.66	0.40689	YES	YES
30	a	92.74	1.13983	YES	YES
31	a	96.67	0.43128	YES	YES
32	a	99.44	0.31997	YES	YES
33	a	102.50	0.12127	YES	YES
34	a	105.42	0.72602	YES	YES
35	a	110.89	0.52767	YES	YES
36	a	115.93	0.33925	YES	YES
37	a	123.31	1.36639	YES	YES
38	a	135.35	3.28838	YES	YES
39	a	157.34	3.32097	YES	YES
40	a	165.22	1.42062	YES	YES
41	a	172.99	1.28049	YES	YES
42	a	187.34	5.38873	YES	YES
43	a	189.15	10.17812	YES	YES
44	a	197.62	0.76420	YES	YES
45	a	200.99	5.09803	YES	YES
46	a	208.02	1.87623	YES	YES
47	a	212.79	0.98978	YES	YES
48	a	222.88	1.41203	YES	YES
49	a	225.08	3.34111	YES	YES
50	a	236.45	68.27474	YES	YES
51	a	243.42	0.97282	YES	YES
52	a	247.89	0.45130	YES	YES
53	a	248.78	0.62380	YES	YES
54	a	249.51	1.31809	YES	YES
55	a	253.30	1.57553	YES	YES
56	a	267.26	0.16726	YES	YES
57	a	270.35	1.35126	YES	YES
58	a	276.60	1.26003	YES	YES
59	a	296.68	27.32451	YES	YES
60	a	304.68	1.46643	YES	YES
61	a	321.90	13.97804	YES	YES
62	a	386.52	123.24957	YES	YES
63	a	396.29	3.36561	YES	YES
64	a	397.84	1.04485	YES	YES
65	a	398.87	5.38935	YES	YES
66	a	400.37	1.46181	YES	YES
67	a	403.46	0.67984	YES	YES
68	a	408.06	0.55834	YES	YES
69	a	410.47	0.18499	YES	YES
70	a	412.81	20.36925	YES	YES
71	a	420.97	12.28065	YES	YES
72	a	424.07	16.32616	YES	YES
73	a	434.98	7.87070	YES	YES
74	a	447.47	29.57729	YES	YES
75	a	455.41	6.05970	YES	YES
76	a	463.97	25.55678	YES	YES
77	a	478.92	16.61057	YES	YES
78	a	486.54	15.87802	YES	YES
79	a	490.12	17.46177	YES	YES
80	a	497.46	37.32751	YES	YES
81	a	502.22	19.62290	YES	YES
82	a	507.05	35.15449	YES	YES
83	a	512.71	23.17414	YES	YES
84	a	515.43	111.30865	YES	YES
85	a	520.90	39.96087	YES	YES
86	a	526.45	193.22414	YES	YES
87	a	552.28	24.80166	YES	YES
88	a	596.30	6.48632	YES	YES
89	a	599.28	1.51389	YES	YES
90	a	608.71	0.09081	YES	YES
91	a	609.01	0.43060	YES	YES
92	a	610.00	0.04147	YES	YES
93	a	610.39	2.70845	YES	YES
94	a	611.36	0.14957	YES	YES
95	a	612.12	0.42366	YES	YES
96	a	612.68	1.19985	YES	YES
97	a	660.92	20.09216	YES	YES
98	a	666.50	46.09414	YES	YES
99	a	670.36	12.88904	YES	YES
100	a	672.39	29.58887	YES	YES
101	a	680.57	10.73656	YES	YES
102	a	680.59	11.07730	YES	YES
103	a	684.65	23.99666	YES	YES
104	a	687.05	20.99150	YES	YES
105	a	692.05	44.97382	YES	YES
106	a	692.69	14.71590	YES	YES
107	a	695.15	31.70195	YES	YES
108	a	698.24	28.88925	YES	YES
109	a	698.70	60.72118	YES	YES
110	a	703.44	14.56225	YES	YES
111	a	704.74	13.60569	YES	YES
112	a	712.36	409.70599	YES	YES
113	a	737.61	12.55167	YES	YES
114	a	738.86	0.50663	YES	YES
115	a	739.79	10.18396	YES	YES
116	a	743.70	10.58023	YES	YES
117	a	746.23	6.04565	YES	YES
118	a	748.49	4.72829	YES	YES
119	a	764.72	17.74931	YES	YES
120	a	771.14	0.41862	YES	YES
121	a	828.80	2.66508	YES	YES
122	a	833.02	0.43407	YES	YES
123	a	833.93	0.54676	YES	YES
124	a	834.53	2.03730	YES	YES
125	a	838.57	0.30514	YES	YES
126	a	839.16	1.76715	YES	YES
127	a	841.98	0.49746	YES	YES
128	a	902.78	0.34190	YES	YES
129	a	907.31	0.73776	YES	YES
130	a	912.46	0.71423	YES	YES
131	a	913.17	0.99855	YES	YES
132	a	914.15	0.20433	YES	YES
133	a	914.36	1.67069	YES	YES
134	a	916.94	5.10572	YES	YES
135	a	920.23	3.13073	YES	YES
136	a	939.81	18.50721	YES	YES
137	a	953.50	0.37419	YES	YES
138	a	959.60	0.19391	YES	YES
139	a	960.90	2.38291	YES	YES
140	a	962.04	0.33065	YES	YES
141	a	963.40	0.77162	YES	YES
142	a	965.28	1.38202	YES	YES
143	a	967.60	0.55986	YES	YES
144	a	978.63	0.17145	YES	YES
145	a	980.69	0.98403	YES	YES
146	a	981.11	1.84467	YES	YES
147	a	981.88	2.32389	YES	YES
148	a	982.85	2.37340	YES	YES
149	a	983.39	1.99301	YES	YES
150	a	983.50	1.52337	YES	YES
151	a	983.68	0.76783	YES	YES
152	a	984.18	1.74427	YES	YES
153	a	984.84	1.00458	YES	YES
154	a	985.35	5.89917	YES	YES
155	a	986.81	2.21647	YES	YES
156	a	987.20	0.49033	YES	YES
157	a	988.25	2.01760	YES	YES
158	a	991.03	1.63893	YES	YES
159	a	994.73	1.87052	YES	YES
160	a	1020.43	5.69238	YES	YES
161	a	1022.82	1.44379	YES	YES
162	a	1023.31	9.98389	YES	YES
163	a	1023.41	0.84901	YES	YES
164	a	1023.79	4.64128	YES	YES
165	a	1024.02	1.49575	YES	YES
166	a	1024.90	1.08323	YES	YES

167	a	1025.11	1.14862	YES	YES
168	a	1025.76	0.63586	YES	YES
169	a	1066.13	29.56453	YES	YES
170	a	1068.18	5.76008	YES	YES
171	a	1070.99	10.45443	YES	YES
172	a	1071.11	7.76998	YES	YES
173	a	1072.90	16.18947	YES	YES
174	a	1074.05	4.90276	YES	YES
175	a	1074.25	14.18316	YES	YES
176	a	1074.50	17.29578	YES	YES
177	a	1076.98	0.76626	YES	YES
178	a	1078.08	9.66462	YES	YES
179	a	1079.26	6.84308	YES	YES
180	a	1080.70	12.59202	YES	YES
181	a	1081.79	7.53612	YES	YES
182	a	1140.38	0.36230	YES	YES
183	a	1140.64	0.45366	YES	YES
184	a	1141.13	0.12837	YES	YES
185	a	1141.43	0.40701	YES	YES
186	a	1141.67	0.08996	YES	YES
187	a	1142.43	0.55121	YES	YES
188	a	1143.25	0.50920	YES	YES
189	a	1158.86	0.95871	YES	YES
190	a	1164.47	1.74489	YES	YES
191	a	1167.44	4.51525	YES	YES
192	a	1169.81	3.22681	YES	YES
193	a	1172.11	2.17713	YES	YES
194	a	1173.16	12.06663	YES	YES
195	a	1174.55	10.93584	YES	YES
196	a	1213.69	2.74179	YES	YES
197	a	1284.25	25.16251	YES	YES
198	a	1287.48	120.20081	YES	YES

* zero point VIBRATIONAL energy : 0.7433283 Hartree *

Cis 3_pfbx



bp86-SVP SCF energy: -2931.4112960650
pbe-TZVPP SCF energy: -2930.957647045

XYZ Coordinates
97

C	1.16546	-3.44491	-0.93657
C	0.65016	-2.33324	-1.19225
C	1.77613	-4.67249	-0.57664
H	0.08979	-1.82114	-2.01091
C	3.00129	-7.12853	0.12964
C	1.80484	-6.73084	0.75590
C	1.19209	-5.52145	0.40777
C	2.99079	-5.08648	-1.19789
C	3.58851	-6.30300	-0.84778
H	3.47733	-8.08434	0.40435
H	1.34508	-7.37305	1.52532
H	0.25979	-5.20382	0.90069
H	3.44573	-4.43744	-1.96296
H	4.52503	-6.61290	-1.34061
C	2.79434	-0.84651	0.20487
C	4.12031	-1.40025	0.66214
H	4.15457	-2.48850	0.42844
H	4.23235	-1.27847	1.75862
H	4.95564	-0.90199	0.13009
C	-0.67858	1.35488	-3.00496
C	-1.06343	1.33037	-4.48513
H	-1.11820	2.36454	-4.88013
H	-2.06214	0.85176	-4.59815
H	-0.34159	0.72852	-5.07603
C	2.17662	1.98840	1.52471
C	3.55306	1.96649	1.19662
H	3.86512	1.96308	0.14191
C	4.53766	1.96274	2.19914
H	5.60250	1.95446	1.91175
C	4.17201	1.97631	3.55509
H	4.94431	1.98073	4.34232
C	2.80988	1.99659	3.89516
H	2.50273	2.01680	4.95422
C	1.82516	1.99680	2.89194
H	0.77167	2.02931	3.19935
C	-0.40390	3.11109	0.74864
C	-1.15647	2.75363	1.89008
H	-1.03101	1.76158	2.35134
C	-2.10395	3.63520	2.43443
H	-2.67178	3.33701	3.33081
C	-2.34432	4.87548	1.82216
H	-3.08942	5.56901	2.24632
C	-1.65408	5.20924	0.64504
H	-1.86232	6.16316	0.13177
C	-0.69567	4.33442	0.10777
H	-0.18859	4.59572	-0.83160
C	1.89605	2.98381	-1.09806
C	2.36024	4.26645	-0.72699
H	2.11214	4.68019	0.26401
C	3.15402	5.02132	-1.60596
H	3.50131	6.02300	-1.30222
C	3.51202	4.49631	-2.85986
H	4.14032	5.08565	-3.54877
C	3.07205	3.21315	-3.22501
H	3.35706	2.78775	-4.20166
C	2.26672	2.46124	-2.35230
H	1.93624	1.45349	-2.64065
C	-3.04876	0.59067	0.45804
C	-4.03046	0.40163	1.45635
H	-3.96307	-0.44944	2.15012
C	-5.10631	1.29759	1.57940
H	-5.86279	1.13201	2.36523
C	-5.22099	2.39208	0.70554
H	-6.07011	3.08980	0.79900
C	-4.23807	2.59666	-0.27637
H	-4.30116	3.46287	-0.95518
C	-3.15279	1.71086	-0.39553
H	-2.36736	1.91947	-1.14105
C	-2.61459	-1.80338	-1.02494
C	-3.49701	-1.26958	-1.98965
H	-3.71551	-0.19055	-2.00067
C	-4.11882	-2.10266	-2.93510
H	-4.80610	-1.66237	-3.67679
C	-3.87468	-3.48591	-2.93249
H	-4.36689	-4.13952	-3.67186
C	-2.99849	-4.02909	-1.97816
H	-2.79544	-5.11293	-1.96416
C	-2.37052	-3.19594	-1.03730
H	-1.67850	-3.63852	-0.30579
C	-1.70041	-1.62203	1.75569
C	-2.69015	-2.57966	2.08032
H	-3.47965	-2.82782	1.35336
C	-2.68082	-3.22318	3.32998
H	-3.45932	-3.96848	3.56469
C	-1.68847	-2.91531	4.27707
H	-1.68244	-3.42057	5.25747
C	-0.70201	-1.96542	3.96379
H	0.08807	-1.72459	4.69407
C	-0.70403	-1.32625	2.71158
H	0.09751	-0.61634	2.45988
O	1.75666	-0.94430	0.95029
O	2.65744	-0.31469	-0.95167
O	-0.79668	2.39111	-2.32826
O	-0.25807	0.20629	-2.55732
P	0.91275	1.96426	0.11687
P	-1.69618	-0.66947	0.15362
Ru	0.45046	-0.23470	-0.62749

Vibrational Frequencies

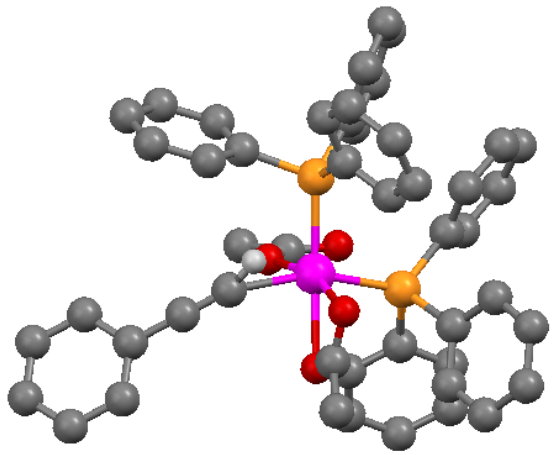
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	3.67	0.03757	YES	YES
8	a	14.57	0.13764	YES	YES
9	a	17.83	0.41796	YES	YES
10	a	24.63	0.11042	YES	YES
11	a	26.43	0.65274	YES	YES
12	a	32.99	0.02452	YES	YES
13	a	33.77	0.11958	YES	YES
14	a	38.28	0.38797	YES	YES
15	a	41.36	0.12038	YES	YES
16	a	44.72	0.05420	YES	YES
17	a	52.14	0.35409	YES	YES
18	a	54.27	0.12237	YES	YES
19	a	58.10	1.17709	YES	YES

20	a	58.81	1.96183	YES	YES
21	a	60.07	0.13097	YES	YES
22	a	63.87	0.60814	YES	YES
23	a	65.09	0.84938	YES	YES
24	a	72.90	2.21345	YES	YES
25	a	74.07	0.54787	YES	YES
26	a	79.78	1.19643	YES	YES
27	a	84.25	0.51759	YES	YES
28	a	89.47	0.03787	YES	YES
29	a	93.52	0.70335	YES	YES
30	a	96.96	0.38570	YES	YES
31	a	99.05	0.36136	YES	YES
32	a	105.49	1.36874	YES	YES
33	a	107.62	0.20210	YES	YES
34	a	114.38	2.48821	YES	YES
35	a	118.41	0.84659	YES	YES
36	a	134.43	6.81111	YES	YES
37	a	137.59	0.29048	YES	YES
38	a	144.03	5.98954	YES	YES
39	a	148.88	11.04399	YES	YES
40	a	171.76	2.20542	YES	YES
41	a	175.35	0.36847	YES	YES
42	a	185.16	8.50025	YES	YES
43	a	191.14	3.74199	YES	YES
44	a	201.76	11.99897	YES	YES
45	a	203.75	1.84293	YES	YES
46	a	204.48	1.89491	YES	YES
47	a	211.09	0.38437	YES	YES
48	a	219.02	11.50282	YES	YES
49	a	222.53	1.58445	YES	YES
50	a	233.01	7.29138	YES	YES
51	a	245.66	0.03575	YES	YES
52	a	250.06	1.12485	YES	YES
53	a	254.29	0.90705	YES	YES
54	a	257.89	1.61590	YES	YES
55	a	261.10	0.84566	YES	YES
56	a	264.13	0.34336	YES	YES
57	a	269.32	0.64298	YES	YES
58	a	276.41	3.90759	YES	YES
59	a	293.54	11.82878	YES	YES
60	a	310.06	14.03471	YES	YES
61	a	326.85	22.27171	YES	YES
62	a	389.48	106.09265	YES	YES
63	a	396.45	2.22337	YES	YES
64	a	397.97	10.28409	YES	YES
65	a	398.80	15.06710	YES	YES
66	a	399.90	1.63101	YES	YES
67	a	403.11	0.79553	YES	YES
68	a	406.12	2.64129	YES	YES
69	a	413.35	0.93308	YES	YES
70	a	416.60	2.67863	YES	YES
71	a	421.50	11.26650	YES	YES
72	a	428.75	33.08523	YES	YES
73	a	435.33	5.16707	YES	YES
74	a	454.10	17.58882	YES	YES
75	a	466.19	18.59303	YES	YES
76	a	473.91	8.07670	YES	YES
77	a	478.12	8.68426	YES	YES
78	a	486.75	8.11507	YES	YES
79	a	493.22	19.60493	YES	YES
80	a	499.82	8.56685	YES	YES
81	a	505.49	24.47477	YES	YES
82	a	508.27	12.51144	YES	YES
83	a	512.52	54.12039	YES	YES
84	a	518.53	116.50493	YES	YES
85	a	528.08	134.73461	YES	YES
86	a	546.57	55.07671	YES	YES
87	a	555.99	16.23607	YES	YES
88	a	594.61	7.56522	YES	YES
89	a	596.76	2.85470	YES	YES
90	a	608.00	0.21227	YES	YES
91	a	609.59	0.85917	YES	YES
92	a	610.26	0.98679	YES	YES
93	a	610.30	1.39727	YES	YES
94	a	611.54	1.46778	YES	YES
95	a	612.28	0.85003	YES	YES
96	a	612.98	0.70613	YES	YES
97	a	656.06	21.63465	YES	YES
98	a	666.65	9.40703	YES	YES
99	a	667.94	37.51464	YES	YES
100	a	670.26	18.82750	YES	YES
101	a	676.78	4.83897	YES	YES
102	a	677.28	47.01886	YES	YES
103	a	686.15	8.52892	YES	YES
104	a	687.43	33.59157	YES	YES
105	a	689.49	12.13916	YES	YES
106	a	694.20	16.53653	YES	YES
107	a	697.78	44.43311	YES	YES
108	a	699.15	106.25578	YES	YES
109	a	701.75	23.88927	YES	YES
110	a	702.57	254.41615	YES	YES
111	a	706.44	12.59079	YES	YES
112	a	706.61	39.22809	YES	YES
113	a	733.42	9.71937	YES	YES
114	a	738.92	6.40332	YES	YES
115	a	742.36	1.59621	YES	YES
116	a	743.85	11.10050	YES	YES
117	a	745.65	5.29854	YES	YES
118	a	749.12	6.05865	YES	YES
119	a	761.83	22.82085	YES	YES
120	a	766.77	0.83431	YES	YES
121	a	828.64	0.20398	YES	YES
122	a	829.02	0.24597	YES	YES
123	a	832.40	1.38014	YES	YES
124	a	833.87	0.08057	YES	YES
125	a	840.78	0.50294	YES	YES
126	a	842.55	0.06032	YES	YES
127	a	846.45	1.25844	YES	YES
128	a	902.37	0.18480	YES	YES
129	a	906.24	0.13115	YES	YES
130	a	908.43	1.36447	YES	YES
131	a	909.36	2.29040	YES	YES
132	a	914.95	0.81784	YES	YES
133	a	919.55	0.29993	YES	YES
134	a	922.68	0.13260	YES	YES
135	a	926.79	7.10951	YES	YES
136	a	943.66	15.76823	YES	YES
137	a	954.90	0.18568	YES	YES
138	a	956.13	0.45671	YES	YES
139	a	957.24	0.11533	YES	YES
140	a	958.89	0.03488	YES	YES
141	a	963.84	0.04605	YES	YES
142	a	966.15	0.05302	YES	YES
143	a	971.43	0.23673	YES	YES
144	a	977.03	0.83115	YES	YES
145	a	979.53	0.30569	YES	YES
146	a	979.76	0.20290	YES	YES
147	a	980.18	2.04421	YES	YES
148	a	981.59	0.53156	YES	YES
149	a	981.84	0.30957	YES	YES
150	a	982.25	0.10186	YES	YES
151	a	983.02	0.97622	YES	YES
152	a	983.70	1.65276	YES	YES
153	a	984.43	0.29481	YES	YES
154	a	984.46	2.32242	YES	YES
155	a	985.35	2.26943	YES	YES
156	a	986.72	0.57024	YES	YES
157	a	988.41	1.38013	YES	YES
158	a	991.69	6.33448	YES	YES
159	a	1003.96	0.06421	YES	YES
160	a	1020.27	6.88383	YES	YES
161	a	1021.01	15.60998	YES	YES
162	a	1022.95	1.78299	YES	YES
163	a	1023.51	0.41396	YES	YES
164	a	1023.61	1.93865	YES	YES
165	a	1024.06	2.58846	YES	YES
166	a	1024.73	1.18428	YES	YES
167	a	1026.33	0.08887	YES	YES

168	a	1027.21	0.28186	YES	YES
169	a	1064.38	13.54634	YES	YES
170	a	1067.00	15.47395	YES	YES
171	a	1070.52	9.31894	YES	YES
172	a	1070.87	15.86353	YES	YES
173	a	1071.98	5.84716	YES	YES
174	a	1073.51	12.12093	YES	YES
175	a	1075.22	4.49038	YES	YES
176	a	1077.36	0.78927	YES	YES
177	a	1078.21	6.99250	YES	YES
178	a	1078.32	17.28890	YES	YES
179	a	1081.05	10.36940	YES	YES
180	a	1081.27	5.98974	YES	YES
181	a	1086.14	0.58464	YES	YES
182	a	1140.21	0.01185	YES	YES
183	a	1140.96	0.89674	YES	YES
184	a	1141.20	0.23087	YES	YES
185	a	1141.83	0.29343	YES	YES
186	a	1142.17	0.31907	YES	YES
187	a	1142.62	0.09026	YES	YES
188	a	1143.09	0.72631	YES	YES
189	a	1157.72	0.11968	YES	YES
190	a	1166.84	2.30229	YES	YES
191	a	1167.92	6.19402	YES	YES
192	a	1169.71	5.70659	YES	YES
193	a	1173.25	2.66919	YES	YES
194	a	1175.41	2.82068	YES	YES
195	a	1183.03	2.50049	YES	YES
196	a	1209.63	4.86237	YES	YES
197	a	1287.56	0.30287	YES	YES
198	a	1288.17	3.58325	YES	YES

* zero point VIBRATIONAL energy : 0.7439283 Hartree *

Cis 3_pfby



bp86-SVP SCF energy: -2931.4071428010
pbe-TZVPP SCF energy: -2930.954634423

XYZ Coordinates
97

C	0.74675	3.76647	-0.40905
C	0.30237	2.61675	-0.58649
C	1.27727	5.05262	-0.12513
H	-0.45298	2.05848	-1.21209
C	2.32685	7.62005	0.44950
C	2.92812	6.81709	-0.53785
C	2.41329	5.54728	-0.82613
C	0.67979	5.87582	0.87131
C	1.20335	7.14397	1.15123
H	2.73571	8.61924	0.67381
H	3.80991	7.18696	-1.08715
H	2.88304	4.91307	-1.59433
H	-0.19802	5.49500	1.41656
H	0.73197	7.76981	1.92730
C	2.02948	0.66301	-2.23470
C	2.90843	0.94449	-3.42745
H	2.65518	1.94943	-3.83445
H	2.72580	0.19617	-4.22561
H	3.97727	0.94368	-3.13399
C	0.52963	0.47802	2.77868
C	0.54996	1.33577	4.04656
H	1.05194	0.78597	4.86820
H	-0.49675	1.55399	4.35708
H	1.05286	2.30830	3.86490
C	1.91747	-2.49136	-1.35924
C	3.21127	-2.12573	-1.80356
H	3.80732	-1.40928	-1.21974
C	3.75974	-2.67508	-2.97465
H	4.77441	-2.37697	-3.28800
C	3.03073	-3.60575	-3.73350
H	3.46347	-4.04281	-4.64873
C	1.74867	-3.98190	-3.30308
H	1.16609	-4.72316	-3.87550
C	1.19987	-3.43119	-2.13108
H	0.20678	-3.77597	-1.81290
C	0.25113	-3.05822	0.95582
C	-0.91244	-3.51740	0.29912
H	-1.28196	-3.00766	-0.60430
C	-1.64238	-4.60804	0.80040
H	-2.54399	-4.94983	0.26626
C	-1.23829	-5.23863	1.98719
H	-1.80982	-6.09386	2.38478
C	-0.11657	-4.75180	2.68006
H	0.19041	-5.21498	3.63286
C	0.61945	-3.66794	2.17464
H	1.47118	-3.27502	2.74681
C	2.84495	-1.62664	1.15655
C	3.58521	-2.81648	1.33736
H	3.20266	-3.77265	0.94480
C	4.82105	-2.79429	2.00519
H	5.38119	-3.73390	2.14570
C	5.34313	-1.57944	2.48101
H	6.31588	-1.55983	3.00060
C	4.62245	-0.38969	2.28254
H	5.02858	0.57061	2.64142
C	3.37991	-0.41130	1.62704
H	2.82589	0.52532	1.47089
C	-2.88519	-1.03487	0.91209
C	-4.16189	-1.52750	0.55818
H	-4.59224	-1.30638	-0.43020
C	-4.89990	-2.31260	1.45929
H	-5.89392	-2.68804	1.16326
C	-4.37666	-2.61467	2.72836
H	-4.95872	-3.22793	3.43679
C	-3.10159	-2.14341	3.07864
H	-2.66617	-2.39268	4.06017
C	-2.35429	-1.36578	2.17638
H	-1.33273	-1.06106	2.45348
C	-2.81313	1.73822	0.20717
C	-3.22917	1.99586	1.53097
H	-3.12812	1.21518	2.30104
C	-3.78286	3.23964	1.87821
H	-4.10494	3.41906	2.91764
C	-3.93293	4.24550	0.90893
H	-4.37366	5.21899	1.18119
C	-3.51847	4.00125	-0.41144
H	-3.63026	4.78227	-1.18192
C	-2.95766	2.76107	-0.75802
H	-2.64308	2.59237	-1.80191
C	-2.65535	-0.28733	-1.89440
C	-3.93414	0.14104	-2.32401
H	-4.54793	0.78828	-1.67717
C	-4.43435	-0.24575	-3.57909
H	-5.43186	0.10018	-3.89784
C	-3.66772	-1.06721	-4.42358
H	-4.05985	-1.36800	-5.40945
C	-2.39495	-1.49265	-4.00872
H	-1.77724	-2.12388	-4.66867
C	-1.88961	-1.10182	-2.75682
H	-0.87306	-1.40339	-2.46202
O	0.81681	0.27435	-2.40124
O	2.44143	0.85352	-1.04056
O	0.64240	-0.76143	2.85338
O	0.35269	1.16349	1.69242
P	1.24121	-1.67256	0.21135
P	-1.95434	0.13223	-0.21766
Ru	0.35117	0.47037	-0.29934

Vibrational Frequencies

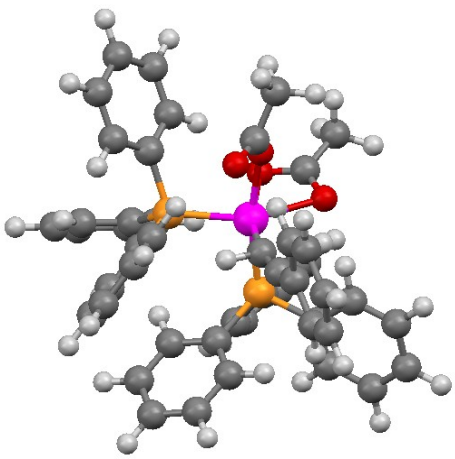
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	3.95	0.10301	YES	YES
8	a	11.96	0.07868	YES	YES
9	a	16.18	0.18251	YES	YES
10	a	19.98	0.01301	YES	YES
11	a	22.24	0.00143	YES	YES
12	a	28.78	0.10632	YES	YES
13	a	30.89	0.01081	YES	YES
14	a	36.77	0.24011	YES	YES
15	a	43.59	0.68260	YES	YES
16	a	46.30	0.20355	YES	YES
17	a	50.00	0.66820	YES	YES
18	a	55.76	0.22720	YES	YES

19	a	58.01	0.01996	YES	YES
20	a	60.42	0.03408	YES	YES
21	a	61.75	0.30741	YES	YES
22	a	65.09	0.94301	YES	YES
23	a	68.46	0.09771	YES	YES
24	a	73.42	0.26053	YES	YES
25	a	76.20	0.55045	YES	YES
26	a	80.13	0.76324	YES	YES
27	a	82.69	1.35447	YES	YES
28	a	87.53	0.58737	YES	YES
29	a	89.88	1.85232	YES	YES
30	a	92.61	1.42341	YES	YES
31	a	95.00	0.60838	YES	YES
32	a	100.76	1.43462	YES	YES
33	a	107.95	0.34827	YES	YES
34	a	109.24	0.87436	YES	YES
35	a	114.30	1.70413	YES	YES
36	a	130.49	0.70567	YES	YES
37	a	139.64	1.11756	YES	YES
38	a	146.87	6.13600	YES	YES
39	a	159.82	1.38456	YES	YES
40	a	171.15	4.73437	YES	YES
41	a	172.73	3.76638	YES	YES
42	a	183.79	4.44011	YES	YES
43	a	191.15	1.39502	YES	YES
44	a	200.55	7.25557	YES	YES
45	a	205.82	2.15088	YES	YES
46	a	207.38	7.38578	YES	YES
47	a	212.72	0.81655	YES	YES
48	a	221.30	13.34177	YES	YES
49	a	227.54	5.62551	YES	YES
50	a	231.58	36.58627	YES	YES
51	a	244.40	0.76326	YES	YES
52	a	246.65	0.72084	YES	YES
53	a	249.36	2.45272	YES	YES
54	a	254.84	0.32227	YES	YES
55	a	259.79	1.03678	YES	YES
56	a	262.13	3.36503	YES	YES
57	a	267.49	1.81641	YES	YES
58	a	269.98	0.09291	YES	YES
59	a	303.28	18.69072	YES	YES
60	a	321.79	5.23834	YES	YES
61	a	328.21	15.04180	YES	YES
62	a	382.59	84.32978	YES	YES
63	a	394.94	0.45795	YES	YES
64	a	397.23	4.44120	YES	YES
65	a	398.61	12.06980	YES	YES
66	a	399.66	8.58863	YES	YES
67	a	401.79	9.37063	YES	YES
68	a	405.72	4.37208	YES	YES
69	a	411.63	2.76337	YES	YES
70	a	416.56	2.36967	YES	YES
71	a	418.09	10.75491	YES	YES
72	a	429.84	27.19589	YES	YES
73	a	433.76	13.07850	YES	YES
74	a	451.69	21.34880	YES	YES
75	a	466.23	8.24758	YES	YES
76	a	470.77	20.76670	YES	YES
77	a	476.91	4.91340	YES	YES
78	a	486.39	8.66281	YES	YES
79	a	491.49	44.98203	YES	YES
80	a	497.05	54.90357	YES	YES
81	a	504.37	16.42912	YES	YES
82	a	508.84	8.71919	YES	YES
83	a	510.59	60.98925	YES	YES
84	a	517.33	91.73390	YES	YES
85	a	518.76	50.08058	YES	YES
86	a	528.74	115.71564	YES	YES
87	a	556.22	12.44226	YES	YES
88	a	598.84	4.57172	YES	YES
89	a	600.97	6.72160	YES	YES
90	a	607.89	0.48046	YES	YES
91	a	609.41	0.89559	YES	YES
92	a	609.84	0.64346	YES	YES
93	a	610.28	1.02737	YES	YES
94	a	611.85	1.54826	YES	YES
95	a	612.29	0.02278	YES	YES
96	a	612.33	0.44240	YES	YES
97	a	661.69	8.60230	YES	YES
98	a	663.64	8.59035	YES	YES
99	a	668.42	50.74149	YES	YES
100	a	670.79	19.62044	YES	YES
101	a	676.66	14.21868	YES	YES
102	a	679.01	20.34021	YES	YES
103	a	686.12	13.50689	YES	YES
104	a	687.45	27.83212	YES	YES
105	a	690.62	14.01406	YES	YES
106	a	691.85	31.64482	YES	YES
107	a	696.78	33.54804	YES	YES
108	a	699.77	33.35283	YES	YES
109	a	700.46	48.77170	YES	YES
110	a	704.68	4.64216	YES	YES
111	a	706.87	26.43690	YES	YES
112	a	733.62	7.37557	YES	YES
113	a	737.94	1.20561	YES	YES
114	a	741.06	2.17110	YES	YES
115	a	742.69	5.54001	YES	YES
116	a	744.91	5.58057	YES	YES
117	a	748.32	13.27728	YES	YES
118	a	762.47	28.81686	YES	YES
119	a	767.68	4.58887	YES	YES
120	a	794.02	462.47438	YES	YES
121	a	824.86	0.98681	YES	YES
122	a	829.02	0.31401	YES	YES
123	a	833.09	2.15293	YES	YES
124	a	835.62	16.81809	YES	YES
125	a	839.45	1.40804	YES	YES
126	a	843.65	0.06745	YES	YES
127	a	844.51	0.60441	YES	YES
128	a	898.61	0.53396	YES	YES
129	a	905.66	4.09923	YES	YES
130	a	908.75	0.97956	YES	YES
131	a	910.17	2.07372	YES	YES
132	a	913.62	0.04911	YES	YES
133	a	919.77	0.39184	YES	YES
134	a	922.56	0.09985	YES	YES
135	a	926.92	4.18187	YES	YES
136	a	943.82	18.56107	YES	YES
137	a	953.32	0.53938	YES	YES
138	a	956.53	0.82486	YES	YES
139	a	957.16	0.54412	YES	YES
140	a	958.45	0.05755	YES	YES
141	a	962.47	0.10382	YES	YES
142	a	966.74	0.00803	YES	YES
143	a	970.79	0.23366	YES	YES
144	a	978.05	0.76127	YES	YES
145	a	979.95	0.14671	YES	YES
146	a	980.76	0.65984	YES	YES
147	a	980.82	0.94423	YES	YES
148	a	981.06	0.12435	YES	YES
149	a	981.10	1.84540	YES	YES
150	a	981.88	0.31543	YES	YES
151	a	982.02	2.66510	YES	YES
152	a	983.30	0.47978	YES	YES
153	a	984.03	1.63597	YES	YES
154	a	984.39	2.12734	YES	YES
155	a	985.42	1.95311	YES	YES
156	a	987.64	1.87783	YES	YES
157	a	987.93	0.24916	YES	YES
158	a	992.21	2.58355	YES	YES
159	a	1003.76	0.00252	YES	YES
160	a	1022.21	4.57438	YES	YES
161	a	1022.72	3.52366	YES	YES
162	a	1022.85	8.35785	YES	YES
163	a	1023.28	2.76640	YES	YES
164	a	1023.55	1.91799	YES	YES
165	a	1024.16	3.19237	YES	YES
166	a	1024.47	2.68081	YES	YES

167	a	1025.93	0.78287	YES	YES
168	a	1026.53	1.37613	YES	YES
169	a	1061.10	16.52965	YES	YES
170	a	1067.13	17.79101	YES	YES
171	a	1068.98	6.28491	YES	YES
172	a	1070.21	5.05779	YES	YES
173	a	1072.07	13.18216	YES	YES
174	a	1072.61	10.21883	YES	YES
175	a	1074.99	2.24582	YES	YES
176	a	1075.13	4.57809	YES	YES
177	a	1078.25	7.91397	YES	YES
178	a	1078.56	18.09822	YES	YES
179	a	1080.14	1.15530	YES	YES
180	a	1081.86	14.02301	YES	YES
181	a	1082.31	1.31523	YES	YES
182	a	1140.24	0.19373	YES	YES
183	a	1140.51	0.59860	YES	YES
184	a	1140.86	0.02070	YES	YES
185	a	1141.38	0.26119	YES	YES
186	a	1141.83	0.08046	YES	YES
187	a	1142.06	0.40404	YES	YES
188	a	1143.56	0.62713	YES	YES
189	a	1156.49	0.21298	YES	YES
190	a	1162.92	2.47218	YES	YES
191	a	1167.91	1.84169	YES	YES
192	a	1168.61	4.00662	YES	YES
193	a	1170.40	5.47559	YES	YES
194	a	1174.63	2.32586	YES	YES
195	a	1177.16	3.54840	YES	YES
196	a	1211.66	3.93188	YES	YES
197	a	1284.98	3.05670	YES	YES
198	a	1287.41	0.20755	YES	YES

* zero point VIBRATIONAL energy : 0.7434533 Hartree *

Cis TS_{35}_afam



bp86-SVP SCF energy: -2931.4151319570
pbe-TZVPP SCF energy: -2930.963902493

XYZ Coordinates
97

C	1.26067	0.56633	-2.64059
C	0.80619	0.63809	-1.44053
C	2.13000	0.63667	-3.76584
H	1.52675	-0.28220	-1.31447
C	3.88343	0.81664	-5.96824
C	4.29457	1.28224	-4.70379
C	3.42828	1.20695	-3.60657
C	1.72991	0.16043	-5.04545
C	2.60023	0.26185	-6.13766
H	4.56869	0.88685	-6.82975
H	5.30046	1.71630	-4.57724
H	3.72053	1.56641	-2.60422
H	0.72598	-0.27748	-5.16238
H	2.28244	-0.09987	-7.12946
C	-1.19556	3.32342	1.02192
C	-1.60961	4.67756	1.54562
H	-0.69416	5.23585	1.84375
H	-2.25143	4.56962	2.44450
H	-2.13142	5.26066	0.75965
C	2.71968	2.54865	0.26719
C	3.43847	3.87110	0.56294
H	4.53591	3.73717	0.47788
H	3.17687	4.24816	1.57378
H	3.11267	4.63851	-0.17498
C	-3.59369	0.26422	0.44426
C	-4.00525	1.60023	0.66371
H	-3.39737	2.42547	0.26228
C	-5.20103	1.88431	1.34004
H	-5.50310	2.93363	1.49427
C	-6.01499	0.83817	1.80959
H	-6.95426	1.06019	2.34294
C	-5.62915	-0.49109	1.57720
H	-6.26875	-1.32210	1.91915
C	-4.43052	-0.77749	0.89710
H	-4.16968	-1.82892	0.70688
C	-1.87920	-1.76689	-0.86242
C	-1.98014	-2.72910	0.16898
H	-2.11373	-2.41101	1.21424
C	-1.90100	-4.10267	-0.11928
H	-2.00849	-4.83482	0.69887
C	-1.67501	-4.54043	-1.43475
H	-1.61156	-5.61811	-1.65985
C	-1.52004	-3.59176	-2.45905
H	-1.32239	-3.92017	-3.49302
C	-1.62820	-2.21938	-2.17824
H	-1.52225	-1.49080	-2.99648
C	-2.61547	0.70767	-2.14948
C	-3.79835	0.16378	-2.70318
H	-4.33447	-0.64115	-2.17393
C	-4.30436	0.64087	-3.92192
H	-5.22734	0.20427	-4.33883
C	-3.64006	1.67773	-4.60297
H	-4.03884	2.05725	-5.55873
C	-2.47319	2.23238	-4.05376
H	-1.95178	3.05350	-4.57302
C	-1.96169	1.75185	-2.83326
H	-1.06344	2.21059	-2.39867
C	1.86886	-1.82018	0.67749
C	1.42374	-3.15846	0.64971
H	0.53060	-3.45731	1.21679
C	2.10938	-4.12380	-0.10811
H	1.74355	-5.16394	-0.11778
C	3.24611	-3.76751	-0.85210
H	3.78166	-4.52727	-1.44559
C	3.69138	-2.43467	-0.83882
H	4.58030	-2.14054	-1.42156
C	3.01093	-1.46180	-0.08467
H	3.36147	-0.41180	-0.08640
C	2.22578	0.26624	2.70609
C	3.47329	-0.33882	2.96061
H	3.78033	-1.23899	2.40561
C	4.34157	0.20359	3.92481
H	5.31683	-0.27743	4.10971
C	3.97045	1.34957	4.64556
H	4.65209	1.77382	5.40186
C	2.72503	1.95371	4.39709
H	2.42616	2.85519	4.95806
C	1.85570	1.42052	3.43263
H	0.88709	1.90738	3.23466
C	-0.09654	-1.28030	2.83915
C	0.39353	-2.35074	3.62161
H	1.39906	-2.76131	3.43335
C	-0.38653	-2.88866	4.65756
H	0.00515	-3.72903	5.25512
C	-1.65392	-2.34855	4.94309
H	-2.26113	-2.76795	5.76282
C	-2.13159	-1.26160	4.19328
H	-3.11355	-0.81601	4.42252
C	-1.35778	-0.72884	3.14608
H	-1.72570	0.14012	2.57678
O	-0.98283	2.35262	1.83129
O	-1.02939	3.12804	-0.23070
O	3.31528	1.63058	-0.32702
O	1.48629	2.54035	0.67814
P	-1.98844	0.05807	-0.50510
P	0.95659	-0.45387	1.54183
Ru	-0.06323	1.16418	0.23897

Vibrational Frequencies

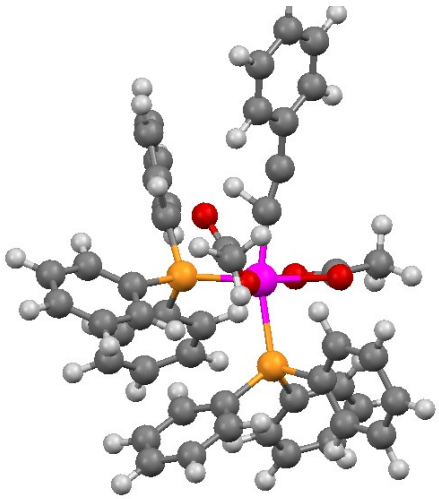
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-471.90	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	6.26	0.00318	YES	YES
9	a	18.63	0.10679	YES	YES
10	a	21.69	0.02590	YES	YES
11	a	25.43	0.46376	YES	YES
12	a	29.06	0.05165	YES	YES
13	a	34.11	0.49925	YES	YES
14	a	39.84	0.18281	YES	YES

15	a	43.14	0.03375	YES	YES
16	a	46.40	0.11635	YES	YES
17	a	47.24	0.05488	YES	YES
18	a	49.61	0.27821	YES	YES
19	a	52.02	0.07686	YES	YES
20	a	53.29	0.26449	YES	YES
21	a	57.18	0.20217	YES	YES
22	a	61.01	0.25323	YES	YES
23	a	61.81	0.19393	YES	YES
24	a	65.53	0.17818	YES	YES
25	a	67.18	0.22873	YES	YES
26	a	75.51	1.17127	YES	YES
27	a	75.71	0.30547	YES	YES
28	a	79.94	2.26867	YES	YES
29	a	84.27	1.88886	YES	YES
30	a	91.39	1.06753	YES	YES
31	a	91.86	0.30764	YES	YES
32	a	97.47	3.72901	YES	YES
33	a	104.11	1.59867	YES	YES
34	a	106.17	0.80980	YES	YES
35	a	109.74	2.51828	YES	YES
36	a	112.72	1.05124	YES	YES
37	a	125.40	0.30887	YES	YES
38	a	134.09	4.85931	YES	YES
39	a	149.81	6.14380	YES	YES
40	a	159.24	1.08197	YES	YES
41	a	171.86	1.29057	YES	YES
42	a	184.46	0.85397	YES	YES
43	a	187.17	0.59176	YES	YES
44	a	195.79	2.00680	YES	YES
45	a	200.07	3.20363	YES	YES
46	a	209.87	0.42898	YES	YES
47	a	212.69	0.36428	YES	YES
48	a	217.86	4.04939	YES	YES
49	a	221.33	3.68374	YES	YES
50	a	225.82	1.23958	YES	YES
51	a	242.07	0.79478	YES	YES
52	a	243.64	0.71785	YES	YES
53	a	244.27	2.07941	YES	YES
54	a	248.66	8.87838	YES	YES
55	a	253.14	0.35837	YES	YES
56	a	264.44	6.11869	YES	YES
57	a	268.09	3.69966	YES	YES
58	a	269.74	9.87100	YES	YES
59	a	280.33	4.11469	YES	YES
60	a	287.94	48.64546	YES	YES
61	a	314.43	0.34179	YES	YES
62	a	337.80	8.66197	YES	YES
63	a	392.76	18.04613	YES	YES
64	a	396.27	0.39683	YES	YES
65	a	397.28	0.14656	YES	YES
66	a	401.21	0.22870	YES	YES
67	a	403.28	2.30350	YES	YES
68	a	410.82	29.90034	YES	YES
69	a	411.14	11.30926	YES	YES
70	a	413.71	20.03519	YES	YES
71	a	415.42	11.04771	YES	YES
72	a	419.97	7.67626	YES	YES
73	a	427.28	8.34346	YES	YES
74	a	429.79	20.85018	YES	YES
75	a	446.55	11.49044	YES	YES
76	a	459.60	17.73910	YES	YES
77	a	465.84	7.40308	YES	YES
78	a	472.77	9.92309	YES	YES
79	a	480.40	7.84166	YES	YES
80	a	491.93	24.78365	YES	YES
81	a	496.45	25.94453	YES	YES
82	a	501.43	9.07136	YES	YES
83	a	509.82	5.61550	YES	YES
84	a	512.43	88.88397	YES	YES
85	a	514.90	187.65917	YES	YES
86	a	526.52	112.42651	YES	YES
87	a	552.82	7.75592	YES	YES
88	a	585.45	48.10450	YES	YES
89	a	591.71	2.48566	YES	YES
90	a	594.71	9.46066	YES	YES
91	a	607.48	0.20064	YES	YES
92	a	609.24	0.83725	YES	YES
93	a	609.39	0.56316	YES	YES
94	a	610.33	2.90916	YES	YES
95	a	610.46	1.61643	YES	YES
96	a	611.12	1.86228	YES	YES
97	a	612.60	0.46825	YES	YES
98	a	653.23	24.25652	YES	YES
99	a	667.17	64.78002	YES	YES
100	a	670.59	13.07018	YES	YES
101	a	673.43	16.99489	YES	YES
102	a	678.40	8.41596	YES	YES
103	a	680.24	10.26888	YES	YES
104	a	685.70	11.66503	YES	YES
105	a	691.69	25.68542	YES	YES
106	a	694.68	34.51018	YES	YES
107	a	696.86	24.35458	YES	YES
108	a	697.08	27.87636	YES	YES
109	a	699.00	61.34047	YES	YES
110	a	700.77	41.89172	YES	YES
111	a	707.20	6.67623	YES	YES
112	a	715.57	20.92721	YES	YES
113	a	736.80	11.77491	YES	YES
114	a	738.24	8.94282	YES	YES
115	a	740.53	8.39037	YES	YES
116	a	743.48	1.65110	YES	YES
117	a	746.49	2.36061	YES	YES
118	a	747.22	2.08868	YES	YES
119	a	768.13	18.27066	YES	YES
120	a	794.09	18.23810	YES	YES
121	a	833.01	0.00338	YES	YES
122	a	834.97	0.32061	YES	YES
123	a	835.79	0.06861	YES	YES
124	a	839.44	1.35963	YES	YES
125	a	844.34	2.38315	YES	YES
126	a	845.54	0.58325	YES	YES
127	a	855.84	1.08088	YES	YES
128	a	905.64	0.58882	YES	YES
129	a	908.39	0.13079	YES	YES
130	a	909.76	0.26994	YES	YES
131	a	912.99	0.79831	YES	YES
132	a	914.34	0.08761	YES	YES
133	a	917.88	3.37718	YES	YES
134	a	929.22	1.91851	YES	YES
135	a	933.31	0.70992	YES	YES
136	a	938.10	32.32632	YES	YES
137	a	957.95	0.10400	YES	YES
138	a	958.55	0.21599	YES	YES
139	a	959.16	0.05459	YES	YES
140	a	962.07	0.40452	YES	YES
141	a	965.17	0.93587	YES	YES
142	a	975.53	1.34632	YES	YES
143	a	976.55	0.03087	YES	YES
144	a	978.79	1.24716	YES	YES
145	a	979.65	0.92547	YES	YES
146	a	980.76	0.09286	YES	YES
147	a	981.34	1.64645	YES	YES
148	a	981.56	0.12479	YES	YES
149	a	982.05	0.16003	YES	YES
150	a	982.46	0.26063	YES	YES
151	a	982.80	1.63915	YES	YES
152	a	984.36	0.52767	YES	YES
153	a	984.83	3.31996	YES	YES
154	a	986.61	1.12923	YES	YES
155	a	986.90	0.96203	YES	YES
156	a	988.42	0.24391	YES	YES
157	a	990.84	7.20159	YES	YES
158	a	1010.76	2.31748	YES	YES
159	a	1015.50	4.72023	YES	YES
160	a	1020.27	5.51071	YES	YES
161	a	1022.50	1.71471	YES	YES
162	a	1022.69	0.49746	YES	YES

163	a	1022.89	5.51057	YES	YES
164	a	1023.33	10.51611	YES	YES
165	a	1024.53	2.61174	YES	YES
166	a	1024.62	2.25679	YES	YES
167	a	1026.02	0.09495	YES	YES
168	a	1026.30	0.54289	YES	YES
169	a	1067.37	16.92604	YES	YES
170	a	1070.46	1.96083	YES	YES
171	a	1070.95	7.56240	YES	YES
172	a	1071.13	13.38344	YES	YES
173	a	1071.35	4.21132	YES	YES
174	a	1073.25	22.94205	YES	YES
175	a	1074.19	3.62853	YES	YES
176	a	1075.15	10.87762	YES	YES
177	a	1078.48	2.51328	YES	YES
178	a	1079.54	3.40859	YES	YES
179	a	1080.32	31.91399	YES	YES
180	a	1081.05	7.08323	YES	YES
181	a	1086.60	5.30124	YES	YES
182	a	1139.45	0.19329	YES	YES
183	a	1141.04	0.29065	YES	YES
184	a	1141.24	0.34025	YES	YES
185	a	1141.97	0.84413	YES	YES
186	a	1142.30	0.72003	YES	YES
187	a	1142.77	0.06796	YES	YES
188	a	1143.27	0.34714	YES	YES
189	a	1158.71	12.29974	YES	YES
190	a	1165.20	6.78611	YES	YES
191	a	1166.69	4.50622	YES	YES
192	a	1169.52	4.65427	YES	YES
193	a	1174.20	10.01440	YES	YES
194	a	1175.57	0.95508	YES	YES
195	a	1182.93	0.93786	YES	YES
196	a	1206.86	27.29754	YES	YES
197	a	1288.46	2.51429	YES	YES
198	a	1290.85	5.29414	YES	YES

* zero point VIBRATIONAL energy : 0.7406808 Hartree *

Cis TS_{35}_pfam



bp86-SVP SCF energy: -2931.4029957440
pbe-TZVPP SCF energy: -2930.952782715

XYZ Coordinates
97

C	1.84530	-3.35301	-0.25601
C	1.29953	-2.21546	-0.03872
C	2.27832	-4.55405	-0.90191
H	0.39035	-2.98495	-0.17632
C	3.04946	-6.92312	-2.22365
C	2.40015	-5.89938	-2.94007
C	2.02468	-4.71438	-2.29505
C	2.92796	-5.59530	-0.18724
C	3.31913	-6.76546	-0.85103
H	3.34711	-7.85199	-2.73861
H	2.19128	-6.02595	-4.01552
H	1.52136	-3.89205	-2.83295
H	3.11727	-5.46858	0.89046
H	3.82792	-7.56913	-0.29350
C	2.41390	-0.62513	2.32620
C	3.27248	-0.96509	3.52226
H	3.41752	-2.06783	3.56331
H	2.77175	-0.65201	4.46147
H	4.27015	-0.48879	3.43556
C	1.00612	-0.73148	-2.73371
C	1.63588	-0.25607	-4.04784
H	0.97734	-0.52727	-4.89911
H	2.60631	-0.78348	-4.19222
H	1.83227	0.83568	-4.04550
C	0.95183	2.80683	2.28399
C	2.03703	2.47702	3.13090
H	2.88407	1.89916	2.72886
C	2.06930	2.91615	4.46335
H	2.93012	2.65554	5.10177
C	1.01781	3.69477	4.97882
H	1.04426	4.04375	6.02459
C	-0.05871	4.03558	4.14483
H	-0.88303	4.65927	4.52935
C	-0.09257	3.59574	2.80884
H	-0.93848	3.89513	2.17279
C	-0.16278	3.25262	-0.39356
C	-1.54790	3.22741	-0.10882
H	-1.94375	2.54410	0.65846
C	-2.44209	4.05005	-0.81224
H	-3.51613	4.01629	-0.56657
C	-1.97391	4.89225	-1.83473
H	-2.67653	5.53369	-2.39245
C	-0.60518	4.89983	-2.14999
H	-0.22677	5.54600	-2.95994
C	0.29494	4.09073	-1.43445
H	1.36428	4.11397	-1.69312
C	2.66013	2.78139	0.00084
C	3.10872	4.05014	0.43728
H	2.48414	4.65380	1.11568
C	4.34926	4.55301	0.01369
H	4.68465	5.54392	0.36305
C	5.15988	3.79367	-0.84908
H	6.13723	4.18526	-1.17788
C	4.71832	2.53495	-1.28839
H	5.34871	1.93264	-1.96370
C	3.47500	2.02773	-0.86881
H	3.12020	1.05049	-1.22647
C	-2.33417	-0.25186	-1.49172
C	-3.52989	-0.92413	-1.83616
H	-3.92272	-1.72397	-1.18781
C	-4.22384	-0.59257	-3.01158
H	-5.15249	-1.13057	-3.26667
C	-3.73239	0.41279	-3.86181
H	-4.27372	0.66807	-4.78837
C	-2.54317	1.08156	-3.52958
H	-2.14289	1.86515	-4.19383
C	-1.84733	0.75164	-2.35421
H	-0.90128	1.25943	-2.11744
C	-1.86302	-2.45316	0.30632
C	-1.67378	-3.35599	-0.77093
H	-1.32309	-2.97371	-1.74463
C	-1.92219	-4.72967	-0.59549
H	-1.77571	-5.41895	-1.44368
C	-2.35456	-5.22151	0.64851
H	-2.54809	-6.29884	0.78307
C	-2.53699	-4.33105	1.71991
H	-2.87378	-4.70666	2.70070
C	-2.29333	-2.95622	1.55183
H	-2.44161	-2.27262	2.40238
C	-2.44077	0.14834	1.40112
C	-3.78717	0.52562	1.19547
H	-4.25602	0.38863	0.20840
C	-4.53766	1.09076	2.24057
H	-5.58623	1.38292	2.06117
C	-3.95748	1.28190	3.50677
H	-4.54874	1.72428	4.32607
C	-2.61958	0.91023	3.71898
H	-2.15155	1.06158	4.70570
C	-1.86059	0.35182	2.67430
H	-0.80879	0.07170	2.84880
O	1.13566	-0.69201	2.41190
O	2.93335	-0.30106	1.20616
O	0.39704	-1.81305	-2.68767
O	1.21154	0.08917	-1.73755
P	0.99630	2.13397	0.54105
P	-1.39847	-0.65669	0.07035
Ru	0.85930	-0.32084	0.29523

Vibrational Frequencies

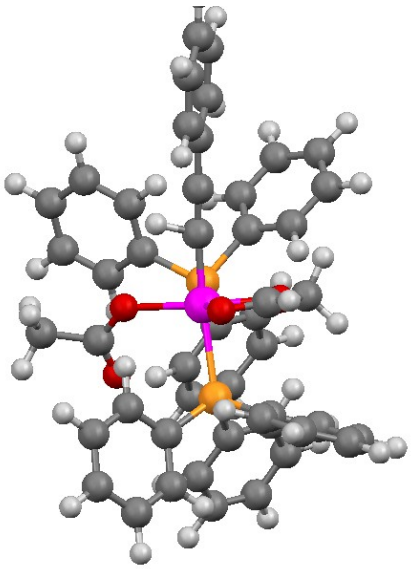
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-494.13	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	10.82	0.01124	YES	YES
9	a	18.95	0.08922	YES	YES
10	a	20.63	0.11344	YES	YES
11	a	21.31	0.31173	YES	YES
12	a	30.74	0.07031	YES	YES
13	a	33.64	0.07214	YES	YES
14	a	38.97	0.01065	YES	YES

15	a	40.49	0.40682	YES	YES
16	a	44.33	0.10460	YES	YES
17	a	46.34	0.01866	YES	YES
18	a	49.74	0.16596	YES	YES
19	a	54.04	0.79671	YES	YES
20	a	56.89	0.01995	YES	YES
21	a	59.94	0.04260	YES	YES
22	a	61.61	0.29035	YES	YES
23	a	62.59	0.16133	YES	YES
24	a	68.89	0.54213	YES	YES
25	a	70.58	0.89463	YES	YES
26	a	74.28	0.35461	YES	YES
27	a	77.65	0.71043	YES	YES
28	a	84.73	2.10215	YES	YES
29	a	85.50	1.28606	YES	YES
30	a	85.85	1.56839	YES	YES
31	a	89.27	0.83976	YES	YES
32	a	91.25	3.11221	YES	YES
33	a	91.80	0.18178	YES	YES
34	a	101.23	0.29227	YES	YES
35	a	106.16	3.78716	YES	YES
36	a	112.23	0.96434	YES	YES
37	a	123.01	3.68998	YES	YES
38	a	131.28	0.03848	YES	YES
39	a	147.12	5.30427	YES	YES
40	a	157.16	0.88564	YES	YES
41	a	170.35	2.26714	YES	YES
42	a	176.69	0.18616	YES	YES
43	a	192.39	0.40074	YES	YES
44	a	194.88	0.81201	YES	YES
45	a	197.27	1.19361	YES	YES
46	a	202.08	2.11373	YES	YES
47	a	207.31	2.76946	YES	YES
48	a	209.43	1.20222	YES	YES
49	a	220.75	4.28552	YES	YES
50	a	223.63	2.29885	YES	YES
51	a	231.97	2.19519	YES	YES
52	a	245.60	0.64611	YES	YES
53	a	247.25	1.82728	YES	YES
54	a	249.26	0.07192	YES	YES
55	a	250.25	0.48507	YES	YES
56	a	263.46	9.86119	YES	YES
57	a	265.49	0.03716	YES	YES
58	a	267.23	0.12743	YES	YES
59	a	275.40	6.13134	YES	YES
60	a	293.61	16.85633	YES	YES
61	a	316.20	12.36463	YES	YES
62	a	320.65	15.79680	YES	YES
63	a	390.27	1.33537	YES	YES
64	a	397.37	0.20300	YES	YES
65	a	397.92	0.57252	YES	YES
66	a	399.07	0.36161	YES	YES
67	a	400.96	0.49154	YES	YES
68	a	404.28	28.07317	YES	YES
69	a	406.27	1.18886	YES	YES
70	a	409.06	5.16658	YES	YES
71	a	411.29	1.83577	YES	YES
72	a	424.29	27.56661	YES	YES
73	a	426.32	8.28877	YES	YES
74	a	433.54	13.67900	YES	YES
75	a	445.14	15.76274	YES	YES
76	a	451.14	8.68684	YES	YES
77	a	459.55	21.93779	YES	YES
78	a	472.84	5.11774	YES	YES
79	a	482.05	23.62987	YES	YES
80	a	487.75	31.50934	YES	YES
81	a	496.63	24.90437	YES	YES
82	a	501.94	2.01086	YES	YES
83	a	507.37	32.79123	YES	YES
84	a	510.91	42.09134	YES	YES
85	a	517.28	165.74441	YES	YES
86	a	528.56	109.14283	YES	YES
87	a	543.14	1.56628	YES	YES
88	a	596.33	7.99746	YES	YES
89	a	600.21	0.68760	YES	YES
90	a	600.64	23.59368	YES	YES
91	a	608.28	0.30463	YES	YES
92	a	609.35	1.64800	YES	YES
93	a	609.92	0.16272	YES	YES
94	a	610.17	1.35262	YES	YES
95	a	610.78	2.38769	YES	YES
96	a	611.99	4.66221	YES	YES
97	a	612.35	0.27950	YES	YES
98	a	663.34	29.41639	YES	YES
99	a	666.03	36.28827	YES	YES
100	a	670.53	6.29328	YES	YES
101	a	671.69	15.20719	YES	YES
102	a	679.82	16.55034	YES	YES
103	a	681.82	5.99305	YES	YES
104	a	684.93	12.00937	YES	YES
105	a	685.90	13.76544	YES	YES
106	a	695.88	31.10297	YES	YES
107	a	696.30	35.82977	YES	YES
108	a	698.97	89.73766	YES	YES
109	a	699.53	8.05330	YES	YES
110	a	702.97	31.71114	YES	YES
111	a	704.68	18.01922	YES	YES
112	a	705.07	7.48847	YES	YES
113	a	738.03	8.64343	YES	YES
114	a	741.23	3.37334	YES	YES
115	a	742.17	2.67945	YES	YES
116	a	744.30	3.66478	YES	YES
117	a	746.65	7.36586	YES	YES
118	a	749.08	9.00132	YES	YES
119	a	767.80	19.53894	YES	YES
120	a	788.69	10.53222	YES	YES
121	a	835.63	0.53999	YES	YES
122	a	836.81	0.12344	YES	YES
123	a	837.74	1.68168	YES	YES
124	a	843.69	2.03341	YES	YES
125	a	844.61	1.57778	YES	YES
126	a	846.70	1.44012	YES	YES
127	a	848.93	2.94038	YES	YES
128	a	907.71	0.76027	YES	YES
129	a	909.53	1.55207	YES	YES
130	a	914.78	0.45816	YES	YES
131	a	914.90	1.61785	YES	YES
132	a	915.56	1.73128	YES	YES
133	a	918.06	4.33447	YES	YES
134	a	921.78	0.15880	YES	YES
135	a	931.92	1.04217	YES	YES
136	a	941.02	20.06370	YES	YES
137	a	958.15	0.86918	YES	YES
138	a	960.23	0.03967	YES	YES
139	a	963.17	1.13772	YES	YES
140	a	965.37	1.74276	YES	YES
141	a	967.15	1.70036	YES	YES
142	a	971.51	0.70465	YES	YES
143	a	975.81	0.19769	YES	YES
144	a	979.71	1.05156	YES	YES
145	a	980.83	0.62851	YES	YES
146	a	981.62	0.91322	YES	YES
147	a	981.91	1.82597	YES	YES
148	a	982.33	0.46383	YES	YES
149	a	982.58	1.39642	YES	YES
150	a	983.69	0.60598	YES	YES
151	a	983.98	2.86395	YES	YES
152	a	984.41	0.82648	YES	YES
153	a	984.88	1.17979	YES	YES
154	a	986.90	3.91877	YES	YES
155	a	987.02	1.38555	YES	YES
156	a	987.81	1.54794	YES	YES
157	a	989.15	2.09421	YES	YES
158	a	990.93	0.11952	YES	YES
159	a	1006.99	0.83841	YES	YES
160	a	1017.90	5.50059	YES	YES
161	a	1023.48	9.35428	YES	YES
162	a	1023.67	1.58430	YES	YES

163	a	1023.74	0.77889	YES	YES
164	a	1024.10	1.73878	YES	YES
165	a	1024.40	4.65593	YES	YES
166	a	1024.55	2.72538	YES	YES
167	a	1024.79	1.64315	YES	YES
168	a	1025.60	1.13647	YES	YES
169	a	1068.02	17.10955	YES	YES
170	a	1069.19	11.76528	YES	YES
171	a	1069.60	12.35595	YES	YES
172	a	1070.57	4.94696	YES	YES
173	a	1073.00	2.66472	YES	YES
174	a	1073.51	6.13890	YES	YES
175	a	1074.06	0.99834	YES	YES
176	a	1075.30	20.00519	YES	YES
177	a	1076.57	11.00710	YES	YES
178	a	1077.04	5.64123	YES	YES
179	a	1079.10	5.85509	YES	YES
180	a	1080.08	13.85382	YES	YES
181	a	1082.00	10.90479	YES	YES
182	a	1139.59	0.35731	YES	YES
183	a	1140.45	0.49266	YES	YES
184	a	1140.96	0.27210	YES	YES
185	a	1141.92	0.18346	YES	YES
186	a	1142.22	0.89510	YES	YES
187	a	1142.49	0.27211	YES	YES
188	a	1142.73	0.30586	YES	YES
189	a	1158.32	10.86141	YES	YES
190	a	1166.82	1.59582	YES	YES
191	a	1168.59	2.14456	YES	YES
192	a	1169.79	14.28525	YES	YES
193	a	1171.68	4.74837	YES	YES
194	a	1172.97	3.43908	YES	YES
195	a	1173.71	4.70556	YES	YES
196	a	1203.08	17.74841	YES	YES
197	a	1289.57	4.06131	YES	YES
198	a	1290.17	3.48137	YES	YES

* zero point VIBRATIONAL energy : 0.7400821 Hartree *

Cis TS_{35}_pfbx



bp86-SVP SCF energy: -2931.3906714370
pbe-TZVPP SCF energy: -2930.938938199

XYZ Coordinates
97

C	0.90124	-3.62994	0.57779
C	0.65501	-2.39919	0.31251
C	1.08487	-5.00991	0.88963
H	0.54789	-3.03776	-0.71329
C	1.44991	-7.73466	1.55440
C	0.39219	-7.00537	2.12900
C	0.19767	-5.65926	1.79500
C	2.15962	-5.75466	0.32674
C	2.32742	-7.10627	0.64994
H	1.59306	-8.79662	1.81388
H	-0.29383	-7.49507	2.83979
H	-0.63083	-5.08512	2.23879
H	2.85334	-5.25280	-0.36645
H	3.15837	-7.67534	0.20148
C	3.07072	-0.65648	0.76426
C	4.44220	-0.86282	1.35814
H	4.39488	-1.66123	2.13130
H	4.78062	0.07022	1.85699
H	5.16811	-1.14799	0.57212
C	-1.00948	-0.13326	-2.59942
C	-1.60305	-0.73205	-3.87447
H	-1.78764	0.07038	-4.61765
H	-2.57924	-1.20468	-3.62258
H	-0.94673	-1.51649	-4.30493
C	2.96199	2.34838	0.00383
C	4.12979	1.94667	-0.68846
H	4.04530	1.36924	-1.62059
C	5.40776	2.28014	-0.21028
H	6.29760	1.96174	-0.77902
C	5.55311	3.01728	0.97668
H	6.55584	3.28642	1.34866
C	4.40397	3.41146	1.68037
H	4.49562	3.99390	2.61256
C	3.12468	3.07832	1.20051
H	2.25054	3.42125	1.77066
C	0.23285	3.30380	-0.25565
C	-0.04771	3.51112	1.11535
H	0.26018	2.75954	1.85989
C	-0.74071	4.65528	1.54153
H	-0.93384	4.80591	2.61623
C	-1.20945	5.58664	0.60017
H	-1.75412	6.48575	0.93319
C	-1.01411	5.34321	-0.76936
H	-1.41775	6.04349	-1.51991
C	-0.30251	4.20875	-1.19663
H	-0.17492	4.02288	-2.27324
C	1.75148	2.11336	-2.50521
C	2.20196	3.37615	-2.95681
H	2.22752	4.23548	-2.26733
C	2.64859	3.54627	-4.27689
H	2.98824	4.54020	-4.61354
C	2.67833	2.45177	-5.15941
H	3.03458	2.58411	-6.19489
C	2.26766	1.18749	-4.70789
H	2.30474	0.31818	-5.38539
C	1.80824	1.01706	-3.38926
H	1.49885	0.02089	-3.03929
C	-2.74522	-1.40726	-0.05639
C	-3.82793	-0.83145	-0.75240
H	-3.97698	0.25737	-0.74634
C	-4.74344	-1.63538	-1.45670
H	-5.58283	-1.15734	-1.98906
C	-4.59762	-3.03099	-1.47636
H	-5.31782	-3.66011	-2.02574
C	-3.52608	-3.61829	-0.78133
H	-3.40016	-4.71412	-0.77906
C	-2.61170	-2.81502	-0.08251
H	-1.78657	-3.29453	0.46506
C	-1.48747	-1.26718	2.52974
C	-2.67565	-1.84233	3.03649
H	-3.60187	-1.80929	2.44044
C	-2.69043	-2.45622	4.30016
H	-3.62554	-2.90212	4.67936
C	-1.51999	-2.49817	5.07928
H	-1.53218	-2.97934	6.07184
C	-0.33730	-1.92368	4.58483
H	0.58602	-1.95237	5.18735
C	-0.31709	-1.31310	3.31689
H	0.62097	-0.88434	2.92886
C	-2.41307	1.15357	1.27275
C	-2.84247	1.44046	2.58842
H	-2.54974	0.78788	3.42426
C	-3.66180	2.55350	2.84709
H	-3.99115	2.75575	3.88038
C	-4.07272	3.38964	1.79656
H	-4.73281	4.25022	1.99776
C	-3.62093	3.13158	0.49144
H	-3.91285	3.79656	-0.33755
C	-2.77967	2.03767	0.22962
H	-2.39832	1.86092	-0.79010
O	2.09488	-0.29256	1.51586
O	2.83861	-0.85437	-0.47699
O	-1.27526	1.03231	-2.25884
O	-0.23990	-0.95619	-1.94043
P	1.28269	1.84847	-0.72057
P	-1.45280	-0.39945	0.87275
Ru	0.65185	-0.49067	-0.09708

Vibrational Frequencies

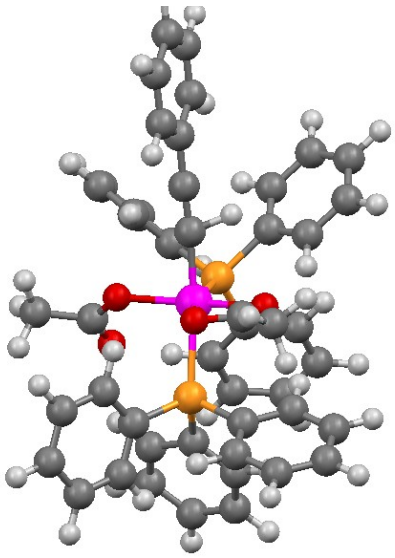
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-785.84	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	8.21	0.16707	YES	YES
9	a	13.76	0.09015	YES	YES
10	a	18.87	0.40837	YES	YES
11	a	20.69	0.19534	YES	YES
12	a	30.46	0.02075	YES	YES

13	a	33.95	0.73272	YES	YES
14	a	34.94	0.26315	YES	YES
15	a	39.41	0.20454	YES	YES
16	a	44.65	0.05737	YES	YES
17	a	48.99	0.19481	YES	YES
18	a	50.48	1.08156	YES	YES
19	a	56.98	0.09259	YES	YES
20	a	58.83	0.75269	YES	YES
21	a	60.48	0.05251	YES	YES
22	a	62.89	0.27024	YES	YES
23	a	64.41	0.47833	YES	YES
24	a	71.05	0.58640	YES	YES
25	a	74.30	0.70022	YES	YES
26	a	76.71	0.42246	YES	YES
27	a	81.34	0.56714	YES	YES
28	a	85.73	2.92352	YES	YES
29	a	89.65	1.52144	YES	YES
30	a	95.61	0.10738	YES	YES
31	a	97.35	0.98050	YES	YES
32	a	102.75	0.43935	YES	YES
33	a	109.00	2.26927	YES	YES
34	a	109.64	0.25998	YES	YES
35	a	115.24	2.57795	YES	YES
36	a	123.18	0.72791	YES	YES
37	a	127.26	5.32194	YES	YES
38	a	136.81	3.09727	YES	YES
39	a	142.97	0.30578	YES	YES
40	a	157.09	4.40409	YES	YES
41	a	179.99	2.44235	YES	YES
42	a	184.58	4.61754	YES	YES
43	a	187.99	2.48362	YES	YES
44	a	195.91	0.15972	YES	YES
45	a	201.60	0.51740	YES	YES
46	a	208.90	2.77759	YES	YES
47	a	211.13	0.56754	YES	YES
48	a	214.09	3.70503	YES	YES
49	a	219.15	1.44784	YES	YES
50	a	229.67	0.88413	YES	YES
51	a	247.52	0.02834	YES	YES
52	a	254.68	0.22361	YES	YES
53	a	255.22	2.05265	YES	YES
54	a	259.62	1.31278	YES	YES
55	a	260.45	1.23186	YES	YES
56	a	266.10	0.28469	YES	YES
57	a	269.64	2.03992	YES	YES
58	a	278.08	9.64952	YES	YES
59	a	284.13	14.52216	YES	YES
60	a	299.43	34.10174	YES	YES
61	a	313.41	16.75056	YES	YES
62	a	328.68	22.00395	YES	YES
63	a	383.37	3.21433	YES	YES
64	a	386.41	47.77612	YES	YES
65	a	395.01	0.35838	YES	YES
66	a	396.08	0.93690	YES	YES
67	a	402.55	1.51794	YES	YES
68	a	403.66	0.84787	YES	YES
69	a	405.46	4.64273	YES	YES
70	a	413.93	0.30984	YES	YES
71	a	418.29	4.01901	YES	YES
72	a	421.60	9.11876	YES	YES
73	a	425.53	21.69811	YES	YES
74	a	429.74	20.10366	YES	YES
75	a	451.35	7.36639	YES	YES
76	a	459.23	33.84009	YES	YES
77	a	462.21	19.40034	YES	YES
78	a	475.89	5.79989	YES	YES
79	a	480.68	16.78760	YES	YES
80	a	485.23	15.15347	YES	YES
81	a	493.07	15.27865	YES	YES
82	a	502.98	5.26325	YES	YES
83	a	508.40	32.03856	YES	YES
84	a	513.09	19.41307	YES	YES
85	a	519.19	165.58390	YES	YES
86	a	524.30	112.03217	YES	YES
87	a	552.31	34.95400	YES	YES
88	a	567.67	39.54380	YES	YES
89	a	595.60	7.12524	YES	YES
90	a	605.15	4.48752	YES	YES
91	a	607.98	0.09008	YES	YES
92	a	609.86	0.54151	YES	YES
93	a	610.36	2.84951	YES	YES
94	a	610.81	1.04773	YES	YES
95	a	611.06	0.30925	YES	YES
96	a	612.59	0.28510	YES	YES
97	a	613.09	0.57216	YES	YES
98	a	663.05	4.87674	YES	YES
99	a	665.43	63.72807	YES	YES
100	a	666.89	7.44799	YES	YES
101	a	668.98	16.02873	YES	YES
102	a	676.57	7.11790	YES	YES
103	a	678.69	16.18905	YES	YES
104	a	684.60	9.59709	YES	YES
105	a	688.84	29.68532	YES	YES
106	a	690.78	13.86221	YES	YES
107	a	691.13	32.63400	YES	YES
108	a	694.58	33.17120	YES	YES
109	a	701.72	57.46256	YES	YES
110	a	703.25	28.64746	YES	YES
111	a	708.99	19.49909	YES	YES
112	a	711.26	15.32946	YES	YES
113	a	734.38	12.29973	YES	YES
114	a	740.18	4.58899	YES	YES
115	a	743.39	3.91629	YES	YES
116	a	746.69	7.26138	YES	YES
117	a	747.61	0.50776	YES	YES
118	a	749.09	7.84380	YES	YES
119	a	760.22	24.99198	YES	YES
120	a	788.51	11.76201	YES	YES
121	a	825.73	0.94468	YES	YES
122	a	829.85	0.91545	YES	YES
123	a	831.56	0.21739	YES	YES
124	a	836.75	2.31230	YES	YES
125	a	845.85	0.37276	YES	YES
126	a	847.66	0.91941	YES	YES
127	a	851.30	2.53028	YES	YES
128	a	900.28	0.84027	YES	YES
129	a	904.88	0.05706	YES	YES
130	a	909.48	2.10852	YES	YES
131	a	912.49	1.37753	YES	YES
132	a	921.70	0.23196	YES	YES
133	a	923.51	2.94177	YES	YES
134	a	924.99	1.44717	YES	YES
135	a	927.25	1.34061	YES	YES
136	a	941.48	20.06124	YES	YES
137	a	952.97	0.32904	YES	YES
138	a	955.88	0.37736	YES	YES
139	a	960.54	0.97186	YES	YES
140	a	960.96	0.16084	YES	YES
141	a	969.82	0.48782	YES	YES
142	a	971.14	0.86166	YES	YES
143	a	973.39	0.19312	YES	YES
144	a	977.93	0.03829	YES	YES
145	a	979.03	0.27301	YES	YES
146	a	979.79	0.04267	YES	YES
147	a	981.00	0.10282	YES	YES
148	a	981.38	2.14728	YES	YES
149	a	981.71	0.41155	YES	YES
150	a	983.51	0.38848	YES	YES
151	a	984.10	2.18276	YES	YES
152	a	984.34	0.49378	YES	YES
153	a	985.04	0.32742	YES	YES
154	a	986.02	2.54017	YES	YES
155	a	986.53	3.00338	YES	YES
156	a	989.60	3.25075	YES	YES
157	a	990.58	4.37233	YES	YES
158	a	992.27	0.76908	YES	YES
159	a	1016.24	0.42797	YES	YES
160	a	1020.58	11.76968	YES	YES

161	a	1022.84	4.26730	YES	YES
162	a	1023.29	1.35355	YES	YES
163	a	1023.70	0.82658	YES	YES
164	a	1024.29	1.96672	YES	YES
165	a	1024.54	1.86825	YES	YES
166	a	1026.42	1.94961	YES	YES
167	a	1027.28	8.89846	YES	YES
168	a	1027.84	1.05348	YES	YES
169	a	1062.23	11.09114	YES	YES
170	a	1067.34	16.90040	YES	YES
171	a	1070.28	2.16283	YES	YES
172	a	1072.37	5.84501	YES	YES
173	a	1073.09	15.97513	YES	YES
174	a	1074.38	4.97203	YES	YES
175	a	1074.73	4.50781	YES	YES
176	a	1075.15	1.60220	YES	YES
177	a	1078.05	21.23617	YES	YES
178	a	1078.59	7.46162	YES	YES
179	a	1081.75	1.34396	YES	YES
180	a	1081.88	10.44021	YES	YES
181	a	1083.42	8.68895	YES	YES
182	a	1140.21	0.53674	YES	YES
183	a	1140.80	0.37242	YES	YES
184	a	1140.90	0.18319	YES	YES
185	a	1140.96	0.35599	YES	YES
186	a	1141.53	0.02852	YES	YES
187	a	1142.08	1.02222	YES	YES
188	a	1142.98	0.08975	YES	YES
189	a	1157.58	0.92856	YES	YES
190	a	1166.47	6.20109	YES	YES
191	a	1169.43	4.09364	YES	YES
192	a	1170.94	4.74605	YES	YES
193	a	1171.45	4.37335	YES	YES
194	a	1177.09	3.73248	YES	YES
195	a	1178.56	9.83960	YES	YES
196	a	1203.12	6.10141	YES	YES
197	a	1288.04	0.29735	YES	YES
198	a	1288.79	0.31836	YES	YES

* zero point VIBRATIONAL energy : 0.7410730 Hartree *

Cis TS_{35}_pfby



bp86-SVP SCF energy: -2931.4000753760
pbe-TZVPP SCF energy: -2930.949404370

XYZ Coordinates
97

C	0.57308	-3.61498	0.41515
C	0.77126	-2.36590	0.20581
C	0.33454	-4.99201	0.69902
H	1.04176	-2.56917	1.35915
C	-0.14652	-7.72487	1.23304
C	0.98161	-7.34344	0.48177
C	1.23014	-5.99039	0.22135
C	-0.80814	-5.39200	1.44931
C	-1.03584	-6.74667	1.71797
H	-0.33419	-8.79117	1.44145
H	1.67543	-8.11051	0.10061
H	2.11290	-5.68030	-0.36009
H	-1.50231	-4.61983	1.81630
H	-1.91856	-7.04641	2.30594
C	3.57053	-0.95132	0.54917
C	4.95511	-1.19430	1.09786
H	4.90182	-1.53456	2.15275
H	5.52327	-0.23754	1.07607
H	5.49388	-1.93810	0.47686
C	-0.49520	-0.18193	-2.80370
C	-0.88376	-0.74378	-4.17234
H	-0.25449	-0.25535	-4.95012
H	-1.94244	-0.49042	-4.38921
H	-0.72901	-1.84028	-4.23390
C	3.60081	2.08359	-0.24358
C	4.87805	2.19057	-0.83244
H	5.00368	2.00953	-1.91117
C	5.99933	2.52909	-0.05297
H	6.98945	2.61051	-0.53235
C	5.86008	2.76660	1.32464
H	6.73873	3.03856	1.93324
C	4.59365	2.64665	1.92424
H	4.47390	2.81787	3.00711
C	3.47631	2.29453	1.14964
H	2.49236	2.18025	1.63261
C	1.30036	3.37826	-1.36650
C	1.71271	4.46560	-0.56685
H	2.45980	4.32336	0.22733
C	1.19606	5.75577	-0.78436
H	1.53611	6.58845	-0.14612
C	0.27092	5.98493	-1.81421
H	-0.12122	7.00005	-1.99501
C	-0.14984	4.90649	-2.61215
H	-0.88156	5.06841	-3.42176
C	0.34915	3.61408	-2.38700
H	-0.01905	2.77322	-2.99374
C	2.71292	1.44764	-2.93907
C	3.11562	2.56351	-3.71072
H	3.01231	3.58209	-3.30485
C	3.65116	2.38916	-4.99703
H	3.95922	3.27151	-5.58293
C	3.79100	1.09778	-5.53520
H	4.20706	0.96148	-6.54769
C	3.39660	-0.01508	-4.77529
H	3.50177	-1.03268	-5.18696
C	2.86269	0.15415	-3.48493
H	2.55352	-0.72349	-2.90222
C	-2.41933	-0.45984	0.02069
C	-3.62783	0.23847	0.23969
H	-3.62824	1.17565	0.81746
C	-4.84137	-0.25200	-0.27308
H	-5.77372	0.30969	-0.09444
C	-4.86740	-1.44820	-1.00911
H	-5.81918	-1.83008	-1.41510
C	-3.67057	-2.15149	-1.22755
H	-3.67720	-3.08884	-1.80888
C	-2.45606	-1.66269	-0.71723
H	-1.52142	-2.20674	-0.91420
C	-0.91632	-0.68071	2.46488
C	-2.13243	-1.17168	2.98908
H	-3.05383	-1.11814	2.38889
C	-2.18470	-1.73651	4.27620
H	-3.14544	-2.11531	4.66426
C	-1.02431	-1.81803	5.06421
H	-1.06701	-2.26088	6.07341
C	0.19112	-1.33281	4.55272
H	1.11044	-1.39201	5.15953
C	0.24862	-0.77193	3.26356
H	1.21474	-0.41951	2.86850
C	-1.12391	1.88492	1.15642
C	-0.91173	2.40827	2.45111
H	-0.54391	1.75724	3.25952
C	-1.19051	3.75795	2.72806
H	-1.02275	4.15044	3.74514
C	-1.69702	4.59522	1.72044
H	-1.92872	5.65074	1.94115
C	-1.90259	4.08153	0.42839
H	-2.28747	4.73433	-0.37133
C	-1.60563	2.74000	0.13848
H	-1.74786	2.34057	-0.87833
O	2.64745	-0.48209	1.31300
O	3.29106	-1.17198	-0.67336
O	-0.88599	0.94381	-2.45058
O	0.27676	-0.96861	-2.11010
P	2.05590	1.66478	-1.20575
P	-0.79463	0.10030	0.75612
Ru	1.15629	-0.50801	-0.27760

Vibrational Frequencies

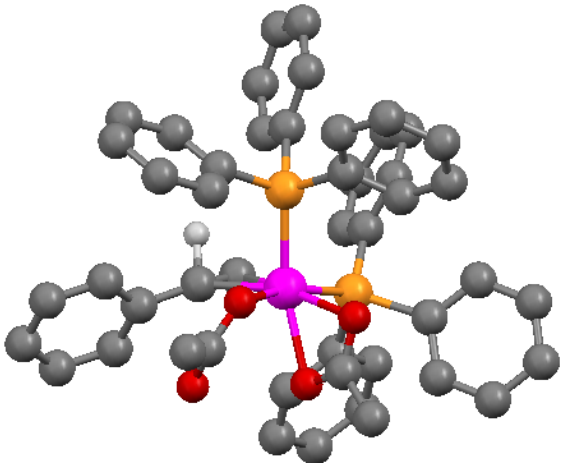
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-735.19	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	12.77	0.11652	YES	YES
9	a	16.91	0.18762	YES	YES
10	a	17.91	0.25142	YES	YES
11	a	21.44	0.17203	YES	YES
12	a	24.65	0.14498	YES	YES

13	a	29.18	0.12431	YES	YES
14	a	33.76	1.40576	YES	YES
15	a	36.12	0.06770	YES	YES
16	a	41.29	0.65102	YES	YES
17	a	47.31	0.17179	YES	YES
18	a	50.09	0.01094	YES	YES
19	a	51.47	0.12112	YES	YES
20	a	55.53	1.13552	YES	YES
21	a	59.05	0.02828	YES	YES
22	a	59.48	1.55748	YES	YES
23	a	64.68	0.08065	YES	YES
24	a	67.02	0.06363	YES	YES
25	a	72.22	0.54044	YES	YES
26	a	74.11	0.02465	YES	YES
27	a	76.76	1.94914	YES	YES
28	a	81.36	1.25046	YES	YES
29	a	82.69	2.19076	YES	YES
30	a	83.58	2.44238	YES	YES
31	a	85.95	0.53297	YES	YES
32	a	91.81	0.12195	YES	YES
33	a	94.55	0.48097	YES	YES
34	a	101.42	1.25010	YES	YES
35	a	103.77	0.69922	YES	YES
36	a	108.94	0.44136	YES	YES
37	a	112.32	1.24025	YES	YES
38	a	117.58	1.40455	YES	YES
39	a	141.35	10.22557	YES	YES
40	a	157.89	3.90514	YES	YES
41	a	165.91	0.81421	YES	YES
42	a	182.92	1.14606	YES	YES
43	a	188.94	3.57153	YES	YES
44	a	196.36	12.17922	YES	YES
45	a	199.22	1.96227	YES	YES
46	a	201.78	22.90058	YES	YES
47	a	212.43	20.68582	YES	YES
48	a	215.87	6.53088	YES	YES
49	a	220.59	2.70893	YES	YES
50	a	229.78	0.83820	YES	YES
51	a	233.30	1.86108	YES	YES
52	a	245.06	0.56151	YES	YES
53	a	246.72	0.52825	YES	YES
54	a	250.91	0.08886	YES	YES
55	a	255.25	0.18384	YES	YES
56	a	258.36	1.57073	YES	YES
57	a	263.42	0.65650	YES	YES
58	a	265.57	0.30849	YES	YES
59	a	277.86	1.87246	YES	YES
60	a	288.74	14.40145	YES	YES
61	a	295.51	23.24771	YES	YES
62	a	325.33	17.50993	YES	YES
63	a	381.20	8.76211	YES	YES
64	a	394.82	1.10194	YES	YES
65	a	400.19	0.82128	YES	YES
66	a	400.81	0.43495	YES	YES
67	a	401.16	0.89503	YES	YES
68	a	405.45	35.30563	YES	YES
69	a	405.87	4.00576	YES	YES
70	a	406.30	1.02515	YES	YES
71	a	409.01	1.54683	YES	YES
72	a	421.53	17.37061	YES	YES
73	a	424.24	2.72876	YES	YES
74	a	437.82	36.57880	YES	YES
75	a	441.51	3.75326	YES	YES
76	a	450.36	27.15601	YES	YES
77	a	454.86	19.40040	YES	YES
78	a	470.53	2.27711	YES	YES
79	a	474.15	0.43141	YES	YES
80	a	493.34	22.45169	YES	YES
81	a	497.45	13.79134	YES	YES
82	a	501.57	2.14931	YES	YES
83	a	503.19	63.49573	YES	YES
84	a	509.51	23.19968	YES	YES
85	a	516.92	142.16330	YES	YES
86	a	527.05	126.41826	YES	YES
87	a	550.06	31.88595	YES	YES
88	a	567.32	41.44229	YES	YES
89	a	591.83	3.45720	YES	YES
90	a	599.98	6.10570	YES	YES
91	a	609.30	1.33623	YES	YES
92	a	609.37	0.10468	YES	YES
93	a	610.13	1.79598	YES	YES
94	a	610.49	0.15552	YES	YES
95	a	610.75	0.24002	YES	YES
96	a	611.11	0.51710	YES	YES
97	a	611.61	1.27708	YES	YES
98	a	664.89	16.90015	YES	YES
99	a	666.20	49.47725	YES	YES
100	a	669.24	13.89899	YES	YES
101	a	672.15	17.26101	YES	YES
102	a	676.88	6.36237	YES	YES
103	a	680.02	11.84306	YES	YES
104	a	684.63	6.88716	YES	YES
105	a	687.21	11.75110	YES	YES
106	a	688.29	31.03266	YES	YES
107	a	693.59	29.56049	YES	YES
108	a	694.09	78.11928	YES	YES
109	a	697.83	19.52060	YES	YES
110	a	699.79	36.48523	YES	YES
111	a	700.97	13.11933	YES	YES
112	a	705.09	21.67741	YES	YES
113	a	739.62	13.65276	YES	YES
114	a	742.14	5.11033	YES	YES
115	a	743.06	5.50866	YES	YES
116	a	744.44	2.12683	YES	YES
117	a	747.08	4.87238	YES	YES
118	a	749.03	5.86654	YES	YES
119	a	763.82	22.38194	YES	YES
120	a	789.36	11.14317	YES	YES
121	a	830.07	0.17713	YES	YES
122	a	831.79	0.25658	YES	YES
123	a	833.84	2.38841	YES	YES
124	a	834.49	0.83344	YES	YES
125	a	837.97	1.34856	YES	YES
126	a	839.95	1.19221	YES	YES
127	a	847.16	1.93949	YES	YES
128	a	906.47	0.18999	YES	YES
129	a	907.06	1.30011	YES	YES
130	a	908.97	0.68415	YES	YES
131	a	911.73	1.75150	YES	YES
132	a	913.38	0.31223	YES	YES
133	a	918.51	0.99358	YES	YES
134	a	920.37	0.92137	YES	YES
135	a	926.91	5.24904	YES	YES
136	a	943.57	18.65222	YES	YES
137	a	955.91	0.07941	YES	YES
138	a	957.53	0.42820	YES	YES
139	a	958.92	1.00526	YES	YES
140	a	962.07	1.80665	YES	YES
141	a	963.55	0.04435	YES	YES
142	a	963.82	1.00493	YES	YES
143	a	970.39	2.79602	YES	YES
144	a	979.15	0.14248	YES	YES
145	a	980.33	0.11527	YES	YES
146	a	980.97	0.26634	YES	YES
147	a	982.14	0.07853	YES	YES
148	a	982.46	0.80771	YES	YES
149	a	982.56	0.51307	YES	YES
150	a	982.71	0.75410	YES	YES
151	a	983.28	0.61443	YES	YES
152	a	984.00	0.81472	YES	YES
153	a	984.68	1.05780	YES	YES
154	a	985.65	3.93880	YES	YES
155	a	986.35	2.91768	YES	YES
156	a	987.26	0.02900	YES	YES
157	a	987.45	1.28679	YES	YES
158	a	989.55	2.53242	YES	YES
159	a	989.71	1.25819	YES	YES
160	a	1019.42	10.02052	YES	YES

161	a	1022.21	4.42216	YES	YES
162	a	1023.45	0.75675	YES	YES
163	a	1023.96	14.66983	YES	YES
164	a	1024.17	0.56856	YES	YES
165	a	1024.80	2.69791	YES	YES
166	a	1025.11	1.15724	YES	YES
167	a	1025.61	0.78887	YES	YES
168	a	1026.57	1.75696	YES	YES
169	a	1066.81	12.88841	YES	YES
170	a	1070.00	21.82548	YES	YES
171	a	1071.17	4.58774	YES	YES
172	a	1073.22	16.33556	YES	YES
173	a	1073.34	17.79321	YES	YES
174	a	1074.30	2.27286	YES	YES
175	a	1075.71	1.45122	YES	YES
176	a	1077.21	0.68853	YES	YES
177	a	1077.47	3.04312	YES	YES
178	a	1077.59	10.48946	YES	YES
179	a	1080.89	15.60665	YES	YES
180	a	1081.30	11.54866	YES	YES
181	a	1081.97	3.97397	YES	YES
182	a	1140.72	0.33664	YES	YES
183	a	1140.84	0.37499	YES	YES
184	a	1141.07	0.44159	YES	YES
185	a	1141.51	0.62193	YES	YES
186	a	1142.16	0.38622	YES	YES
187	a	1142.73	0.47542	YES	YES
188	a	1143.24	0.15978	YES	YES
189	a	1155.53	2.65910	YES	YES
190	a	1170.72	1.68038	YES	YES
191	a	1171.07	5.90494	YES	YES
192	a	1172.48	4.92042	YES	YES
193	a	1173.82	9.25579	YES	YES
194	a	1174.17	6.18069	YES	YES
195	a	1179.85	10.54889	YES	YES
196	a	1203.86	8.94954	YES	YES
197	a	1287.56	0.03314	YES	YES
198	a	1293.49	2.13984	YES	YES

* zero point VIBRATIONAL energy : 0.7405843 Hartree *

Cis TS_{25}_afay



bp86-SVP SCF energy: -2931.3447904250
pbe-TZVPP SCF energy: -2930.897400013

XYZ Coordinates
97

C	-0.43800	-0.21424	-2.23088
C	-0.69668	0.88794	-1.50879
C	-0.42588	-0.74553	-3.60786
H	-1.58228	-0.19304	-1.79573
C	-0.52201	-1.67646	-6.26902
C	-0.75608	-2.56115	-5.20180
C	-0.70463	-2.10324	-3.87729
C	-0.20107	0.14338	-4.68426
C	-0.24245	-0.32402	-6.00496
H	-0.55686	-2.04134	-7.30907
H	-0.97714	-3.62276	-5.40172
H	-0.87968	-2.79815	-3.04194
H	0.01267	1.20229	-4.47193
H	-0.05656	0.37592	-6.83660
C	3.31018	-0.21714	-0.04119
C	4.79757	-0.39839	0.11998
H	5.08580	-1.37644	-0.32598
H	5.07346	-0.41405	1.19412
H	5.34874	0.40001	-0.41624
C	2.15468	-2.26417	-2.35200
C	2.69394	-3.68562	-2.57618
H	3.37802	-3.69054	-3.44855
H	1.84772	-4.38017	-2.77640
H	3.22385	-4.06105	-1.67400
C	1.95072	2.19861	1.92442
C	3.25968	2.48739	1.46789
H	3.46544	2.52447	0.38736
C	4.30105	2.74810	2.37230
H	5.30882	2.97598	1.98672
C	4.06098	2.73212	3.75678
H	4.87729	2.94263	4.46758
C	2.76581	2.45970	4.22303
H	2.55318	2.46293	5.30534
C	1.72234	2.19519	3.31713
H	0.71666	2.01740	3.72218
C	-0.93438	2.41716	1.40600
C	-1.40570	1.80705	2.59157
H	-0.88394	0.93603	3.01689
C	-2.56602	2.27333	3.23072
H	-2.90470	1.79005	4.16159
C	-3.30448	3.32811	2.67038
H	-4.21757	3.69369	3.16888
C	-2.88582	3.89459	1.45497
H	-3.47459	4.70088	0.98630
C	-1.71168	3.44466	0.82708
H	-1.39945	3.89735	-0.12512
C	1.08182	3.21877	-0.55090
C	1.12272	4.54519	-0.06188
H	0.86982	4.75428	0.99065
C	1.49088	5.60761	-0.90234
H	1.51274	6.63568	-0.50381
C	1.83846	5.35879	-2.24194
H	2.13409	6.19151	-2.90189
C	1.82141	4.04230	-2.72923
H	2.11324	3.83181	-3.77137
C	1.44582	2.97682	-1.89114
H	1.47700	1.94941	-2.27990
C	-2.45649	-1.01635	1.27570
C	-3.13690	-1.67457	2.32567
H	-2.63942	-2.47896	2.88921
C	-4.45228	-1.31636	2.66376
H	-4.96379	-1.84202	3.48741
C	-5.11562	-0.30150	1.95195
H	-6.15222	-0.02827	2.21105
C	-4.44360	0.36890	0.91749
H	-4.94277	1.18087	0.36432
C	-3.12075	0.02295	0.58953
H	-2.59458	0.59840	-0.18976
C	-1.31167	-3.14342	-0.22967
C	-2.60394	-3.24065	-0.79227
H	-3.34011	-2.43730	-0.63356
C	-2.97419	-4.36602	-1.55093
H	-3.98813	-4.42193	-1.98055
C	-2.06148	-5.41407	-1.75081
H	-2.35362	-6.30061	-2.33801
C	-0.77310	-5.32751	-1.19264
H	-0.04998	-6.14661	-1.34178
C	-0.39446	-4.20006	-0.44568
H	0.61948	-4.13730	-0.02747
C	-0.07194	-2.33602	2.28292
C	-0.38077	-3.64126	2.73051
H	-1.01985	-4.29873	2.12084
C	0.12386	-4.11620	3.95330
H	-0.12567	-5.13835	4.28355
C	0.94201	-3.29572	4.74802
H	1.34043	-3.67065	5.70552
C	1.25849	-1.99952	4.30848
H	1.91404	-1.35150	4.91342
C	0.76105	-1.52503	3.08334
H	1.05628	-0.52592	2.73196
O	2.49844	-0.74257	0.80777
O	2.82090	0.41414	-1.03418
O	2.35879	-1.36613	-3.16606
O	1.46297	-2.17393	-1.22904
P	0.64204	1.83033	0.61679
P	-0.77474	-1.62459	0.71207
Ru	0.79056	-0.33913	-0.43010

Vibrational Frequencies

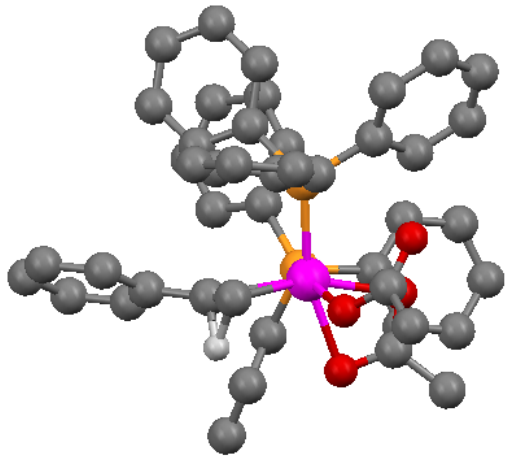
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-725.94	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	7.39	0.23259	YES	YES
9	a	20.87	0.13017	YES	YES
10	a	22.27	0.00837	YES	YES
11	a	28.87	0.22796	YES	YES
12	a	32.06	0.14564	YES	YES
13	a	35.05	0.37642	YES	YES
14	a	41.24	0.20156	YES	YES
15	a	47.27	0.02040	YES	YES
16	a	50.10	0.14828	YES	YES
17	a	54.42	0.00444	YES	YES
18	a	56.14	0.21064	YES	YES

19	a	58.24	0.17420	YES	YES
20	a	59.35	0.39729	YES	YES
21	a	62.10	0.38621	YES	YES
22	a	63.30	0.21985	YES	YES
23	a	70.94	1.08992	YES	YES
24	a	77.27	0.37044	YES	YES
25	a	78.42	0.25162	YES	YES
26	a	82.01	0.23844	YES	YES
27	a	87.25	0.07975	YES	YES
28	a	88.88	0.57393	YES	YES
29	a	95.41	2.75217	YES	YES
30	a	100.09	0.91892	YES	YES
31	a	102.16	1.58508	YES	YES
32	a	103.72	0.65030	YES	YES
33	a	110.75	0.77799	YES	YES
34	a	112.55	0.72697	YES	YES
35	a	114.63	0.12635	YES	YES
36	a	117.94	2.28665	YES	YES
37	a	129.75	0.74203	YES	YES
38	a	143.72	1.13654	YES	YES
39	a	150.21	3.15226	YES	YES
40	a	169.16	3.06708	YES	YES
41	a	182.41	3.70669	YES	YES
42	a	190.83	0.99571	YES	YES
43	a	191.67	2.64005	YES	YES
44	a	197.68	3.08077	YES	YES
45	a	201.53	0.27945	YES	YES
46	a	207.54	0.76074	YES	YES
47	a	214.04	3.64469	YES	YES
48	a	219.49	3.40080	YES	YES
49	a	224.12	1.83169	YES	YES
50	a	228.26	2.92098	YES	YES
51	a	233.66	3.41274	YES	YES
52	a	245.58	0.19448	YES	YES
53	a	251.37	0.88071	YES	YES
54	a	255.87	0.21825	YES	YES
55	a	260.49	0.65201	YES	YES
56	a	263.63	0.02888	YES	YES
57	a	268.03	1.41950	YES	YES
58	a	270.21	0.74441	YES	YES
59	a	277.57	7.15310	YES	YES
60	a	301.71	17.37216	YES	YES
61	a	318.42	8.14699	YES	YES
62	a	383.77	20.62215	YES	YES
63	a	392.46	16.14561	YES	YES
64	a	399.04	0.16420	YES	YES
65	a	399.40	0.07608	YES	YES
66	a	400.79	0.28608	YES	YES
67	a	402.00	0.41865	YES	YES
68	a	403.10	1.32933	YES	YES
69	a	411.98	0.74470	YES	YES
70	a	412.81	1.32447	YES	YES
71	a	418.01	12.40167	YES	YES
72	a	423.90	8.13074	YES	YES
73	a	429.28	22.51009	YES	YES
74	a	436.79	3.56324	YES	YES
75	a	448.92	17.68078	YES	YES
76	a	464.29	14.94562	YES	YES
77	a	473.53	3.21869	YES	YES
78	a	482.44	8.98083	YES	YES
79	a	492.37	0.98484	YES	YES
80	a	497.33	15.19810	YES	YES
81	a	500.29	12.02678	YES	YES
82	a	508.32	39.14621	YES	YES
83	a	513.68	42.46186	YES	YES
84	a	518.28	136.48646	YES	YES
85	a	529.15	92.02673	YES	YES
86	a	542.24	23.51093	YES	YES
87	a	586.51	4.60028	YES	YES
88	a	592.43	8.80994	YES	YES
89	a	597.48	2.35544	YES	YES
90	a	607.80	0.20796	YES	YES
91	a	609.19	1.42647	YES	YES
92	a	609.40	0.46219	YES	YES
93	a	610.29	0.27586	YES	YES
94	a	612.20	0.67317	YES	YES
95	a	612.46	1.41534	YES	YES
96	a	615.14	0.95666	YES	YES
97	a	652.72	16.98747	YES	YES
98	a	666.38	9.20291	YES	YES
99	a	672.66	6.68948	YES	YES
100	a	674.35	59.72328	YES	YES
101	a	678.50	10.31618	YES	YES
102	a	679.24	10.04795	YES	YES
103	a	685.99	24.25962	YES	YES
104	a	687.48	16.64688	YES	YES
105	a	688.89	15.53669	YES	YES
106	a	695.18	36.35945	YES	YES
107	a	696.89	52.40237	YES	YES
108	a	698.83	40.67216	YES	YES
109	a	701.77	35.03094	YES	YES
110	a	704.06	8.06879	YES	YES
111	a	704.79	20.81106	YES	YES
112	a	734.87	9.03910	YES	YES
113	a	739.63	5.13239	YES	YES
114	a	741.00	1.89209	YES	YES
115	a	742.69	6.27526	YES	YES
116	a	745.19	4.47753	YES	YES
117	a	745.71	16.10601	YES	YES
118	a	748.39	8.39192	YES	YES
119	a	771.02	4.33229	YES	YES
120	a	822.53	0.34743	YES	YES
121	a	830.96	0.10684	YES	YES
122	a	831.38	1.11347	YES	YES
123	a	834.11	0.88520	YES	YES
124	a	837.94	0.52446	YES	YES
125	a	838.80	0.27559	YES	YES
126	a	843.55	0.21228	YES	YES
127	a	889.74	4.63181	YES	YES
128	a	903.62	1.39141	YES	YES
129	a	905.08	0.49972	YES	YES
130	a	905.24	0.54221	YES	YES
131	a	909.63	0.64805	YES	YES
132	a	912.68	0.38503	YES	YES
133	a	913.76	0.57287	YES	YES
134	a	920.14	1.54906	YES	YES
135	a	936.18	23.77576	YES	YES
136	a	947.20	7.60695	YES	YES
137	a	950.49	0.15732	YES	YES
138	a	954.44	0.16390	YES	YES
139	a	956.41	0.49790	YES	YES
140	a	958.33	0.49015	YES	YES
141	a	959.74	0.25730	YES	YES
142	a	961.14	0.15980	YES	YES
143	a	967.25	1.38102	YES	YES
144	a	976.45	1.16946	YES	YES
145	a	977.77	11.11327	YES	YES
146	a	979.41	0.05212	YES	YES
147	a	980.28	0.91697	YES	YES
148	a	980.94	2.39921	YES	YES
149	a	981.41	0.80131	YES	YES
150	a	981.93	0.23581	YES	YES
151	a	982.94	1.38059	YES	YES
152	a	983.56	2.25566	YES	YES
153	a	983.95	0.21848	YES	YES
154	a	985.33	1.37691	YES	YES
155	a	986.18	0.65506	YES	YES
156	a	986.41	0.25948	YES	YES
157	a	987.28	2.91848	YES	YES
158	a	988.27	1.70722	YES	YES
159	a	990.11	0.08206	YES	YES
160	a	1013.13	3.99932	YES	YES
161	a	1023.69	1.41276	YES	YES
162	a	1023.98	1.57478	YES	YES
163	a	1024.25	0.51697	YES	YES
164	a	1024.46	2.02503	YES	YES
165	a	1025.71	2.07455	YES	YES
166	a	1025.93	2.76406	YES	YES

167	a	1026.27	1.30794	YES	YES
168	a	1026.69	8.01328	YES	YES
169	a	1066.29	16.29889	YES	YES
170	a	1070.61	12.60721	YES	YES
171	a	1070.94	2.85452	YES	YES
172	a	1071.66	18.18069	YES	YES
173	a	1072.65	15.71858	YES	YES
174	a	1075.75	12.74721	YES	YES
175	a	1076.20	13.23936	YES	YES
176	a	1076.71	3.83908	YES	YES
177	a	1077.24	1.68735	YES	YES
178	a	1079.85	15.13695	YES	YES
179	a	1081.00	6.58072	YES	YES
180	a	1082.00	0.65576	YES	YES
181	a	1084.25	3.84925	YES	YES
182	a	1140.36	0.26549	YES	YES
183	a	1141.27	0.21529	YES	YES
184	a	1141.94	0.31915	YES	YES
185	a	1142.36	0.52217	YES	YES
186	a	1142.57	0.19890	YES	YES
187	a	1143.13	0.28117	YES	YES
188	a	1143.73	0.97697	YES	YES
189	a	1152.44	1.26979	YES	YES
190	a	1166.80	1.19693	YES	YES
191	a	1167.27	3.33656	YES	YES
192	a	1168.70	4.93286	YES	YES
193	a	1170.38	2.58157	YES	YES
194	a	1172.53	1.58736	YES	YES
195	a	1178.41	5.81287	YES	YES
196	a	1179.74	3.03113	YES	YES
197	a	1259.83	329.12743	YES	YES
198	a	1287.41	4.03116	YES	YES

* zero point VIBRATIONAL energy : 0.7411098 Hartree *

Cis TS_{25}_afbx



bp86-SVP SCF energy: -2931.3240787300
pbe-TZVPP SCF energy: -2930.873170987

XYZ Coordinates
97

C	-0.06949	0.17267	-2.53693
C	0.22027	-1.12596	-2.68027
C	-1.01157	1.11660	-3.19364
H	0.92089	-0.13106	-3.28223
C	-2.82947	2.77854	-4.59882
C	-1.85441	3.34333	-3.75972
C	-0.95403	2.52118	-3.06286
C	-1.99994	0.55739	-4.04784
C	-2.89823	1.38054	-4.74010
H	-3.53613	3.42644	-5.14378
H	-1.78883	4.43804	-3.64658
H	-0.18628	2.97443	-2.42287
H	-2.04569	-0.53745	-4.15727
H	-3.65801	0.92590	-5.39742
C	3.44086	-0.68683	-0.06106
C	4.88691	-0.95315	0.26334
H	5.14863	-1.96631	-0.11543
H	5.04820	-0.94287	1.36020
H	5.54388	-0.21488	-0.23986
C	2.06909	-3.61212	-0.62812
C	2.99004	-4.64857	-1.28864
H	3.43760	-5.30207	-0.51156
H	3.78209	-4.16942	-1.90065
H	2.37743	-5.28214	-1.96867
C	1.92637	1.61400	1.86216
C	3.30710	1.85343	1.66819
H	3.70881	1.95512	0.64846
C	4.17974	1.98399	2.75935
H	5.25043	2.17634	2.57721
C	3.69288	1.88087	4.07342
H	4.37609	1.98944	4.93192
C	2.32476	1.64934	4.27940
H	1.92111	1.57945	5.30323
C	1.44987	1.51647	3.18551
H	0.38183	1.36109	3.39016
C	-0.77208	2.18161	0.93537
C	-1.50402	1.47287	1.91725
H	-1.16021	0.48505	2.26053
C	-2.68850	1.99988	2.45538
H	-3.23156	1.43162	3.22733
C	-3.19013	3.22712	1.99162
H	-4.12443	3.63838	2.40803
C	-2.50291	3.91515	0.97906
H	-2.89580	4.86939	0.59043
C	-1.30291	3.40010	0.45783
H	-0.77685	3.96737	-0.32325
C	1.62442	2.86722	-0.61840
C	1.73519	4.14357	-0.01495
H	1.32681	4.31515	0.99421
C	2.37946	5.19752	-0.68104
H	2.44997	6.18574	-0.19662
C	2.94566	4.98952	-1.95196
H	3.45945	5.81532	-2.47175
C	2.86626	3.72063	-2.54608
H	3.32303	3.53939	-3.53291
C	2.21117	2.66653	-1.88346
H	2.17773	1.67045	-2.34487
C	-2.55119	-1.02836	0.31158
C	-3.53648	-1.49611	1.21041
H	-3.31482	-2.32729	1.89556
C	-4.81208	-0.90844	1.25009
H	-5.56353	-1.29360	1.95996
C	-5.13374	0.15522	0.38943
H	-6.13830	0.60969	0.41725
C	-4.15981	0.63856	-0.49801
H	-4.38464	1.48108	-1.17178
C	-2.88126	0.05610	-0.52450
H	-2.12493	0.46682	-1.20496
C	-1.47617	-3.30395	-0.96238
C	-2.41657	-3.03001	-1.98155
H	-2.82215	-2.01404	-2.10436
C	-2.86750	-4.04649	-2.83908
H	-3.60239	-3.80708	-3.62588
C	-2.39359	-5.35998	-2.68879
H	-2.75083	-6.16089	-3.35765
C	-1.46092	-5.64231	-1.67755
H	-1.07841	-6.66896	-1.54868
C	-0.99793	-4.62551	-0.82370
H	-0.23756	-4.85130	-0.06125
C	-0.67701	-2.61807	1.82009
C	-1.40202	-3.74837	2.25941
H	-2.07506	-4.28178	1.56997
C	-1.26078	-4.21898	3.57615
H	-1.82900	-5.10788	3.89848
C	-0.39870	-3.56791	4.47382
H	-0.28602	-3.94155	5.50534
C	0.33141	-2.44862	4.04078
H	1.03176	-1.94246	4.72583
C	0.19777	-1.98037	2.72360
H	0.82231	-1.14174	2.38116
O	2.51857	-1.07798	0.74411
O	3.09174	-0.11178	-1.14719
O	1.52356	-3.85563	0.45710
O	1.92232	-2.54121	-1.35564
P	0.83344	1.45763	0.32994
P	-0.88374	-1.89363	0.12280
Ru	0.98700	-0.72341	-0.71623

Vibrational Frequencies

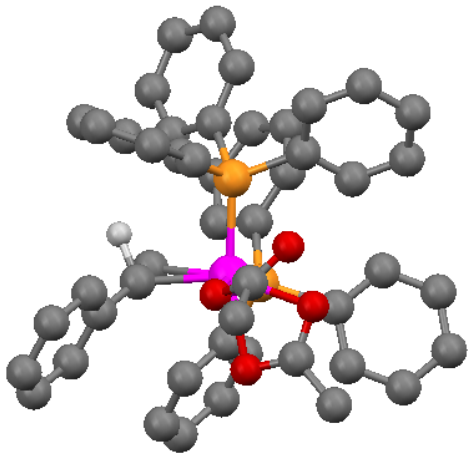
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-838.36	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	13.26	0.13707	YES	YES
9	a	21.54	0.11508	YES	YES
10	a	30.11	0.01965	YES	YES
11	a	33.88	0.00409	YES	YES
12	a	40.03	0.03634	YES	YES
13	a	42.19	0.07718	YES	YES
14	a	43.98	0.24990	YES	YES
15	a	47.55	0.27674	YES	YES
16	a	52.19	0.24749	YES	YES
17	a	54.44	0.27896	YES	YES
18	a	55.46	0.19146	YES	YES

19	a	60.77	1.68006	YES	YES
20	a	62.45	0.12360	YES	YES
21	a	63.57	0.30958	YES	YES
22	a	68.03	0.07787	YES	YES
23	a	70.00	0.16450	YES	YES
24	a	73.24	1.09157	YES	YES
25	a	74.94	0.40051	YES	YES
26	a	80.04	1.36682	YES	YES
27	a	84.76	1.02497	YES	YES
28	a	92.08	0.24227	YES	YES
29	a	94.54	1.09904	YES	YES
30	a	96.17	0.70613	YES	YES
31	a	97.54	0.09897	YES	YES
32	a	104.29	0.73795	YES	YES
33	a	111.41	8.24393	YES	YES
34	a	113.23	1.17231	YES	YES
35	a	114.18	0.10127	YES	YES
36	a	125.49	0.60354	YES	YES
37	a	136.13	0.99923	YES	YES
38	a	146.50	4.57642	YES	YES
39	a	152.34	5.45013	YES	YES
40	a	154.32	3.95851	YES	YES
41	a	168.57	0.15838	YES	YES
42	a	177.31	2.45537	YES	YES
43	a	186.29	0.76209	YES	YES
44	a	197.99	4.25529	YES	YES
45	a	200.13	3.62486	YES	YES
46	a	208.56	1.41705	YES	YES
47	a	210.31	1.12323	YES	YES
48	a	217.68	4.92258	YES	YES
49	a	220.64	0.57836	YES	YES
50	a	230.67	1.55409	YES	YES
51	a	236.73	2.57660	YES	YES
52	a	250.80	0.50444	YES	YES
53	a	251.73	1.31122	YES	YES
54	a	256.91	0.53341	YES	YES
55	a	260.36	1.46965	YES	YES
56	a	263.83	0.25476	YES	YES
57	a	268.48	2.37417	YES	YES
58	a	272.41	0.43985	YES	YES
59	a	290.85	10.24918	YES	YES
60	a	297.98	7.51583	YES	YES
61	a	327.34	11.42088	YES	YES
62	a	372.60	17.73996	YES	YES
63	a	398.24	4.73095	YES	YES
64	a	399.92	12.85391	YES	YES
65	a	401.06	10.62514	YES	YES
66	a	402.61	3.18233	YES	YES
67	a	404.32	0.73661	YES	YES
68	a	409.79	1.54781	YES	YES
69	a	411.75	11.39718	YES	YES
70	a	414.88	1.66149	YES	YES
71	a	419.53	5.87684	YES	YES
72	a	426.50	23.86764	YES	YES
73	a	428.19	1.22231	YES	YES
74	a	443.69	6.61344	YES	YES
75	a	452.56	19.36798	YES	YES
76	a	462.85	18.40938	YES	YES
77	a	470.36	8.25201	YES	YES
78	a	473.28	1.83947	YES	YES
79	a	481.08	8.67699	YES	YES
80	a	488.91	16.41916	YES	YES
81	a	497.65	28.90409	YES	YES
82	a	506.69	34.62984	YES	YES
83	a	510.85	41.24762	YES	YES
84	a	516.90	138.95527	YES	YES
85	a	526.18	38.40003	YES	YES
86	a	542.35	22.04401	YES	YES
87	a	558.78	17.41180	YES	YES
88	a	588.46	4.78541	YES	YES
89	a	600.10	2.65784	YES	YES
90	a	608.66	0.09957	YES	YES
91	a	609.64	0.95770	YES	YES
92	a	610.35	0.54326	YES	YES
93	a	610.78	0.24542	YES	YES
94	a	612.39	0.27349	YES	YES
95	a	612.72	0.53546	YES	YES
96	a	613.18	1.37411	YES	YES
97	a	652.10	10.43185	YES	YES
98	a	666.35	7.27975	YES	YES
99	a	669.67	7.49917	YES	YES
100	a	672.28	10.45956	YES	YES
101	a	672.86	58.60011	YES	YES
102	a	674.66	14.96809	YES	YES
103	a	685.13	15.38748	YES	YES
104	a	689.33	17.00962	YES	YES
105	a	694.22	44.43411	YES	YES
106	a	695.72	48.85112	YES	YES
107	a	697.22	8.66031	YES	YES
108	a	698.88	49.06837	YES	YES
109	a	700.07	32.49992	YES	YES
110	a	705.48	9.14721	YES	YES
111	a	709.35	16.62120	YES	YES
112	a	733.97	9.65023	YES	YES
113	a	736.13	2.38417	YES	YES
114	a	738.47	11.41887	YES	YES
115	a	742.60	7.29463	YES	YES
116	a	746.24	5.42836	YES	YES
117	a	747.22	1.99632	YES	YES
118	a	754.82	14.93149	YES	YES
119	a	772.58	11.59646	YES	YES
120	a	828.69	0.56691	YES	YES
121	a	830.02	0.49810	YES	YES
122	a	834.32	0.50912	YES	YES
123	a	836.40	0.05990	YES	YES
124	a	837.53	1.87723	YES	YES
125	a	841.86	0.49873	YES	YES
126	a	842.33	0.47174	YES	YES
127	a	881.95	30.99668	YES	YES
128	a	903.47	0.44893	YES	YES
129	a	906.90	1.31831	YES	YES
130	a	908.73	1.98710	YES	YES
131	a	910.70	0.47259	YES	YES
132	a	912.86	3.47946	YES	YES
133	a	916.79	1.22773	YES	YES
134	a	920.69	1.94120	YES	YES
135	a	928.18	6.60391	YES	YES
136	a	942.20	20.39065	YES	YES
137	a	954.78	0.16073	YES	YES
138	a	956.92	0.87103	YES	YES
139	a	958.87	0.27603	YES	YES
140	a	961.56	1.10307	YES	YES
141	a	962.53	0.19788	YES	YES
142	a	964.62	0.47466	YES	YES
143	a	967.75	1.45273	YES	YES
144	a	976.65	0.11092	YES	YES
145	a	980.73	3.11519	YES	YES
146	a	981.92	0.38095	YES	YES
147	a	982.28	1.41529	YES	YES
148	a	982.60	1.56985	YES	YES
149	a	983.53	0.14263	YES	YES
150	a	983.91	1.36428	YES	YES
151	a	984.00	3.03023	YES	YES
152	a	984.39	2.55376	YES	YES
153	a	985.14	3.98312	YES	YES
154	a	985.47	0.76246	YES	YES
155	a	985.74	0.31089	YES	YES
156	a	986.83	1.21795	YES	YES
157	a	987.40	0.86427	YES	YES
158	a	989.37	0.49716	YES	YES
159	a	992.86	7.43873	YES	YES
160	a	1016.01	7.02869	YES	YES
161	a	1022.30	9.28383	YES	YES
162	a	1023.30	0.29092	YES	YES
163	a	1024.17	0.98763	YES	YES
164	a	1024.47	1.52744	YES	YES
165	a	1025.18	0.95899	YES	YES
166	a	1026.50	0.66575	YES	YES

167	a	1026.76	0.21873	YES	YES
168	a	1027.74	3.77655	YES	YES
169	a	1063.31	14.63874	YES	YES
170	a	1065.75	14.90701	YES	YES
171	a	1069.13	26.83929	YES	YES
172	a	1071.83	10.73433	YES	YES
173	a	1073.20	3.81627	YES	YES
174	a	1074.61	9.54364	YES	YES
175	a	1074.94	5.75511	YES	YES
176	a	1076.56	4.00285	YES	YES
177	a	1078.46	4.25099	YES	YES
178	a	1079.04	7.83941	YES	YES
179	a	1080.22	3.11263	YES	YES
180	a	1082.58	12.00242	YES	YES
181	a	1083.43	0.11631	YES	YES
182	a	1140.26	0.27105	YES	YES
183	a	1140.73	0.29637	YES	YES
184	a	1141.11	0.62388	YES	YES
185	a	1141.86	0.13434	YES	YES
186	a	1142.06	0.84273	YES	YES
187	a	1142.42	0.50746	YES	YES
188	a	1142.74	0.24562	YES	YES
189	a	1154.23	10.69443	YES	YES
190	a	1166.60	3.22742	YES	YES
191	a	1167.29	1.22497	YES	YES
192	a	1168.78	4.76250	YES	YES
193	a	1170.84	3.65826	YES	YES
194	a	1173.77	1.87162	YES	YES
195	a	1177.58	4.10830	YES	YES
196	a	1178.06	1.43451	YES	YES
197	a	1288.06	1.05540	YES	YES
198	a	1288.51	0.95017	YES	YES

* zero point VIBRATIONAL energy : 0.7416159 Hartree *

Cis TS_{25}_afby



bp86-SVP SCF energy: -2931.3480799490
pbe-TZVPP SCF energy: -2930.900520405

XYZ Coordinates
97

C	-0.39381	-0.24449	-2.25259
C	-0.80575	0.80952	-1.53885
C	-0.14500	-0.81663	-3.58237
H	-1.58810	-0.29521	-1.89324
C	0.31881	-1.84039	-6.16994
C	-0.02998	-2.70666	-5.11819
C	-0.25077	-2.20472	-3.82745
C	0.19538	0.05292	-4.64597
C	0.43332	-0.46010	-5.92997
H	0.50012	-2.24222	-7.18073
H	-0.12436	-3.78941	-5.30328
H	-0.51280	-2.88141	-3.00188
H	0.26627	1.13533	-4.45652
H	0.70222	0.22585	-6.75035
C	3.33011	-0.10665	-0.39984
C	4.83121	-0.23699	-0.42173
H	5.09512	-1.25240	-0.79310
H	5.24355	-0.13197	0.60265
H	5.27922	0.51323	-1.10434
C	2.04968	-3.08740	-0.86903
C	2.82522	-3.94947	-1.87682
H	3.44547	-4.69352	-1.33717
H	3.45807	-3.32262	-2.54007
H	2.10470	-4.48983	-2.53100
C	2.15550	2.22940	1.71866
C	3.39032	2.59231	1.12980
H	3.46874	2.68979	0.03587
C	4.52196	2.84808	1.92018
H	5.46933	3.13508	1.43385
C	4.44717	2.74969	3.31994
H	5.33368	2.95576	3.94228
C	3.22745	2.39583	3.91665
H	3.14554	2.32704	5.01423
C	2.09412	2.13615	3.12482
H	1.15229	1.88629	3.63146
C	-0.76384	2.45088	1.53948
C	-1.09884	1.79186	2.74469
H	-0.54321	0.89568	3.06322
C	-2.16429	2.24173	3.53964
H	-2.39682	1.71893	4.48148
C	-2.94502	3.33131	3.12144
H	-3.78480	3.68361	3.74320
C	-2.66630	3.94906	1.89180
H	-3.29291	4.78420	1.53592
C	-1.58573	3.51395	1.10586
H	-1.38583	4.01078	0.14482
C	1.00427	3.29927	-0.61601
C	1.10064	4.61628	-0.10707
H	0.97412	4.80199	0.97211
C	1.36734	5.69719	-0.96143
H	1.43524	6.71645	-0.54596
C	1.55656	5.47899	-2.33793
H	1.77097	6.32712	-3.00944
C	1.48611	4.17333	-2.84782
H	1.65431	3.98805	-3.92175
C	1.21276	3.08975	-1.99308
H	1.20122	2.06948	-2.39860
C	-2.36076	-0.81125	1.44791
C	-2.98984	-1.36216	2.58719
H	-2.49114	-2.15143	3.16893
C	-4.25671	-0.91351	2.99795
H	-4.72644	-1.36135	3.88980
C	-4.92298	0.09073	2.27606
H	-5.92163	0.43499	2.59332
C	-4.29821	0.66056	1.15483
H	-4.79731	1.46437	0.58921
C	-3.02537	0.22183	0.75099
H	-2.53436	0.70995	-0.10779
C	-1.52404	-2.93874	-0.21218
C	-2.74400	-2.72860	-0.89736
H	-3.29369	-1.78085	-0.78195
C	-3.29982	-3.73513	-1.70668
H	-4.25156	-3.54577	-2.23054
C	-2.65687	-4.97690	-1.83260
H	-3.09746	-5.77090	-2.45844
C	-1.44972	-5.19904	-1.14746
H	-0.93540	-6.17115	-1.23271
C	-0.88135	-4.19017	-0.35054
H	0.07960	-4.36602	0.15770
C	-0.05318	-2.34245	2.29832
C	-0.53654	-3.56461	2.81634
H	-1.32277	-4.12269	2.28395
C	-0.01379	-4.08746	4.01155
H	-0.39625	-5.04692	4.39815
C	0.99219	-3.39570	4.70702
H	1.40389	-3.80922	5.64279
C	1.47939	-2.18149	4.19471
H	2.28316	-1.63969	4.72003
C	0.96518	-1.66004	2.99633
H	1.39333	-0.73824	2.57633
O	2.65645	-0.57603	0.58638
O	2.69161	0.43044	-1.36978
O	1.95993	-3.42091	0.31797
O	1.49219	-2.04671	-1.43804
P	0.70945	1.88058	0.56193
P	-0.75745	-1.54364	0.78067
Ru	0.79746	-0.30300	-0.45503

Vibrational Frequencies

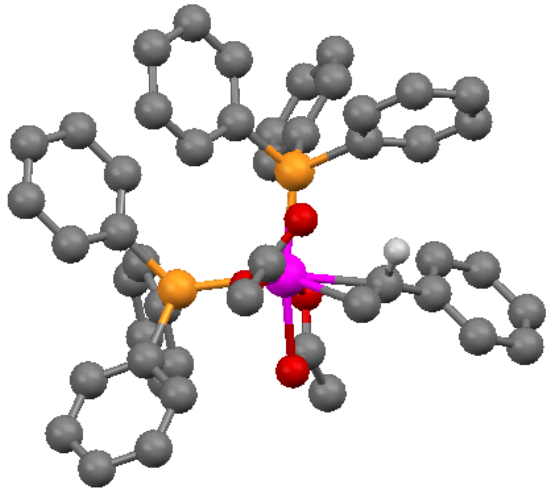
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-792.37	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	12.79	0.17952	YES	YES
9	a	17.59	0.19246	YES	YES
10	a	21.13	0.07057	YES	YES
11	a	26.27	0.17410	YES	YES
12	a	30.31	0.57703	YES	YES
13	a	35.76	0.50853	YES	YES
14	a	41.21	0.14752	YES	YES
15	a	44.51	0.29379	YES	YES
16	a	48.02	0.31272	YES	YES
17	a	48.26	0.44137	YES	YES
18	a	51.74	0.14312	YES	YES

19	a	54.60	0.48508	YES	YES
20	a	55.82	0.70025	YES	YES
21	a	57.60	0.15260	YES	YES
22	a	61.63	0.59234	YES	YES
23	a	66.18	0.45819	YES	YES
24	a	66.59	0.37602	YES	YES
25	a	68.93	0.91121	YES	YES
26	a	72.19	0.54198	YES	YES
27	a	83.30	0.22919	YES	YES
28	a	84.88	0.73913	YES	YES
29	a	93.47	1.14410	YES	YES
30	a	95.76	0.44850	YES	YES
31	a	98.93	0.58353	YES	YES
32	a	100.12	0.89554	YES	YES
33	a	104.82	1.62110	YES	YES
34	a	110.10	0.88135	YES	YES
35	a	115.08	1.60544	YES	YES
36	a	127.33	2.65760	YES	YES
37	a	133.65	0.28074	YES	YES
38	a	137.31	1.12322	YES	YES
39	a	152.88	5.72162	YES	YES
40	a	169.12	1.74831	YES	YES
41	a	179.81	1.92144	YES	YES
42	a	188.56	0.52908	YES	YES
43	a	195.23	5.49786	YES	YES
44	a	198.85	6.46757	YES	YES
45	a	203.62	0.49988	YES	YES
46	a	205.06	1.31756	YES	YES
47	a	214.51	3.26845	YES	YES
48	a	217.55	1.28530	YES	YES
49	a	220.90	0.92801	YES	YES
50	a	228.72	2.38719	YES	YES
51	a	232.35	4.72337	YES	YES
52	a	248.23	0.28423	YES	YES
53	a	251.85	1.23248	YES	YES
54	a	255.45	0.21362	YES	YES
55	a	262.13	1.01175	YES	YES
56	a	263.33	0.71794	YES	YES
57	a	268.34	0.48161	YES	YES
58	a	269.96	1.20552	YES	YES
59	a	277.74	5.76398	YES	YES
60	a	303.48	9.05606	YES	YES
61	a	321.25	11.34530	YES	YES
62	a	385.19	20.02013	YES	YES
63	a	394.05	9.44187	YES	YES
64	a	396.68	0.40364	YES	YES
65	a	400.42	0.68582	YES	YES
66	a	400.82	0.22505	YES	YES
67	a	402.39	2.64842	YES	YES
68	a	404.51	1.85031	YES	YES
69	a	407.63	17.08148	YES	YES
70	a	412.56	0.22715	YES	YES
71	a	413.33	3.57812	YES	YES
72	a	416.13	6.51758	YES	YES
73	a	428.29	22.08192	YES	YES
74	a	436.02	3.21359	YES	YES
75	a	454.28	16.38896	YES	YES
76	a	463.03	18.97777	YES	YES
77	a	473.99	6.50347	YES	YES
78	a	479.96	7.75797	YES	YES
79	a	488.72	6.36487	YES	YES
80	a	493.06	7.15325	YES	YES
81	a	496.35	11.09997	YES	YES
82	a	506.52	33.40002	YES	YES
83	a	510.39	55.97043	YES	YES
84	a	518.00	134.26060	YES	YES
85	a	526.26	90.70768	YES	YES
86	a	537.44	20.53613	YES	YES
87	a	585.02	8.09376	YES	YES
88	a	591.79	3.47355	YES	YES
89	a	599.60	3.21283	YES	YES
90	a	607.67	0.04324	YES	YES
91	a	609.79	1.33066	YES	YES
92	a	610.04	0.29972	YES	YES
93	a	610.40	0.46401	YES	YES
94	a	612.06	0.03637	YES	YES
95	a	612.65	1.63830	YES	YES
96	a	614.45	1.55846	YES	YES
97	a	647.06	10.70682	YES	YES
98	a	667.24	10.06953	YES	YES
99	a	669.38	5.35245	YES	YES
100	a	672.50	9.92051	YES	YES
101	a	673.81	58.09450	YES	YES
102	a	677.67	16.51771	YES	YES
103	a	687.19	13.19289	YES	YES
104	a	688.50	26.67689	YES	YES
105	a	690.68	14.79991	YES	YES
106	a	693.97	39.49809	YES	YES
107	a	695.18	44.61195	YES	YES
108	a	698.84	30.05319	YES	YES
109	a	702.84	45.28270	YES	YES
110	a	703.03	14.82199	YES	YES
111	a	706.49	11.67726	YES	YES
112	a	733.24	8.06093	YES	YES
113	a	738.13	4.36916	YES	YES
114	a	740.36	10.76141	YES	YES
115	a	741.66	4.54120	YES	YES
116	a	744.75	5.41339	YES	YES
117	a	748.35	9.51087	YES	YES
118	a	749.30	11.34654	YES	YES
119	a	764.61	3.46178	YES	YES
120	a	824.09	0.22049	YES	YES
121	a	826.98	0.48459	YES	YES
122	a	829.35	0.88469	YES	YES
123	a	835.58	0.82905	YES	YES
124	a	837.51	0.89317	YES	YES
125	a	844.11	0.77393	YES	YES
126	a	847.78	1.94043	YES	YES
127	a	888.18	13.83283	YES	YES
128	a	901.58	0.16757	YES	YES
129	a	906.03	0.17651	YES	YES
130	a	907.77	3.45696	YES	YES
131	a	909.63	0.85185	YES	YES
132	a	911.63	0.68682	YES	YES
133	a	920.54	4.64374	YES	YES
134	a	921.55	1.54414	YES	YES
135	a	926.56	11.10398	YES	YES
136	a	943.37	16.17972	YES	YES
137	a	951.34	0.42435	YES	YES
138	a	954.04	0.40392	YES	YES
139	a	955.21	0.21685	YES	YES
140	a	958.30	0.22493	YES	YES
141	a	959.28	0.56971	YES	YES
142	a	969.08	1.24232	YES	YES
143	a	971.00	0.95443	YES	YES
144	a	977.62	1.98072	YES	YES
145	a	979.22	0.06773	YES	YES
146	a	979.42	0.93220	YES	YES
147	a	980.17	0.38939	YES	YES
148	a	980.34	0.44217	YES	YES
149	a	981.26	1.05699	YES	YES
150	a	981.68	0.07804	YES	YES
151	a	982.53	0.63455	YES	YES
152	a	983.34	1.82932	YES	YES
153	a	984.47	1.91263	YES	YES
154	a	985.95	2.03781	YES	YES
155	a	986.45	5.83292	YES	YES
156	a	986.57	1.49755	YES	YES
157	a	987.04	2.11166	YES	YES
158	a	990.76	0.09467	YES	YES
159	a	998.69	7.87980	YES	YES
160	a	1017.64	5.21077	YES	YES
161	a	1022.94	8.37410	YES	YES
162	a	1023.62	1.48665	YES	YES
163	a	1023.87	0.46650	YES	YES
164	a	1024.35	1.80765	YES	YES
165	a	1024.72	0.59595	YES	YES
166	a	1025.07	5.41135	YES	YES

167	a	1025.85	0.47019	YES	YES
168	a	1026.94	0.42267	YES	YES
169	a	1064.78	16.96075	YES	YES
170	a	1066.33	16.38634	YES	YES
171	a	1070.91	14.02662	YES	YES
172	a	1071.27	8.78710	YES	YES
173	a	1072.04	9.77892	YES	YES
174	a	1073.97	11.35264	YES	YES
175	a	1074.30	4.43563	YES	YES
176	a	1075.18	6.58002	YES	YES
177	a	1078.11	3.19690	YES	YES
178	a	1079.60	11.47882	YES	YES
179	a	1080.10	1.67036	YES	YES
180	a	1082.57	14.87740	YES	YES
181	a	1083.69	1.06562	YES	YES
182	a	1139.54	0.18534	YES	YES
183	a	1140.68	0.38166	YES	YES
184	a	1141.01	0.08407	YES	YES
185	a	1141.35	0.28573	YES	YES
186	a	1141.90	0.86604	YES	YES
187	a	1142.22	0.32868	YES	YES
188	a	1142.78	0.59895	YES	YES
189	a	1151.80	2.96894	YES	YES
190	a	1164.86	1.61308	YES	YES
191	a	1165.88	4.70392	YES	YES
192	a	1167.21	1.57681	YES	YES
193	a	1168.42	3.54261	YES	YES
194	a	1175.20	4.87506	YES	YES
195	a	1177.50	5.04091	YES	YES
196	a	1178.45	1.23040	YES	YES
197	a	1285.89	5.81775	YES	YES
198	a	1288.36	36.35060	YES	YES

* zero point VIBRATIONAL energy : 0.7403423 Hartree *

Cis TS_{25}_pfax



bp86-SVP SCF energy: -2931.3425178980
pbe-TZVPP SCF energy: -2930.893575489

XYZ Coordinates
97

C	1.53354	-2.11157	-1.52740
C	1.06371	-1.48293	-2.60572
C	2.59350	-3.00957	-1.02325
H	0.52803	-2.65381	-2.00461
C	4.64034	-4.75626	-0.15947
C	3.73911	-4.20852	0.77080
C	2.72295	-3.33881	0.34534
C	3.51086	-3.55819	-1.95296
C	4.52466	-4.42723	-1.52209
H	5.43876	-5.43710	0.17900
H	3.83105	-4.45463	1.84162
H	2.03888	-2.88260	1.07740
H	3.41646	-3.29033	-3.01708
H	5.23107	-4.84781	-2.25584
C	3.20275	0.06576	-0.27840
C	4.67029	0.01006	0.06310
H	5.06012	-0.99589	-0.21187
H	4.82192	0.15176	1.15239
H	5.23554	0.77130	-0.51127
C	-1.31273	0.09435	-3.17535
C	-1.59187	0.83134	-4.48615
H	-0.82072	0.52034	-5.22642
H	-1.52261	1.93262	-4.36612
H	-2.58852	0.54426	-4.87947
C	1.66784	2.59934	1.34950
C	3.01591	2.86475	1.01088
H	3.32884	2.84460	-0.04416
C	3.95930	3.18104	2.00147
H	5.00167	3.39229	1.70953
C	3.57800	3.24060	3.35269
H	4.31749	3.49515	4.13005
C	2.24162	2.98738	3.69986
H	1.92089	3.04846	4.75322
C	1.29563	2.66987	2.70867
H	0.25190	2.50656	3.01261
C	-1.13551	2.84678	0.56734
C	-1.77225	2.26092	1.68682
H	-1.35057	1.35994	2.15832
C	-2.96499	2.79556	2.19875
H	-3.43542	2.32705	3.07819
C	-3.56923	3.89898	1.57359
H	-4.51088	4.31402	1.96933
C	-2.97842	4.45222	0.42596
H	-3.45681	5.30168	-0.08958
C	-1.77035	3.93381	-0.07302
H	-1.32174	4.38425	-0.97054
C	1.04173	3.40990	-1.29381
C	1.21806	4.75494	-0.88644
H	1.00290	5.05166	0.15311
C	1.67575	5.72259	-1.79384
H	1.80480	6.76576	-1.46022
C	1.97582	5.35901	-3.11935
H	2.34153	6.11734	-3.83203
C	1.81245	4.02565	-3.52656
H	2.05176	3.72920	-4.56123
C	1.34639	3.05243	-2.62312
H	1.20151	2.01462	-2.95052
C	-2.80024	-0.49935	0.26652
C	-3.74201	-1.00336	1.19164
H	-3.46842	-1.81677	1.88035
C	-5.04467	-0.48074	1.24676
H	-5.76555	-0.89265	1.97302
C	-5.42879	0.55329	0.37575
H	-6.45433	0.95773	0.41240
C	-4.49457	1.07173	-0.53484
H	-4.77760	1.89183	-1.21468
C	-3.18884	0.55525	-0.58393
H	-2.45486	0.98622	-1.27673
C	-1.56596	-2.95849	-0.56175
C	-2.74407	-3.14551	-1.31642
H	-3.39485	-2.28942	-1.53714
C	-3.07938	-4.41544	-1.81288
H	-4.00492	-4.53767	-2.39983
C	-2.24123	-5.51917	-1.57961
H	-2.50575	-6.51296	-1.97792
C	-1.06339	-5.34506	-0.83589
H	-0.39368	-6.19906	-0.64042
C	-0.73197	-4.07560	-0.32921
H	0.18199	-3.97106	0.27556
C	-0.71610	-1.70823	1.89129
C	-1.27499	-2.83623	2.53976
H	-1.92510	-3.52852	1.98268
C	-0.99907	-3.10251	3.89191
H	-1.44726	-3.98797	4.37316
C	-0.15522	-2.25050	4.62477
H	0.06307	-2.46203	5.68497
C	0.41845	-1.13682	3.99006
H	1.09920	-0.46923	4.54395
C	0.14388	-0.87222	2.63677
H	0.63999	-0.02299	2.14471
O	2.33033	-0.41072	0.53560
O	2.79144	0.52272	-1.39723
O	-1.85870	-0.98057	-2.91476
O	-0.45397	0.72486	-2.40795
P	0.48228	2.15092	-0.03500
P	-1.09855	-1.26684	0.10243
Ru	0.69986	-0.15856	-0.88043

Vibrational Frequencies

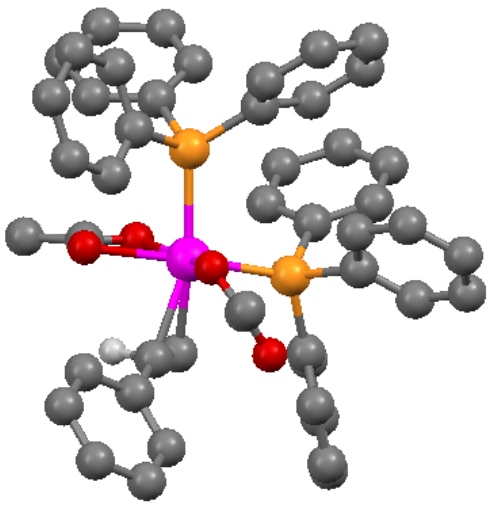
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-633.01	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	17.30	0.03024	YES	YES
9	a	20.50	0.43020	YES	YES
10	a	20.90	0.11620	YES	YES
11	a	29.05	0.15008	YES	YES
12	a	37.90	0.10007	YES	YES
13	a	40.21	0.37810	YES	YES
14	a	43.33	0.03750	YES	YES
15	a	49.85	0.36525	YES	YES
16	a	53.34	0.28419	YES	YES
17	a	56.70	0.34952	YES	YES

18	a	57.66	0.12752	YES	YES
19	a	59.43	0.71212	YES	YES
20	a	63.89	0.22156	YES	YES
21	a	64.27	0.35210	YES	YES
22	a	69.41	1.47906	YES	YES
23	a	71.80	0.04710	YES	YES
24	a	74.98	1.43575	YES	YES
25	a	76.28	0.33933	YES	YES
26	a	83.83	0.37299	YES	YES
27	a	88.63	0.17402	YES	YES
28	a	94.75	1.01582	YES	YES
29	a	97.16	0.55383	YES	YES
30	a	101.60	0.60954	YES	YES
31	a	103.09	0.33918	YES	YES
32	a	105.20	0.29401	YES	YES
33	a	109.11	1.96005	YES	YES
34	a	114.12	0.47894	YES	YES
35	a	119.34	0.09279	YES	YES
36	a	125.02	2.68344	YES	YES
37	a	129.43	0.89813	YES	YES
38	a	144.97	6.36408	YES	YES
39	a	149.74	2.30143	YES	YES
40	a	161.10	2.02766	YES	YES
41	a	183.27	1.38512	YES	YES
42	a	189.73	4.54940	YES	YES
43	a	196.43	1.01689	YES	YES
44	a	201.14	3.32003	YES	YES
45	a	204.72	1.43522	YES	YES
46	a	210.27	0.53070	YES	YES
47	a	216.76	1.49933	YES	YES
48	a	220.76	0.18658	YES	YES
49	a	223.23	3.98838	YES	YES
50	a	227.68	3.39434	YES	YES
51	a	230.28	3.39065	YES	YES
52	a	242.13	2.69775	YES	YES
53	a	246.97	0.74360	YES	YES
54	a	252.30	0.61920	YES	YES
55	a	254.51	0.50686	YES	YES
56	a	260.70	1.58594	YES	YES
57	a	268.39	0.03721	YES	YES
58	a	271.01	0.57532	YES	YES
59	a	281.07	0.10197	YES	YES
60	a	297.17	17.70481	YES	YES
61	a	321.61	18.21441	YES	YES
62	a	387.48	7.12193	YES	YES
63	a	398.87	1.31182	YES	YES
64	a	401.92	3.81368	YES	YES
65	a	402.61	2.46748	YES	YES
66	a	404.89	3.18295	YES	YES
67	a	405.94	10.31664	YES	YES
68	a	406.61	1.68743	YES	YES
69	a	411.84	2.39075	YES	YES
70	a	414.02	0.80938	YES	YES
71	a	417.31	15.18021	YES	YES
72	a	422.65	5.56192	YES	YES
73	a	423.68	7.66169	YES	YES
74	a	434.05	11.39439	YES	YES
75	a	448.15	33.87264	YES	YES
76	a	457.19	12.21467	YES	YES
77	a	461.86	4.82973	YES	YES
78	a	471.99	5.43736	YES	YES
79	a	480.52	10.14349	YES	YES
80	a	493.43	24.18272	YES	YES
81	a	499.53	2.34083	YES	YES
82	a	508.10	31.26062	YES	YES
83	a	514.97	48.63004	YES	YES
84	a	516.99	130.75752	YES	YES
85	a	523.07	92.53285	YES	YES
86	a	539.26	6.26314	YES	YES
87	a	583.29	4.14275	YES	YES
88	a	586.37	7.61330	YES	YES
89	a	601.57	3.34675	YES	YES
90	a	609.28	0.28760	YES	YES
91	a	609.58	0.68880	YES	YES
92	a	610.25	0.07367	YES	YES
93	a	610.59	1.63323	YES	YES
94	a	612.45	1.62627	YES	YES
95	a	612.54	1.95058	YES	YES
96	a	612.75	0.06498	YES	YES
97	a	659.72	20.67563	YES	YES
98	a	667.74	44.73055	YES	YES
99	a	669.71	12.08582	YES	YES
100	a	670.34	9.92514	YES	YES
101	a	676.77	11.05393	YES	YES
102	a	679.29	1.54278	YES	YES
103	a	679.91	21.01939	YES	YES
104	a	687.31	15.65431	YES	YES
105	a	696.67	50.31435	YES	YES
106	a	697.52	52.03117	YES	YES
107	a	698.03	32.94450	YES	YES
108	a	699.19	16.50954	YES	YES
109	a	700.62	28.92090	YES	YES
110	a	702.96	11.42732	YES	YES
111	a	706.45	24.19063	YES	YES
112	a	735.08	10.35924	YES	YES
113	a	738.25	3.66355	YES	YES
114	a	739.50	3.57780	YES	YES
115	a	743.85	4.65666	YES	YES
116	a	746.56	2.45122	YES	YES
117	a	746.74	20.39579	YES	YES
118	a	748.58	14.51861	YES	YES
119	a	766.92	10.31398	YES	YES
120	a	832.13	0.98448	YES	YES
121	a	832.89	0.51184	YES	YES
122	a	835.62	0.23603	YES	YES
123	a	837.15	0.82944	YES	YES
124	a	837.92	0.36116	YES	YES
125	a	838.69	1.56027	YES	YES
126	a	842.32	1.32877	YES	YES
127	a	857.51	41.01409	YES	YES
128	a	905.64	0.57391	YES	YES
129	a	908.27	2.00048	YES	YES
130	a	910.85	0.53526	YES	YES
131	a	915.07	1.30135	YES	YES
132	a	917.95	0.83090	YES	YES
133	a	919.34	2.97589	YES	YES
134	a	923.51	6.22913	YES	YES
135	a	927.17	4.89780	YES	YES
136	a	943.70	16.75664	YES	YES
137	a	957.02	0.55651	YES	YES
138	a	957.67	0.33042	YES	YES
139	a	960.13	0.14383	YES	YES
140	a	963.09	0.92459	YES	YES
141	a	963.32	0.74737	YES	YES
142	a	965.35	0.39161	YES	YES
143	a	966.50	0.71388	YES	YES
144	a	980.75	0.68913	YES	YES
145	a	981.83	1.09239	YES	YES
146	a	981.99	1.85784	YES	YES
147	a	982.67	1.85190	YES	YES
148	a	982.86	1.49049	YES	YES
149	a	983.00	0.99231	YES	YES
150	a	983.38	0.89012	YES	YES
151	a	984.05	1.13986	YES	YES
152	a	984.47	0.39559	YES	YES
153	a	985.83	2.32198	YES	YES
154	a	986.17	2.76751	YES	YES
155	a	986.34	3.98682	YES	YES
156	a	987.39	2.07294	YES	YES
157	a	987.58	1.28048	YES	YES
158	a	987.70	4.61603	YES	YES
159	a	990.19	0.45651	YES	YES
160	a	1015.91	5.90079	YES	YES
161	a	1022.60	1.05265	YES	YES
162	a	1023.80	13.63881	YES	YES
163	a	1023.88	0.72448	YES	YES
164	a	1024.65	3.74515	YES	YES
165	a	1024.78	2.24584	YES	YES

166	a	1025.03	3.23351	YES	YES
167	a	1025.50	0.68758	YES	YES
168	a	1026.54	1.44192	YES	YES
169	a	1063.62	19.83376	YES	YES
170	a	1068.39	9.89180	YES	YES
171	a	1069.23	22.23395	YES	YES
172	a	1070.66	4.73464	YES	YES
173	a	1073.46	7.68491	YES	YES
174	a	1074.31	16.57026	YES	YES
175	a	1074.70	14.10833	YES	YES
176	a	1075.48	1.85476	YES	YES
177	a	1076.16	2.33367	YES	YES
178	a	1078.41	2.70213	YES	YES
179	a	1079.80	11.15528	YES	YES
180	a	1080.49	10.21201	YES	YES
181	a	1083.10	4.49747	YES	YES
182	a	1139.70	0.28612	YES	YES
183	a	1140.37	0.45767	YES	YES
184	a	1140.59	0.04011	YES	YES
185	a	1140.95	0.32702	YES	YES
186	a	1141.43	0.78523	YES	YES
187	a	1142.31	0.49856	YES	YES
188	a	1143.00	0.38224	YES	YES
189	a	1153.63	8.55683	YES	YES
190	a	1165.02	1.76934	YES	YES
191	a	1165.60	1.44327	YES	YES
192	a	1169.99	2.00940	YES	YES
193	a	1171.04	6.40652	YES	YES
194	a	1172.69	5.25543	YES	YES
195	a	1176.36	8.43605	YES	YES
196	a	1178.06	7.91109	YES	YES
197	a	1283.37	13.87747	YES	YES
198	a	1286.76	195.45763	YES	YES

* zero point VIBRATIONAL energy : 0.7399447 Hartree *

Cis TS_{25}_pfay



bp86-SVP SCF energy: -2931.3515461090
pbe-TZVPP SCF energy: -2930.904234490

XYZ Coordinates
97

C	2.20766	1.81714	-1.41357
C	1.09649	2.00036	-2.12025
C	3.46483	2.23755	-0.78246
H	2.34966	1.31983	-2.50311
C	5.91594	3.05753	0.34040
C	5.74544	1.72588	-0.07838
C	4.52496	1.31301	-0.63472
C	3.63848	3.57494	-0.35763
C	4.86039	3.97747	0.19999
H	6.87538	3.38114	0.77743
H	6.56996	1.00195	0.02954
H	4.37638	0.27253	-0.96466
H	2.80719	4.28558	-0.46853
H	4.99031	5.02205	0.52812
C	1.49195	-1.05707	-2.87291
C	1.97817	-1.65981	-4.16927
H	2.33585	-0.84359	-4.83663
H	1.14731	-2.18004	-4.68811
H	2.82105	-2.35684	-3.98765
C	1.69671	1.65426	1.74033
C	2.48817	1.55052	3.04450
H	2.05890	2.24900	3.79279
H	3.53668	1.86994	2.84969
H	2.50296	0.51669	3.44614
C	-0.62964	-3.13438	-1.11817
C	0.29777	-3.78040	-1.96960
H	1.37639	-3.59922	-1.84217
C	-0.13473	-4.67618	-2.96018
H	0.60953	-5.17457	-3.60393
C	-1.50420	-4.94597	-3.12350
H	-1.84408	-5.65411	-3.89746
C	-2.43294	-4.31193	-2.28376
H	-3.51066	-4.51895	-2.39110
C	-2.00102	-3.41306	-1.29238
H	-2.75530	-2.94684	-0.64409
C	-1.14285	-2.11178	1.58846
C	-2.48942	-1.69708	1.46787
H	-2.84717	-1.23006	0.53834
C	-3.38452	-1.83305	2.54089
H	-4.43046	-1.50783	2.41654
C	-2.94491	-2.35566	3.76833
H	-3.64585	-2.45669	4.61344
C	-1.59941	-2.73076	3.91466
H	-1.23498	-3.12511	4.87801
C	-0.70562	-2.61306	2.83571
H	0.34299	-2.91513	2.97306
C	1.50831	-2.89212	0.75681
C	1.38549	-4.28522	0.97672
H	0.42675	-4.79395	0.78422
C	2.47760	-5.03441	1.44120
H	2.36412	-6.11902	1.60604
C	3.70944	-4.40369	1.69274
H	4.56921	-4.99248	2.05424
C	3.83587	-3.02172	1.48226
H	4.79667	-2.51774	1.67967
C	2.74352	-2.26615	1.01753
H	2.83660	-1.18019	0.87571
C	-1.68998	2.00758	1.44738
C	-2.49058	3.14684	1.69546
H	-2.79685	3.79959	0.86295
C	-2.89580	3.46783	3.00221
H	-3.51742	4.36266	3.17412
C	-2.50478	2.65976	4.08300
H	-2.81786	2.91554	5.10920
C	-1.70383	1.53031	3.84681
H	-1.38136	0.89229	4.68592
C	-1.29976	1.20751	2.54043
H	-0.65043	0.33721	2.37338
C	-1.22775	3.23006	-1.12431
C	-0.47530	4.30069	-0.58646
H	0.13184	4.13170	0.31553
C	-0.49836	5.56181	-1.20542
H	0.08870	6.38862	-0.77072
C	-1.26024	5.77446	-2.36725
H	-1.27335	6.76546	-2.85148
C	-2.00712	4.71377	-2.90576
H	-2.60999	4.86533	-3.81679
C	-1.99464	3.45186	-2.28822
H	-2.58547	2.63472	-2.72805
C	-2.76136	0.80725	-0.97485
C	-4.02461	1.01922	-0.37640
H	-4.10365	1.59782	0.55644
C	-5.18961	0.48813	-0.95562
H	-6.16571	0.66288	-0.47234
C	-5.11396	-0.25683	-2.14564
H	-6.03001	-0.66874	-2.60176
C	-3.86300	-0.47168	-2.74748
H	-3.78872	-1.05607	-3.67957
C	-2.69262	0.05015	-2.16654
H	-1.71859	-0.13613	-2.64430
O	0.32169	-0.55562	-2.78753
O	2.25795	-0.98291	-1.84509
O	1.29879	2.75020	1.32772
O	1.52999	0.50719	1.13287
P	0.03080	-1.92401	0.14944
P	-1.17917	1.55104	-0.29050
Ru	0.69036	0.23329	-0.76544

Vibrational Frequencies

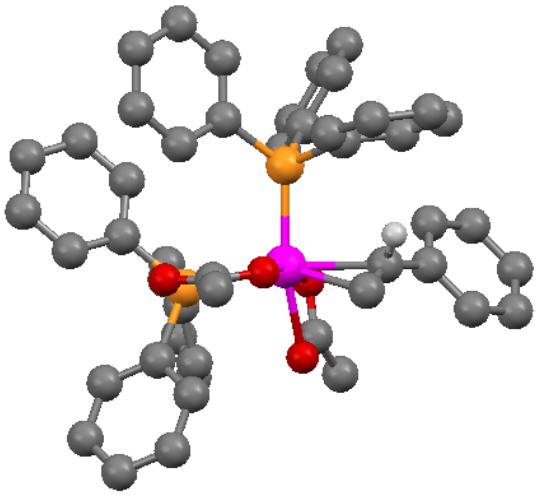
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-543.11	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	9.77	0.19680	YES	YES
9	a	13.47	0.01231	YES	YES
10	a	21.93	0.06104	YES	YES
11	a	26.56	0.01421	YES	YES
12	a	30.40	0.01519	YES	YES
13	a	33.00	0.25243	YES	YES
14	a	33.72	0.14521	YES	YES
15	a	36.63	0.67943	YES	YES

16	a	46.07	0.37166	YES	YES
17	a	48.84	0.24653	YES	YES
18	a	52.43	0.02709	YES	YES
19	a	54.78	0.80807	YES	YES
20	a	59.81	0.21183	YES	YES
21	a	62.25	0.12270	YES	YES
22	a	62.90	0.18834	YES	YES
23	a	65.35	0.22962	YES	YES
24	a	68.39	0.09240	YES	YES
25	a	70.95	0.23260	YES	YES
26	a	76.58	0.80846	YES	YES
27	a	80.37	0.08447	YES	YES
28	a	83.20	0.07307	YES	YES
29	a	86.53	0.57672	YES	YES
30	a	88.48	1.07567	YES	YES
31	a	96.00	1.76360	YES	YES
32	a	101.31	1.43502	YES	YES
33	a	102.84	0.98517	YES	YES
34	a	107.22	1.05971	YES	YES
35	a	117.45	6.74617	YES	YES
36	a	119.40	0.73329	YES	YES
37	a	121.08	1.39355	YES	YES
38	a	139.20	1.43591	YES	YES
39	a	148.52	3.75573	YES	YES
40	a	154.18	6.07703	YES	YES
41	a	167.79	6.35312	YES	YES
42	a	183.27	10.04211	YES	YES
43	a	195.63	0.42088	YES	YES
44	a	198.94	4.04331	YES	YES
45	a	201.34	1.18451	YES	YES
46	a	205.17	0.51751	YES	YES
47	a	208.75	3.52135	YES	YES
48	a	211.68	0.63004	YES	YES
49	a	222.13	7.18682	YES	YES
50	a	226.81	2.90923	YES	YES
51	a	234.31	3.85561	YES	YES
52	a	246.85	1.19826	YES	YES
53	a	248.95	0.29777	YES	YES
54	a	251.60	0.14823	YES	YES
55	a	252.22	0.02912	YES	YES
56	a	256.42	1.53063	YES	YES
57	a	264.06	0.20235	YES	YES
58	a	266.79	0.08673	YES	YES
59	a	276.12	0.09543	YES	YES
60	a	291.87	22.22848	YES	YES
61	a	306.13	18.45739	YES	YES
62	a	341.37	7.91015	YES	YES
63	a	387.72	19.52835	YES	YES
64	a	395.49	0.44692	YES	YES
65	a	397.32	0.04393	YES	YES
66	a	400.10	0.65720	YES	YES
67	a	401.88	1.48277	YES	YES
68	a	402.47	0.14792	YES	YES
69	a	406.12	4.68550	YES	YES
70	a	407.77	16.12557	YES	YES
71	a	412.53	1.98018	YES	YES
72	a	422.01	20.75980	YES	YES
73	a	423.63	14.52335	YES	YES
74	a	434.85	19.14849	YES	YES
75	a	446.23	10.90271	YES	YES
76	a	453.37	15.01956	YES	YES
77	a	460.47	34.40313	YES	YES
78	a	465.57	4.80565	YES	YES
79	a	479.73	19.20010	YES	YES
80	a	496.32	22.26977	YES	YES
81	a	500.27	3.57733	YES	YES
82	a	506.44	21.95204	YES	YES
83	a	510.89	39.70405	YES	YES
84	a	515.60	94.48273	YES	YES
85	a	518.67	127.04002	YES	YES
86	a	529.20	26.18910	YES	YES
87	a	577.60	13.00713	YES	YES
88	a	596.57	7.36574	YES	YES
89	a	598.99	0.28820	YES	YES
90	a	609.31	0.09104	YES	YES
91	a	609.70	1.61125	YES	YES
92	a	609.80	1.07723	YES	YES
93	a	610.55	1.02962	YES	YES
94	a	611.23	0.83889	YES	YES
95	a	612.39	0.69110	YES	YES
96	a	614.56	0.46285	YES	YES
97	a	663.34	63.45985	YES	YES
98	a	664.79	5.73550	YES	YES
99	a	669.51	7.96774	YES	YES
100	a	671.79	16.68775	YES	YES
101	a	677.92	12.27630	YES	YES
102	a	679.74	7.35466	YES	YES
103	a	683.75	7.35633	YES	YES
104	a	684.25	15.01848	YES	YES
105	a	692.21	45.34231	YES	YES
106	a	695.50	26.06979	YES	YES
107	a	696.57	25.26908	YES	YES
108	a	697.13	32.69709	YES	YES
109	a	701.79	2.26743	YES	YES
110	a	702.43	70.69045	YES	YES
111	a	706.56	18.38545	YES	YES
112	a	736.73	6.38411	YES	YES
113	a	741.26	5.99562	YES	YES
114	a	742.76	4.37672	YES	YES
115	a	744.66	4.43019	YES	YES
116	a	746.62	7.75869	YES	YES
117	a	748.11	3.86649	YES	YES
118	a	749.06	18.04373	YES	YES
119	a	749.36	6.28148	YES	YES
120	a	832.88	0.44828	YES	YES
121	a	833.92	0.58669	YES	YES
122	a	835.80	1.03611	YES	YES
123	a	839.08	0.84279	YES	YES
124	a	839.48	2.71087	YES	YES
125	a	841.02	0.71316	YES	YES
126	a	852.63	1.31143	YES	YES
127	a	896.84	8.19489	YES	YES
128	a	906.18	0.28576	YES	YES
129	a	910.70	1.02802	YES	YES
130	a	913.70	0.75017	YES	YES
131	a	914.74	2.46097	YES	YES
132	a	915.55	1.67514	YES	YES
133	a	925.90	2.44218	YES	YES
134	a	928.63	0.41465	YES	YES
135	a	930.39	5.79047	YES	YES
136	a	943.64	19.60463	YES	YES
137	a	957.59	0.20932	YES	YES
138	a	960.12	0.39945	YES	YES
139	a	961.33	0.52626	YES	YES
140	a	961.86	1.13868	YES	YES
141	a	963.13	1.91762	YES	YES
142	a	968.02	1.76610	YES	YES
143	a	977.76	0.81072	YES	YES
144	a	981.09	0.13258	YES	YES
145	a	981.14	0.91751	YES	YES
146	a	981.69	0.55284	YES	YES
147	a	981.88	1.60672	YES	YES
148	a	982.14	0.46466	YES	YES
149	a	982.67	2.23458	YES	YES
150	a	983.16	0.21468	YES	YES
151	a	983.76	1.47498	YES	YES
152	a	984.92	1.84132	YES	YES
153	a	986.12	2.15551	YES	YES
154	a	986.92	0.95701	YES	YES
155	a	987.20	0.54767	YES	YES
156	a	987.68	1.74028	YES	YES
157	a	988.77	3.42923	YES	YES
158	a	991.81	4.61680	YES	YES
159	a	993.98	0.66762	YES	YES
160	a	1018.60	8.08018	YES	YES
161	a	1023.56	7.06151	YES	YES
162	a	1024.10	0.95889	YES	YES
163	a	1024.37	2.17585	YES	YES

164	a	1024.55	0.51904	YES	YES
165	a	1024.76	8.27124	YES	YES
166	a	1025.03	1.17325	YES	YES
167	a	1025.93	0.89479	YES	YES
168	a	1026.48	0.74765	YES	YES
169	a	1068.45	5.90929	YES	YES
170	a	1069.78	24.70616	YES	YES
171	a	1070.57	2.20174	YES	YES
172	a	1071.27	17.09183	YES	YES
173	a	1072.25	26.15777	YES	YES
174	a	1074.46	2.81985	YES	YES
175	a	1075.20	6.73215	YES	YES
176	a	1076.22	5.29930	YES	YES
177	a	1079.07	6.75697	YES	YES
178	a	1079.47	8.31485	YES	YES
179	a	1079.75	10.60939	YES	YES
180	a	1080.78	6.71936	YES	YES
181	a	1082.58	0.20936	YES	YES
182	a	1140.67	0.36438	YES	YES
183	a	1140.89	0.38129	YES	YES
184	a	1141.55	0.26883	YES	YES
185	a	1141.65	0.25877	YES	YES
186	a	1142.10	0.48926	YES	YES
187	a	1142.30	0.04145	YES	YES
188	a	1142.50	1.10224	YES	YES
189	a	1152.26	11.97977	YES	YES
190	a	1165.19	1.44134	YES	YES
191	a	1169.69	1.98092	YES	YES
192	a	1170.45	8.29363	YES	YES
193	a	1170.97	3.93852	YES	YES
194	a	1176.60	5.80175	YES	YES
195	a	1177.72	3.69966	YES	YES
196	a	1178.70	5.80754	YES	YES
197	a	1290.38	3.19618	YES	YES
198	a	1293.62	16.39318	YES	YES

* zero point VIBRATIONAL energy : 0.7407197 Hartree *

Cis TS_{25}_pfbx



bp86-SVP SCF energy: -2931.3348867360
pbe-TZVPP SCF energy: -2930.885159331

XYZ Coordinates
97

C	1.55237	-2.21485	-1.42630
C	1.20775	-1.60267	-2.55142
C	2.55325	-3.06514	-0.75444
H	0.59970	-2.76730	-1.97164
C	4.53813	-4.68942	0.42868
C	3.40739	-4.30167	1.16911
C	2.42253	-3.49004	0.58607
C	3.69532	-3.45796	-1.49491
C	4.68059	-4.26369	-0.90407
H	5.31435	-5.31988	0.89351
H	3.29579	-4.62174	2.21799
H	1.55856	-3.15521	1.17847
H	3.79995	-3.11719	-2.53721
H	5.56698	-4.55944	-1.48960
C	3.10800	0.04107	-0.26239
C	4.56785	-0.02262	0.10295
H	4.96384	-1.02175	-0.18844
H	4.69808	0.09815	1.19701
H	5.14053	0.75305	-0.44390
C	-1.24543	1.34439	-2.88191
C	-1.89105	1.33878	-4.27007
H	-2.17697	2.36986	-4.56010
H	-2.80721	0.70713	-4.24809
H	-1.20340	0.89836	-5.02169
C	1.64884	2.42586	1.32794
C	2.96714	2.79878	0.97237
H	3.23388	2.92324	-0.08769
C	3.94724	3.03505	1.95081
H	4.96181	3.33511	1.63854
C	3.63799	2.90292	3.31425
H	4.40436	3.09628	4.08332
C	2.33484	2.53510	3.68390
H	2.06599	2.44122	4.74963
C	1.35492	2.30024	2.70327
H	0.33941	2.04740	3.03760
C	-1.14970	2.80514	0.74192
C	-1.72907	2.12083	1.83362
H	-1.32849	1.14745	2.15678
C	-2.84731	2.64345	2.50511
H	-3.27772	2.08984	3.35556
C	-3.42475	3.84839	2.07590
H	-4.30306	4.26181	2.59909
C	-2.89044	4.50872	0.95572
H	-3.35538	5.43843	0.58695
C	-1.76750	3.99089	0.28949
H	-1.38622	4.49757	-0.60780
C	1.01777	3.41824	-1.22251
C	1.16243	4.75320	-0.78364
H	0.87595	5.03477	0.24257
C	1.69048	5.73380	-1.64074
H	1.78768	6.77306	-1.28447
C	2.10363	5.38821	-2.93852
H	2.52479	6.15571	-3.60937
C	1.98530	4.05664	-3.37200
H	2.31674	3.77084	-4.38405
C	1.44232	3.07806	-2.52284
H	1.35604	2.03845	-2.87110
C	-2.90917	-0.56265	0.32034
C	-3.81952	-1.19775	1.19673
H	-3.51278	-2.07449	1.78601
C	-5.13192	-0.71931	1.33863
H	-5.82283	-1.22950	2.03081
C	-5.56194	0.39894	0.60326
H	-6.59430	0.77167	0.71223
C	-4.66098	1.04273	-0.25779
H	-4.97134	1.93498	-0.82582
C	-3.34211	0.57242	-0.39322
H	-2.64544	1.13487	-1.03151
C	-1.70716	-2.76241	-1.00664
C	-2.69733	-2.59524	-2.00023
H	-3.21474	-1.62890	-2.10002
C	-3.03591	-3.65087	-2.86204
H	-3.81497	-3.49736	-3.62695
C	-2.39156	-4.89501	-2.75138
H	-2.66189	-5.72373	-3.42649
C	-1.39900	-5.07337	-1.77445
H	-0.88353	-6.04322	-1.67558
C	-1.05507	-4.01528	-0.91280
H	-0.27799	-4.18507	-0.14992
C	-0.81990	-2.02425	1.69734
C	-1.38824	-3.23300	2.16633
H	-2.05578	-3.82221	1.51807
C	-1.10597	-3.70470	3.46001
H	-1.55813	-4.64970	3.80479
C	-0.25546	-2.97675	4.30981
H	-0.03658	-3.34697	5.32524
C	0.32012	-1.77975	3.85248
H	1.00161	-1.20578	4.50172
C	0.04537	-1.31042	2.55635
H	0.54322	-0.39796	2.19488
O	2.21421	-0.41716	0.53816
O	2.71572	0.48096	-1.39652
O	-1.39673	2.32658	-2.12466
O	-0.60452	0.25622	-2.60684
P	0.38210	2.11138	-0.05519
P	-1.19871	-1.28536	0.02474
Ru	0.62347	-0.17848	-0.90722

Vibrational Frequencies

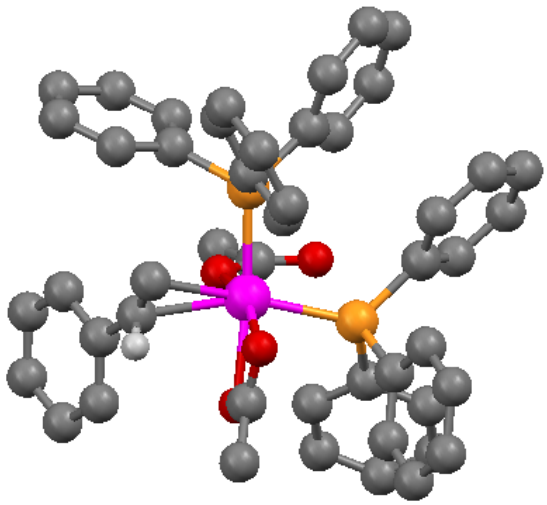
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-570.45	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	19.27	0.03090	YES	YES
9	a	21.89	0.24193	YES	YES
10	a	24.55	0.18763	YES	YES
11	a	28.19	0.04134	YES	YES
12	a	36.48	0.05512	YES	YES
13	a	42.96	0.12058	YES	YES
14	a	44.17	0.15029	YES	YES
15	a	45.55	0.89188	YES	YES
16	a	51.69	0.15248	YES	YES

17	a	52.84	0.08238	YES	YES
18	a	55.73	0.15492	YES	YES
19	a	55.95	0.05917	YES	YES
20	a	59.13	0.05109	YES	YES
21	a	61.00	0.42019	YES	YES
22	a	64.80	0.27674	YES	YES
23	a	68.31	0.40494	YES	YES
24	a	73.96	0.08513	YES	YES
25	a	76.30	0.44589	YES	YES
26	a	82.28	0.47394	YES	YES
27	a	85.91	0.84657	YES	YES
28	a	89.36	1.26133	YES	YES
29	a	93.61	0.74380	YES	YES
30	a	98.84	1.62494	YES	YES
31	a	104.82	0.09933	YES	YES
32	a	105.78	0.72325	YES	YES
33	a	119.42	1.48614	YES	YES
34	a	122.57	3.52467	YES	YES
35	a	127.25	0.69010	YES	YES
36	a	131.85	11.27457	YES	YES
37	a	139.72	5.34404	YES	YES
38	a	143.10	1.91344	YES	YES
39	a	150.88	2.42790	YES	YES
40	a	154.21	0.61958	YES	YES
41	a	162.30	1.27419	YES	YES
42	a	179.84	5.06713	YES	YES
43	a	190.77	3.85943	YES	YES
44	a	195.93	1.30719	YES	YES
45	a	200.03	1.47289	YES	YES
46	a	206.88	2.86162	YES	YES
47	a	214.58	5.01694	YES	YES
48	a	217.43	2.10893	YES	YES
49	a	222.41	1.23068	YES	YES
50	a	229.42	1.84389	YES	YES
51	a	229.90	7.93025	YES	YES
52	a	245.54	1.34614	YES	YES
53	a	248.87	1.57236	YES	YES
54	a	251.64	0.87012	YES	YES
55	a	253.02	2.96351	YES	YES
56	a	256.69	1.97386	YES	YES
57	a	264.49	0.64449	YES	YES
58	a	265.70	0.89462	YES	YES
59	a	271.20	0.50064	YES	YES
60	a	298.09	12.20768	YES	YES
61	a	325.72	15.82382	YES	YES
62	a	356.31	1.31638	YES	YES
63	a	390.21	35.98644	YES	YES
64	a	399.64	1.57011	YES	YES
65	a	400.95	0.54170	YES	YES
66	a	401.70	5.30788	YES	YES
67	a	402.69	3.50490	YES	YES
68	a	407.69	0.95268	YES	YES
69	a	410.76	14.99215	YES	YES
70	a	415.44	6.11122	YES	YES
71	a	418.26	3.23558	YES	YES
72	a	419.07	1.80150	YES	YES
73	a	428.45	21.03123	YES	YES
74	a	434.26	13.75292	YES	YES
75	a	450.42	20.09473	YES	YES
76	a	457.05	5.01350	YES	YES
77	a	468.17	25.94025	YES	YES
78	a	475.29	5.79308	YES	YES
79	a	481.08	13.83842	YES	YES
80	a	493.95	27.25484	YES	YES
81	a	498.78	11.97833	YES	YES
82	a	504.89	70.41523	YES	YES
83	a	508.54	16.74198	YES	YES
84	a	512.86	67.72446	YES	YES
85	a	518.96	87.28746	YES	YES
86	a	528.13	43.76099	YES	YES
87	a	578.33	3.63921	YES	YES
88	a	597.20	8.69567	YES	YES
89	a	598.53	4.45990	YES	YES
90	a	608.71	0.66118	YES	YES
91	a	609.26	1.03230	YES	YES
92	a	610.19	0.99125	YES	YES
93	a	610.45	0.03177	YES	YES
94	a	612.35	1.40430	YES	YES
95	a	612.81	1.28210	YES	YES
96	a	612.90	0.06001	YES	YES
97	a	655.96	10.58249	YES	YES
98	a	661.52	7.27715	YES	YES
99	a	669.00	28.44610	YES	YES
100	a	669.99	30.82302	YES	YES
101	a	675.38	2.41524	YES	YES
102	a	675.88	21.46683	YES	YES
103	a	684.67	11.50455	YES	YES
104	a	690.93	12.08802	YES	YES
105	a	696.06	29.28862	YES	YES
106	a	697.54	30.99178	YES	YES
107	a	700.01	26.32188	YES	YES
108	a	701.35	53.05155	YES	YES
109	a	702.91	35.30014	YES	YES
110	a	708.97	13.98585	YES	YES
111	a	710.52	9.60798	YES	YES
112	a	735.11	9.07109	YES	YES
113	a	738.24	8.18093	YES	YES
114	a	740.20	31.89616	YES	YES
115	a	741.61	9.99796	YES	YES
116	a	743.11	7.28390	YES	YES
117	a	746.19	8.73330	YES	YES
118	a	749.07	4.61152	YES	YES
119	a	758.06	6.87987	YES	YES
120	a	832.13	0.88845	YES	YES
121	a	834.93	7.68034	YES	YES
122	a	835.54	6.82537	YES	YES
123	a	839.89	1.71877	YES	YES
124	a	840.25	0.88685	YES	YES
125	a	842.16	11.37894	YES	YES
126	a	843.41	0.18403	YES	YES
127	a	850.99	0.39510	YES	YES
128	a	903.02	0.40671	YES	YES
129	a	908.74	1.23643	YES	YES
130	a	910.36	0.08680	YES	YES
131	a	919.08	0.34632	YES	YES
132	a	919.86	0.35357	YES	YES
133	a	923.84	0.42897	YES	YES
134	a	925.88	4.60773	YES	YES
135	a	927.35	1.42998	YES	YES
136	a	945.41	16.02058	YES	YES
137	a	955.90	0.39533	YES	YES
138	a	958.26	0.52162	YES	YES
139	a	961.15	0.31376	YES	YES
140	a	964.32	0.16222	YES	YES
141	a	966.13	0.01439	YES	YES
142	a	968.77	0.23470	YES	YES
143	a	972.10	0.17627	YES	YES
144	a	979.46	0.32792	YES	YES
145	a	980.25	1.02507	YES	YES
146	a	980.64	1.18186	YES	YES
147	a	981.74	1.60187	YES	YES
148	a	982.86	1.94374	YES	YES
149	a	983.87	0.67246	YES	YES
150	a	983.99	1.82523	YES	YES
151	a	985.10	0.37838	YES	YES
152	a	985.42	0.39962	YES	YES
153	a	986.63	1.15748	YES	YES
154	a	986.85	0.20836	YES	YES
155	a	987.19	2.49526	YES	YES
156	a	987.65	0.50527	YES	YES
157	a	990.01	1.20346	YES	YES
158	a	995.21	2.00244	YES	YES
159	a	1004.61	0.70078	YES	YES
160	a	1021.75	4.68517	YES	YES
161	a	1022.97	10.03611	YES	YES
162	a	1023.39	1.25983	YES	YES
163	a	1023.87	4.74612	YES	YES
164	a	1024.20	0.86729	YES	YES

165	a	1024.55	6.47432	YES	YES
166	a	1025.25	2.80141	YES	YES
167	a	1025.84	0.35300	YES	YES
168	a	1026.55	1.61204	YES	YES
169	a	1062.22	16.70333	YES	YES
170	a	1065.04	16.30998	YES	YES
171	a	1070.88	1.89187	YES	YES
172	a	1072.03	11.26316	YES	YES
173	a	1072.09	11.34489	YES	YES
174	a	1073.00	3.00895	YES	YES
175	a	1074.86	0.57280	YES	YES
176	a	1076.87	2.29114	YES	YES
177	a	1077.75	5.41969	YES	YES
178	a	1078.12	21.68018	YES	YES
179	a	1081.14	9.97162	YES	YES
180	a	1081.42	2.54685	YES	YES
181	a	1082.82	2.15787	YES	YES
182	a	1140.63	0.19389	YES	YES
183	a	1140.79	0.09973	YES	YES
184	a	1141.19	0.03429	YES	YES
185	a	1141.73	0.25721	YES	YES
186	a	1142.14	1.32396	YES	YES
187	a	1142.18	0.19531	YES	YES
188	a	1142.45	0.16716	YES	YES
189	a	1154.02	6.50306	YES	YES
190	a	1166.30	2.11956	YES	YES
191	a	1167.49	1.71067	YES	YES
192	a	1168.57	5.48969	YES	YES
193	a	1170.80	1.79513	YES	YES
194	a	1171.13	2.92884	YES	YES
195	a	1175.55	2.09885	YES	YES
196	a	1177.86	1.27725	YES	YES
197	a	1287.49	1.18271	YES	YES
198	a	1289.13	2.15663	YES	YES

* zero point VIBRATIONAL energy : 0.7390702 Hartree *

Cis TS_{25}_pfby



bp86-SVP SCF energy: -2931.3476254530
pbe-TZVPP SCF energy: -2930.901069019

XYZ Coordinates
97

C	1.37160	-1.80348	-2.22143
C	2.01390	-2.00503	-1.08917
C	0.71066	-2.13762	-3.47423
H	2.55533	-1.42259	-2.23270
C	-0.59184	-2.82690	-5.87308
C	0.19382	-1.66229	-5.80847
C	0.83766	-1.30959	-4.61355
C	-0.08091	-3.30915	-3.53890
C	-0.72997	-3.64360	-4.73566
H	-1.10103	-3.09834	-6.81272
H	0.29994	-1.01664	-6.69585
H	1.43041	-0.38458	-4.54219
H	-0.18312	-3.94264	-2.64466
H	-1.34811	-4.55551	-4.78150
C	2.65103	1.12961	-1.63690
C	3.88941	1.77772	-2.20587
H	4.58162	0.98739	-2.57528
H	4.41729	2.35023	-1.41658
H	3.62908	2.44292	-3.05317
C	-2.32834	-0.55602	-1.36420
C	-3.36367	-1.34540	-2.16782
H	-4.25954	-0.71690	-2.34700
H	-3.67751	-2.23942	-1.58274
H	-2.94025	-1.70622	-3.12801
C	1.10127	3.16019	0.26441
C	1.55515	3.92508	-0.83666
H	1.08676	3.79911	-1.82390
C	2.59364	4.86206	-0.69493
H	2.91423	5.45043	-1.57123
C	3.21052	5.05692	0.55104
H	4.01801	5.79897	0.66647
C	2.78107	4.29568	1.65016
H	3.25075	4.43365	2.63848
C	1.74481	3.35735	1.50595
H	1.43423	2.79170	2.39397
C	-1.33265	2.15816	1.50160
C	-0.81604	1.84949	2.78012
H	0.16251	1.35547	2.88031
C	-1.55492	2.12112	3.94306
H	-1.12584	1.87748	4.92843
C	-2.84234	2.67263	3.84582
H	-3.42541	2.88659	4.75704
C	-3.39419	2.91675	2.57693
H	-4.42036	3.31070	2.48543
C	-2.65053	2.65647	1.41381
H	-3.11023	2.81845	0.42890
C	-1.15976	2.78499	-1.38269
C	-1.60469	4.11284	-1.19234
H	-1.46144	4.61174	-0.22014
C	-2.21769	4.81932	-2.24040
H	-2.56519	5.85229	-2.07057
C	-2.37660	4.21638	-3.49977
H	-2.85409	4.77186	-4.32437
C	-1.91569	2.90505	-3.70238
H	-2.02646	2.42450	-4.68876
C	-1.31341	2.19294	-2.65148
H	-0.95226	1.16810	-2.81967
C	-0.96360	-1.37244	2.50733
C	-0.73207	-1.73636	3.85360
H	0.26596	-2.06281	4.18125
C	-1.77025	-1.68489	4.79959
H	-1.56527	-1.97447	5.84424
C	-3.05806	-1.27345	4.41872
H	-3.87356	-1.24056	5.16066
C	-3.29045	-0.88596	3.08961
H	-4.28682	-0.53224	2.77788
C	-2.25148	-0.92170	2.14367
H	-2.44757	-0.55181	1.12473
C	-0.04433	-3.35433	0.67529
C	-1.39154	-3.74595	0.50926
H	-2.20340	-3.04646	0.75931
C	-1.71766	-5.03144	0.04612
H	-2.77753	-5.31397	-0.06860
C	-0.70284	-5.95431	-0.25926
H	-0.95913	-6.96632	-0.61514
C	0.64094	-5.57754	-0.09977
H	1.44886	-6.29169	-0.33182
C	0.96997	-4.28921	0.35818
H	2.02836	-4.01215	0.46802
C	1.88786	-1.76105	2.22803
C	2.19384	-2.92876	2.96462
H	1.53772	-3.81150	2.90472
C	3.33309	-2.97795	3.78575
H	3.55877	-3.89894	4.34918
C	4.17894	-1.86051	3.88989
H	5.07451	-1.90101	4.53246
C	3.87832	-0.69476	3.16655
H	4.53931	0.18533	3.23295
C	2.74351	-0.64502	2.33901
H	2.54171	0.25858	1.74483
O	2.65070	0.64927	-0.45329
O	1.58588	0.98720	-2.34042
O	-2.67874	0.39719	-0.64504
O	-1.11431	-1.00478	-1.49689
P	-0.27878	1.88500	-0.00715
P	0.35463	-1.59432	1.18814
Ru	0.66175	-0.21441	-0.68071

Vibrational Frequencies

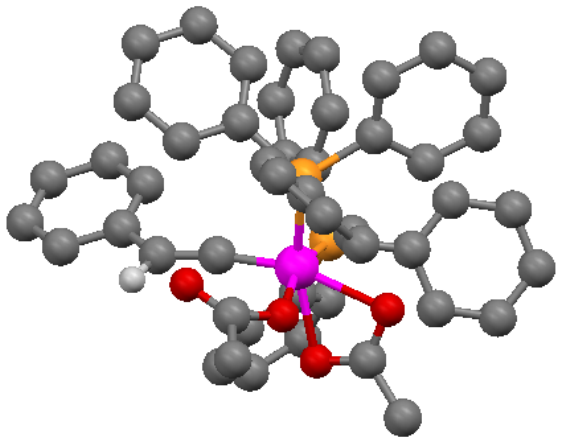
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-620.93	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	10.39	0.12881	YES	YES
9	a	14.76	0.19223	YES	YES
10	a	18.05	0.03343	YES	YES
11	a	27.17	0.19099	YES	YES
12	a	33.74	0.04038	YES	YES
13	a	37.93	0.01579	YES	YES
14	a	40.91	0.04995	YES	YES
15	a	41.97	0.16029	YES	YES
16	a	46.45	0.16655	YES	YES

17	a	50.89	0.08343	YES	YES
18	a	54.20	0.21244	YES	YES
19	a	56.03	0.22873	YES	YES
20	a	58.62	0.55024	YES	YES
21	a	61.52	0.36446	YES	YES
22	a	63.20	0.16718	YES	YES
23	a	65.72	0.10057	YES	YES
24	a	69.66	1.19711	YES	YES
25	a	74.59	0.27810	YES	YES
26	a	77.14	1.36892	YES	YES
27	a	82.57	0.18614	YES	YES
28	a	87.38	2.79526	YES	YES
29	a	90.02	0.79155	YES	YES
30	a	97.65	0.98401	YES	YES
31	a	100.55	0.46689	YES	YES
32	a	102.98	1.84238	YES	YES
33	a	109.99	0.43642	YES	YES
34	a	113.39	1.48053	YES	YES
35	a	118.38	5.53983	YES	YES
36	a	137.62	0.41265	YES	YES
37	a	143.19	3.15167	YES	YES
38	a	145.72	2.93450	YES	YES
39	a	150.21	6.42239	YES	YES
40	a	155.34	8.41917	YES	YES
41	a	171.16	3.94439	YES	YES
42	a	182.22	4.40174	YES	YES
43	a	185.01	3.96656	YES	YES
44	a	193.18	5.46099	YES	YES
45	a	198.58	4.05267	YES	YES
46	a	202.53	2.93608	YES	YES
47	a	210.92	2.68825	YES	YES
48	a	214.54	1.15893	YES	YES
49	a	215.72	1.20350	YES	YES
50	a	225.25	4.40442	YES	YES
51	a	236.51	2.19897	YES	YES
52	a	248.12	0.10827	YES	YES
53	a	250.46	1.64802	YES	YES
54	a	254.43	1.25187	YES	YES
55	a	259.35	1.47261	YES	YES
56	a	260.79	0.11392	YES	YES
57	a	264.12	0.70635	YES	YES
58	a	268.40	3.30604	YES	YES
59	a	269.66	0.88706	YES	YES
60	a	291.59	13.74545	YES	YES
61	a	310.89	15.79190	YES	YES
62	a	329.48	12.65950	YES	YES
63	a	365.26	18.55364	YES	YES
64	a	394.66	28.07535	YES	YES
65	a	395.86	8.62930	YES	YES
66	a	398.93	0.42457	YES	YES
67	a	400.34	0.01998	YES	YES
68	a	404.45	0.21279	YES	YES
69	a	407.14	1.25500	YES	YES
70	a	414.47	4.14694	YES	YES
71	a	416.59	10.44014	YES	YES
72	a	418.44	4.04377	YES	YES
73	a	428.28	24.07279	YES	YES
74	a	432.19	20.03494	YES	YES
75	a	456.03	22.73313	YES	YES
76	a	459.77	12.56509	YES	YES
77	a	468.04	39.14330	YES	YES
78	a	471.15	6.09242	YES	YES
79	a	477.97	9.07865	YES	YES
80	a	490.64	25.16198	YES	YES
81	a	502.58	5.58050	YES	YES
82	a	508.38	17.19471	YES	YES
83	a	512.10	61.97110	YES	YES
84	a	513.47	43.35722	YES	YES
85	a	519.36	133.98654	YES	YES
86	a	529.29	39.49312	YES	YES
87	a	572.89	11.56061	YES	YES
88	a	596.58	0.92955	YES	YES
89	a	600.57	7.84233	YES	YES
90	a	608.70	0.35269	YES	YES
91	a	609.43	0.73659	YES	YES
92	a	609.70	0.42764	YES	YES
93	a	610.52	0.70153	YES	YES
94	a	612.13	1.45990	YES	YES
95	a	613.51	0.74164	YES	YES
96	a	613.93	0.78100	YES	YES
97	a	661.25	7.42201	YES	YES
98	a	663.07	7.67355	YES	YES
99	a	665.38	55.30541	YES	YES
100	a	669.39	16.20541	YES	YES
101	a	674.95	10.34870	YES	YES
102	a	676.45	12.67022	YES	YES
103	a	688.08	16.38720	YES	YES
104	a	689.50	12.25426	YES	YES
105	a	692.63	27.11400	YES	YES
106	a	692.87	30.72407	YES	YES
107	a	696.64	43.49669	YES	YES
108	a	700.97	69.01180	YES	YES
109	a	702.28	18.88278	YES	YES
110	a	706.33	5.68667	YES	YES
111	a	708.52	20.21171	YES	YES
112	a	732.86	7.07444	YES	YES
113	a	737.24	3.87539	YES	YES
114	a	742.42	1.42283	YES	YES
115	a	743.88	7.36748	YES	YES
116	a	745.58	4.53494	YES	YES
117	a	748.23	8.11164	YES	YES
118	a	749.12	18.44149	YES	YES
119	a	751.33	2.83157	YES	YES
120	a	825.93	0.27237	YES	YES
121	a	832.18	1.14785	YES	YES
122	a	832.36	0.97308	YES	YES
123	a	836.27	3.77466	YES	YES
124	a	839.91	0.43575	YES	YES
125	a	843.81	2.71053	YES	YES
126	a	845.69	0.32569	YES	YES
127	a	846.24	1.03606	YES	YES
128	a	899.06	0.23242	YES	YES
129	a	905.82	0.50992	YES	YES
130	a	910.23	0.97032	YES	YES
131	a	914.55	0.92073	YES	YES
132	a	919.39	0.62594	YES	YES
133	a	921.73	0.36041	YES	YES
134	a	923.18	0.10437	YES	YES
135	a	926.39	2.00449	YES	YES
136	a	944.02	18.78740	YES	YES
137	a	953.11	0.15364	YES	YES
138	a	955.75	0.71704	YES	YES
139	a	956.76	0.90478	YES	YES
140	a	962.91	0.48976	YES	YES
141	a	963.11	0.56468	YES	YES
142	a	969.21	0.07455	YES	YES
143	a	969.77	0.25480	YES	YES
144	a	976.70	0.31430	YES	YES
145	a	978.18	0.10610	YES	YES
146	a	979.58	0.40959	YES	YES
147	a	979.63	0.25606	YES	YES
148	a	981.21	2.84463	YES	YES
149	a	981.75	0.86945	YES	YES
150	a	982.50	1.54112	YES	YES
151	a	982.88	0.10004	YES	YES
152	a	983.41	0.36684	YES	YES
153	a	984.74	1.85760	YES	YES
154	a	985.88	0.75618	YES	YES
155	a	986.88	0.12844	YES	YES
156	a	987.11	2.47323	YES	YES
157	a	988.20	0.19298	YES	YES
158	a	992.31	3.50284	YES	YES
159	a	996.47	0.10085	YES	YES
160	a	1021.90	8.93569	YES	YES
161	a	1023.01	1.66307	YES	YES
162	a	1023.74	0.36207	YES	YES
163	a	1023.99	4.29924	YES	YES
164	a	1024.73	3.33099	YES	YES

165	a	1024.85	2.23331	YES	YES
166	a	1025.01	2.71148	YES	YES
167	a	1026.87	0.97859	YES	YES
168	a	1027.19	0.53534	YES	YES
169	a	1062.66	13.76904	YES	YES
170	a	1066.48	15.50027	YES	YES
171	a	1071.46	9.13601	YES	YES
172	a	1072.75	11.08075	YES	YES
173	a	1073.48	0.52865	YES	YES
174	a	1073.74	5.25345	YES	YES
175	a	1075.72	7.00158	YES	YES
176	a	1076.81	1.32646	YES	YES
177	a	1078.71	11.81537	YES	YES
178	a	1079.86	18.94216	YES	YES
179	a	1081.53	6.97006	YES	YES
180	a	1081.93	9.76060	YES	YES
181	a	1084.81	0.38835	YES	YES
182	a	1140.32	0.03557	YES	YES
183	a	1141.14	0.41488	YES	YES
184	a	1141.17	0.40145	YES	YES
185	a	1141.56	0.64225	YES	YES
186	a	1141.81	0.26114	YES	YES
187	a	1141.99	0.15278	YES	YES
188	a	1142.32	0.98682	YES	YES
189	a	1157.16	6.07180	YES	YES
190	a	1167.52	2.76948	YES	YES
191	a	1168.19	3.40869	YES	YES
192	a	1169.53	2.00491	YES	YES
193	a	1171.87	4.78905	YES	YES
194	a	1173.06	3.40323	YES	YES
195	a	1177.10	2.19604	YES	YES
196	a	1180.53	2.51291	YES	YES
197	a	1287.43	1.66459	YES	YES
198	a	1289.40	2.34789	YES	YES

* zero point VIBRATIONAL energy : 0.7391419 Hartree *

Cis 5_afax



bp86-SVP SCF energy: -2931.4631504410
pbe-TZVPP SCF energy: -2931.008888615

XYZ Coordinates
97

C	-2.69865	0.72565	-1.43011
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C	-3.49203	1.79347	-0.81365
H	-3.17166	0.16835	-2.26261
C	-5.11215	3.85078	0.30873
C	-5.45561	3.26873	-0.92472
C	-4.66024	2.25461	-1.47674
C	-3.16830	2.38068	0.43599
C	-3.96441	3.39557	0.98392
H	-5.73845	4.64680	0.74465
H	-6.35682	3.60759	-1.46379
H	-4.93953	1.80468	-2.44476
H	-2.29140	2.01444	0.99229
H	-3.68764	3.82893	1.95995
C	2.31575	-0.09867	-2.63415
C	3.38299	-0.17175	-3.70039
H	3.15724	-1.03686	-4.36282
H	4.37886	-0.34444	-3.24269
H	3.38889	0.74802	-4.31986
C	-1.08047	-2.21724	-3.01492
C	-0.92033	-3.18410	-4.18798
H	-1.88264	-3.28468	-4.72932
H	-0.62856	-4.18136	-3.78999
H	-0.11995	-2.84917	-4.87985
C	2.85048	1.69855	0.48743
C	3.72050	1.91950	-0.60536
H	3.30304	2.08433	-1.61071
C	5.10973	1.97099	-0.41630
H	5.76972	2.15098	-1.28113
C	5.65723	1.80266	0.86778
H	6.74889	1.84704	1.01681
C	4.80134	1.58967	1.95989
H	5.21546	1.47134	2.97510
C	3.40796	1.53866	1.77266
H	2.75773	1.38804	2.64763
C	0.30404	2.09077	1.82191
C	0.28383	1.12035	2.84748
H	0.64687	0.10058	2.64602
C	-0.18274	1.44305	4.13282
H	-0.17651	0.67392	4.92287
C	-0.65907	2.73511	4.40876
H	-1.03033	2.98756	5.41583
C	-0.66845	3.69997	3.38793
H	-1.05106	4.71483	3.58736
C	-0.18898	3.38407	2.10522
H	-0.21135	4.15345	1.31926
C	0.80294	3.20669	-0.81957
C	1.57892	4.34664	-0.49961
H	2.32378	4.30044	0.31114
C	1.41138	5.54575	-1.20983
H	2.02430	6.42429	-0.94798
C	0.46921	5.62260	-2.25107
H	0.33945	6.56351	-2.81157
C	-0.30140	4.49499	-2.57490
H	-1.03991	4.54301	-3.39166
C	-0.13588	3.29162	-1.86679
H	-0.73878	2.41283	-2.13959
C	-1.90841	-1.78372	1.37746
C	-2.02699	-1.52263	2.75965
H	-1.12992	-1.44355	3.39102
C	-3.29302	-1.36451	3.34931
H	-3.36784	-1.16242	4.43085
C	-4.45439	-1.46077	2.56588
H	-5.44724	-1.33462	3.02899
C	-4.34388	-1.70870	1.18706
H	-5.24923	-1.77141	0.56134
C	-3.08261	-1.86233	0.58873
H	-3.00101	-2.03232	-0.49816
C	-0.30231	-3.64855	-0.23162
C	-1.35509	-4.56689	-0.05145
H	-2.26969	-4.26730	0.48237
C	-1.24480	-5.87920	-0.54799
H	-2.07738	-6.58686	-0.39929
C	-0.08455	-6.28463	-1.22629
H	0.00139	-7.31430	-1.61207
C	0.96846	-5.36931	-1.41062
H	1.88332	-5.67749	-1.94370
C	0.86247	-4.05878	-0.92043
H	1.69009	-3.34868	-1.07607
C	0.99472	-2.28713	1.80325
C	0.73918	-3.20390	2.85043
H	-0.25554	-3.66710	2.95124
C	1.75533	-3.55146	3.75401
H	1.53946	-4.26149	4.56978
C	3.04677	-3.01203	3.60875
H	3.84615	-3.29359	4.31443
C	3.31694	-2.13162	2.54925
H	4.33056	-1.72111	2.41041
C	2.29707	-1.76842	1.65030
H	2.52647	-1.09877	0.80614
O	2.39435	-0.82532	-1.58497
O	1.30458	0.67406	-2.78931
O	-2.19679	-1.96144	-2.54282
O	0.06042	-1.75224	-2.57612
P	1.01100	1.63669	0.15911
P	-0.28921	-1.92946	0.49961
Ru	0.26408	-0.30586	-1.08817

Vibrational Frequencies

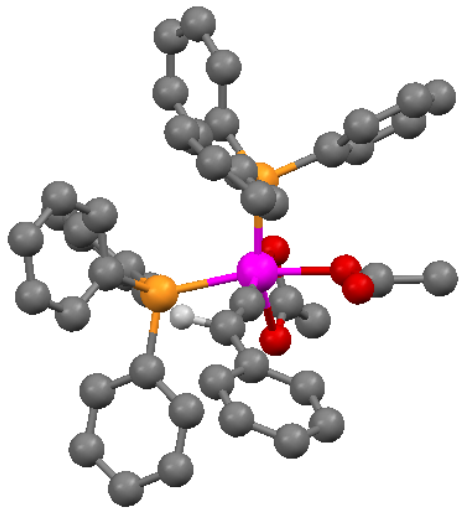
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.52	0.03408	YES	YES
8	a	19.46	0.10694	YES	YES
9	a	22.05	0.09068	YES	YES
10	a	24.07	0.22658	YES	YES
11	a	29.57	0.06050	YES	YES
12	a	38.32	0.61322	YES	YES
13	a	39.17	0.02836	YES	YES
14	a	44.79	0.27445	YES	YES
15	a	47.05	0.33766	YES	YES
16	a	49.17	0.12128	YES	YES
17	a	52.67	0.10725	YES	YES
18	a	54.62	0.03791	YES	YES

19	a	56.04	0.38116	YES	YES
20	a	57.17	0.13315	YES	YES
21	a	60.79	0.43337	YES	YES
22	a	63.63	0.08237	YES	YES
23	a	67.49	0.65244	YES	YES
24	a	71.97	0.45267	YES	YES
25	a	74.79	0.17380	YES	YES
26	a	75.58	0.62851	YES	YES
27	a	78.35	0.46884	YES	YES
28	a	81.68	1.58910	YES	YES
29	a	88.73	1.04044	YES	YES
30	a	91.77	0.12444	YES	YES
31	a	92.91	0.43639	YES	YES
32	a	97.93	0.81891	YES	YES
33	a	100.67	3.92311	YES	YES
34	a	109.47	3.22201	YES	YES
35	a	112.32	0.55798	YES	YES
36	a	118.04	2.86179	YES	YES
37	a	126.72	1.27409	YES	YES
38	a	146.83	8.13271	YES	YES
39	a	161.79	0.92070	YES	YES
40	a	180.30	4.06146	YES	YES
41	a	188.23	1.68093	YES	YES
42	a	191.34	0.51718	YES	YES
43	a	198.82	3.56041	YES	YES
44	a	202.92	0.13267	YES	YES
45	a	208.72	0.43247	YES	YES
46	a	217.46	0.99773	YES	YES
47	a	223.60	0.87907	YES	YES
48	a	229.69	3.68052	YES	YES
49	a	235.62	6.64005	YES	YES
50	a	245.94	1.78261	YES	YES
51	a	246.43	0.81263	YES	YES
52	a	250.75	2.44739	YES	YES
53	a	251.54	2.48139	YES	YES
54	a	253.07	0.89004	YES	YES
55	a	265.64	3.50120	YES	YES
56	a	267.29	1.82059	YES	YES
57	a	269.71	1.71781	YES	YES
58	a	277.00	14.85214	YES	YES
59	a	287.24	7.85020	YES	YES
60	a	320.60	10.05949	YES	YES
61	a	390.25	2.75700	YES	YES
62	a	397.18	0.28837	YES	YES
63	a	399.95	0.37447	YES	YES
64	a	401.76	0.31746	YES	YES
65	a	403.01	0.14037	YES	YES
66	a	405.04	0.03231	YES	YES
67	a	409.75	1.53995	YES	YES
68	a	412.91	30.85494	YES	YES
69	a	415.89	1.08344	YES	YES
70	a	418.11	8.13235	YES	YES
71	a	424.26	17.21888	YES	YES
72	a	430.74	15.07939	YES	YES
73	a	445.52	15.38284	YES	YES
74	a	454.08	15.72478	YES	YES
75	a	467.56	5.52336	YES	YES
76	a	480.70	6.18425	YES	YES
77	a	486.84	10.43288	YES	YES
78	a	495.27	18.07904	YES	YES
79	a	497.06	25.83479	YES	YES
80	a	505.52	18.96862	YES	YES
81	a	508.69	17.41396	YES	YES
82	a	512.46	29.06549	YES	YES
83	a	516.84	143.88010	YES	YES
84	a	525.81	86.62639	YES	YES
85	a	576.48	16.64569	YES	YES
86	a	589.57	7.90325	YES	YES
87	a	593.15	3.72797	YES	YES
88	a	607.86	0.12513	YES	YES
89	a	609.57	0.81576	YES	YES
90	a	609.74	0.08890	YES	YES
91	a	610.20	1.04021	YES	YES
92	a	610.76	2.14202	YES	YES
93	a	611.69	0.44131	YES	YES
94	a	612.63	0.71249	YES	YES
95	a	658.02	35.58220	YES	YES
96	a	669.86	68.45396	YES	YES
97	a	672.11	8.35881	YES	YES
98	a	674.51	16.57731	YES	YES
99	a	680.10	8.60754	YES	YES
100	a	681.15	5.19756	YES	YES
101	a	685.76	12.71391	YES	YES
102	a	688.24	4.65197	YES	YES
103	a	691.77	30.28528	YES	YES
104	a	694.43	20.04673	YES	YES
105	a	697.19	25.36496	YES	YES
106	a	698.41	51.89116	YES	YES
107	a	700.53	31.75788	YES	YES
108	a	702.74	30.89583	YES	YES
109	a	704.00	18.77881	YES	YES
110	a	712.55	11.80172	YES	YES
111	a	724.35	18.30149	YES	YES
112	a	737.11	13.83110	YES	YES
113	a	738.90	4.44065	YES	YES
114	a	740.36	4.59227	YES	YES
115	a	743.76	6.03577	YES	YES
116	a	746.27	3.05939	YES	YES
117	a	747.41	4.94895	YES	YES
118	a	765.37	27.63036	YES	YES
119	a	820.39	5.63559	YES	YES
120	a	822.41	0.85368	YES	YES
121	a	833.18	0.35826	YES	YES
122	a	835.04	0.24635	YES	YES
123	a	839.45	0.30660	YES	YES
124	a	841.99	1.66618	YES	YES
125	a	846.33	0.91372	YES	YES
126	a	850.57	1.02342	YES	YES
127	a	888.05	4.72179	YES	YES
128	a	908.93	0.22488	YES	YES
129	a	909.49	0.05282	YES	YES
130	a	916.26	0.20459	YES	YES
131	a	918.49	1.72493	YES	YES
132	a	922.98	0.51523	YES	YES
133	a	925.13	4.03865	YES	YES
134	a	929.73	0.31251	YES	YES
135	a	936.81	26.51953	YES	YES
136	a	946.99	0.14460	YES	YES
137	a	958.46	0.31603	YES	YES
138	a	959.58	0.34543	YES	YES
139	a	964.60	0.31307	YES	YES
140	a	967.43	0.75848	YES	YES
141	a	968.14	0.63818	YES	YES
142	a	969.35	0.38956	YES	YES
143	a	973.06	0.21253	YES	YES
144	a	979.77	0.08977	YES	YES
145	a	981.22	0.29580	YES	YES
146	a	981.67	1.59149	YES	YES
147	a	982.09	2.69477	YES	YES
148	a	982.57	1.36692	YES	YES
149	a	983.10	1.84387	YES	YES
150	a	983.73	0.53921	YES	YES
151	a	983.78	0.67513	YES	YES
152	a	985.09	1.27691	YES	YES
153	a	985.90	2.13554	YES	YES
154	a	986.32	1.17640	YES	YES
155	a	989.80	0.15521	YES	YES
156	a	991.87	8.03503	YES	YES
157	a	992.36	2.08528	YES	YES
158	a	998.64	0.31133	YES	YES
159	a	1019.52	8.15594	YES	YES
160	a	1022.61	0.74788	YES	YES
161	a	1023.76	2.88111	YES	YES
162	a	1023.99	7.75556	YES	YES
163	a	1024.36	2.93690	YES	YES
164	a	1024.90	1.36682	YES	YES
165	a	1025.78	0.80656	YES	YES
166	a	1026.16	4.24123	YES	YES

167	a	1026.61	0.56261	YES	YES
168	a	1069.07	11.62507	YES	YES
169	a	1069.86	10.97508	YES	YES
170	a	1070.23	15.46096	YES	YES
171	a	1072.24	3.80399	YES	YES
172	a	1074.39	18.54535	YES	YES
173	a	1075.28	6.20198	YES	YES
174	a	1076.71	1.19736	YES	YES
175	a	1078.03	4.28487	YES	YES
176	a	1078.37	15.09320	YES	YES
177	a	1080.20	2.69733	YES	YES
178	a	1081.19	21.66042	YES	YES
179	a	1082.13	12.45367	YES	YES
180	a	1086.87	7.70177	YES	YES
181	a	1132.89	16.31504	YES	YES
182	a	1137.61	1.15062	YES	YES
183	a	1141.63	0.26163	YES	YES
184	a	1141.91	0.28675	YES	YES
185	a	1142.44	0.38567	YES	YES
186	a	1142.66	0.75195	YES	YES
187	a	1142.88	0.20901	YES	YES
188	a	1143.12	0.64205	YES	YES
189	a	1161.18	4.36057	YES	YES
190	a	1167.81	2.73992	YES	YES
191	a	1171.03	2.83215	YES	YES
192	a	1173.08	5.76056	YES	YES
193	a	1173.68	8.44995	YES	YES
194	a	1175.35	1.50483	YES	YES
195	a	1179.50	2.11217	YES	YES
196	a	1232.26	2.03033	YES	YES
197	a	1292.49	3.28012	YES	YES
198	a	1292.86	5.03148	YES	YES

* zero point VIBRATIONAL energy : 0.7460458 Hartree *

Cis 5_afay



bp86-SVP SCF energy: -2931.4665913380
pbe-TZVPP SCF energy: -2931.011484180

XYZ Coordinates
97

C	0.00916	2.71866	0.44545
C	-0.15638	1.59006	-0.26244
C	-0.31918	4.12988	0.22304
H	0.55516	2.50624	1.39249
C	-0.83310	6.91247	-0.10465
C	-0.23780	6.43688	1.07705
C	0.01436	5.06689	1.23814
C	-0.91933	4.62578	-0.96402
C	-1.17171	5.99532	-1.11680
H	-1.03152	7.98947	-0.23650
H	0.03355	7.14018	1.88273
H	0.48260	4.70757	2.16914
H	-1.20738	3.91535	-1.75070
H	-1.63831	6.35535	-2.05025
C	0.90690	-1.16312	-3.14711
C	1.24985	-1.70795	-4.51459
H	0.35349	-1.61337	-5.16780
H	1.51154	-2.78372	-4.44602
H	2.07636	-1.13090	-4.97467
C	-2.35495	1.15081	-2.49728
C	-3.31171	1.11965	-3.68777
H	-3.80627	2.10402	-3.81958
H	-4.09610	0.35956	-3.47795
H	-2.79182	0.81007	-4.61760
C	2.91111	-1.92716	0.05918
C	3.33996	-2.36109	-1.21701
H	3.17822	-1.71467	-2.09497
C	4.01108	-3.58353	-1.36774
H	4.33987	-3.90339	-2.36997
C	4.26880	-4.39346	-0.24742
H	4.79841	-5.35420	-0.36698
C	3.85396	-3.96800	1.02474
H	4.06306	-4.58793	1.91247
C	3.18020	-2.74156	1.17920
H	2.87554	-2.41911	2.18648
C	2.09252	0.12356	1.96325
C	1.28021	-0.59889	2.86592
H	0.61278	-1.39458	2.49544
C	1.31579	-0.32016	4.24323
H	0.68767	-0.90623	4.93386
C	2.14150	0.70494	4.73431
H	2.16374	0.92947	5.81307
C	2.93036	1.44717	3.84214
H	3.57234	2.26214	4.21684
C	2.91112	1.15981	2.46627
H	3.54226	1.74845	1.78293
C	3.35119	0.81592	-0.56055
C	4.71493	0.54502	-0.29814
H	4.99969	-0.33346	0.30286
C	5.71818	1.38986	-0.79854
H	6.77612	1.16702	-0.58202
C	5.37449	2.51420	-1.56998
H	6.16301	3.17753	-1.96344
C	4.02254	2.78982	-1.83295
H	3.74346	3.67006	-2.43559
C	3.01632	1.94683	-1.33501
H	1.96119	2.17292	-1.54410
C	-2.27214	0.16955	1.83849
C	-2.17354	-0.22786	3.19007
H	-1.77137	-1.21774	3.45380
C	-2.60066	0.63054	4.21831
H	-2.52202	0.29975	5.26758
C	-3.12739	1.89610	3.91127
H	-3.46218	2.56804	4.71910
C	-3.21022	2.30616	2.56923
H	-3.60191	3.30398	2.31533
C	-2.78075	1.45555	1.53546
H	-2.83108	1.79810	0.48791
C	-3.26924	-1.27393	-0.51823
C	-4.54147	-0.79132	-0.15188
H	-4.65119	-0.10019	0.69736
C	-5.68569	-1.19415	-0.86651
H	-6.67471	-0.80748	-0.56950
C	-5.56862	-2.08161	-1.94778
H	-6.46696	-2.39760	-2.50549
C	-4.29833	-2.55829	-2.32223
H	-4.19713	-3.24645	-3.17851
C	-3.15316	-2.15432	-1.61959
H	-2.16187	-2.52058	-1.93104
C	-1.44252	-2.58257	1.12998
C	-2.43012	-3.19040	1.93813
H	-3.34661	-2.63699	2.20459
C	-2.26797	-4.51069	2.38592
H	-3.04279	-4.96916	3.02316
C	-1.13026	-5.24877	2.01158
H	-1.00846	-6.28816	2.35864
C	-0.16381	-4.66454	1.17881
H	0.71765	-5.24387	0.85752
C	-0.31902	-3.33771	0.73912
H	0.42536	-2.89910	0.05747
O	0.31804	-1.89199	-2.28012
O	1.18725	0.05650	-2.85947
O	-2.43056	2.04699	-1.64029
O	-1.51749	0.15264	-2.48399
P	2.02799	-0.28656	0.15364
P	-1.70576	-0.88081	0.42038
Ru	-0.04704	-0.06874	-1.01890

Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	7.98	1.82537	YES	YES
8	a	9.89	0.45358	YES	YES
9	a	11.06	0.07933	YES	YES
10	a	19.57	0.06740	YES	YES
11	a	22.21	0.19954	YES	YES
12	a	27.66	0.12325	YES	YES
13	a	36.85	0.61326	YES	YES
14	a	43.47	0.23437	YES	YES
15	a	46.63	0.17433	YES	YES
16	a	46.77	0.12903	YES	YES

17	a	49.44	0.02767	YES	YES
18	a	52.47	0.61138	YES	YES
19	a	53.65	0.18465	YES	YES
20	a	55.22	0.09432	YES	YES
21	a	55.81	0.11924	YES	YES
22	a	62.97	0.57011	YES	YES
23	a	66.63	0.41564	YES	YES
24	a	68.52	0.11444	YES	YES
25	a	70.28	0.20309	YES	YES
26	a	71.29	0.28163	YES	YES
27	a	76.72	0.42721	YES	YES
28	a	80.23	0.08446	YES	YES
29	a	82.07	0.63875	YES	YES
30	a	90.09	1.47200	YES	YES
31	a	93.28	1.94469	YES	YES
32	a	99.74	2.14613	YES	YES
33	a	102.85	1.68400	YES	YES
34	a	106.60	2.26883	YES	YES
35	a	110.56	0.32622	YES	YES
36	a	121.77	2.07226	YES	YES
37	a	130.17	3.10365	YES	YES
38	a	153.07	3.14873	YES	YES
39	a	164.64	0.76358	YES	YES
40	a	184.61	4.56903	YES	YES
41	a	188.19	1.14084	YES	YES
42	a	191.92	3.00595	YES	YES
43	a	200.04	1.01064	YES	YES
44	a	205.58	0.81365	YES	YES
45	a	212.77	0.42649	YES	YES
46	a	222.86	0.55216	YES	YES
47	a	223.40	1.10461	YES	YES
48	a	226.04	3.46409	YES	YES
49	a	241.11	3.62415	YES	YES
50	a	243.60	4.29405	YES	YES
51	a	246.00	0.33522	YES	YES
52	a	247.58	0.90633	YES	YES
53	a	249.34	0.46261	YES	YES
54	a	252.82	0.90165	YES	YES
55	a	258.02	5.59234	YES	YES
56	a	266.02	4.64547	YES	YES
57	a	269.16	6.05667	YES	YES
58	a	271.38	6.71562	YES	YES
59	a	284.34	7.25692	YES	YES
60	a	318.54	12.65207	YES	YES
61	a	386.99	1.69791	YES	YES
62	a	396.47	0.27010	YES	YES
63	a	398.76	0.22496	YES	YES
64	a	400.47	0.04575	YES	YES
65	a	400.64	0.08011	YES	YES
66	a	404.30	0.34384	YES	YES
67	a	407.08	0.99962	YES	YES
68	a	415.78	32.56926	YES	YES
69	a	416.64	0.16523	YES	YES
70	a	419.53	20.33865	YES	YES
71	a	430.20	2.36513	YES	YES
72	a	431.30	23.86378	YES	YES
73	a	443.78	13.26973	YES	YES
74	a	453.85	13.66087	YES	YES
75	a	465.49	4.69152	YES	YES
76	a	472.13	18.90640	YES	YES
77	a	489.21	4.07440	YES	YES
78	a	495.89	23.42316	YES	YES
79	a	498.16	23.54826	YES	YES
80	a	504.42	10.52787	YES	YES
81	a	509.16	10.84118	YES	YES
82	a	512.34	38.68814	YES	YES
83	a	517.30	162.93161	YES	YES
84	a	526.79	90.63708	YES	YES
85	a	580.42	26.64810	YES	YES
86	a	594.45	2.82944	YES	YES
87	a	601.40	6.44198	YES	YES
88	a	607.96	0.48556	YES	YES
89	a	609.23	0.29837	YES	YES
90	a	609.35	0.64620	YES	YES
91	a	610.02	1.42230	YES	YES
92	a	610.64	1.59078	YES	YES
93	a	611.27	0.11347	YES	YES
94	a	613.66	2.85144	YES	YES
95	a	644.19	3.38596	YES	YES
96	a	660.02	34.68783	YES	YES
97	a	670.19	63.88727	YES	YES
98	a	673.28	14.85663	YES	YES
99	a	674.48	14.44561	YES	YES
100	a	681.86	8.24871	YES	YES
101	a	683.74	7.76591	YES	YES
102	a	688.31	23.13983	YES	YES
103	a	688.56	18.22089	YES	YES
104	a	692.94	21.76264	YES	YES
105	a	695.55	27.85815	YES	YES
106	a	695.79	34.87456	YES	YES
107	a	700.01	9.43631	YES	YES
108	a	700.50	76.14130	YES	YES
109	a	704.49	16.77424	YES	YES
110	a	712.17	19.89505	YES	YES
111	a	722.51	17.00356	YES	YES
112	a	738.78	13.04611	YES	YES
113	a	739.99	4.90806	YES	YES
114	a	741.78	7.51109	YES	YES
115	a	744.70	6.06557	YES	YES
116	a	746.98	4.52180	YES	YES
117	a	747.91	2.23860	YES	YES
118	a	761.63	31.16422	YES	YES
119	a	819.70	1.90464	YES	YES
120	a	820.48	8.71995	YES	YES
121	a	833.23	0.26822	YES	YES
122	a	833.36	0.58920	YES	YES
123	a	837.98	1.06924	YES	YES
124	a	839.29	0.59289	YES	YES
125	a	844.07	1.18598	YES	YES
126	a	851.67	0.28887	YES	YES
127	a	888.65	4.83825	YES	YES
128	a	906.75	0.00843	YES	YES
129	a	910.64	0.26724	YES	YES
130	a	912.21	0.72851	YES	YES
131	a	913.55	0.78390	YES	YES
132	a	917.10	0.05175	YES	YES
133	a	927.65	3.87034	YES	YES
134	a	929.77	0.77088	YES	YES
135	a	935.66	27.04607	YES	YES
136	a	946.03	1.19583	YES	YES
137	a	957.23	0.30069	YES	YES
138	a	959.50	0.10761	YES	YES
139	a	960.98	0.10680	YES	YES
140	a	963.55	0.25908	YES	YES
141	a	965.61	0.63105	YES	YES
142	a	970.43	1.47093	YES	YES
143	a	973.63	0.08345	YES	YES
144	a	980.20	0.99341	YES	YES
145	a	980.99	1.53800	YES	YES
146	a	982.32	2.40895	YES	YES
147	a	982.80	0.86857	YES	YES
148	a	983.15	2.11274	YES	YES
149	a	983.30	0.60068	YES	YES
150	a	983.86	0.86987	YES	YES
151	a	984.18	1.23881	YES	YES
152	a	984.31	2.21665	YES	YES
153	a	986.19	0.44575	YES	YES
154	a	987.24	0.27697	YES	YES
155	a	987.54	0.40360	YES	YES
156	a	988.89	1.21942	YES	YES
157	a	993.07	7.20685	YES	YES
158	a	1005.96	0.07444	YES	YES
159	a	1019.09	8.14496	YES	YES
160	a	1023.17	0.74782	YES	YES
161	a	1023.81	1.62312	YES	YES
162	a	1024.31	2.04598	YES	YES
163	a	1024.51	3.10000	YES	YES
164	a	1024.84	1.11125	YES	YES

165	a	1025.58	7.67439	YES	YES
166	a	1026.80	0.52304	YES	YES
167	a	1028.35	5.13182	YES	YES
168	a	1071.58	14.97022	YES	YES
169	a	1071.66	18.56741	YES	YES
170	a	1072.58	9.42127	YES	YES
171	a	1073.29	2.30679	YES	YES
172	a	1073.81	10.14406	YES	YES
173	a	1075.16	16.10062	YES	YES
174	a	1076.50	5.43603	YES	YES
175	a	1077.72	7.25047	YES	YES
176	a	1077.88	6.70439	YES	YES
177	a	1078.47	0.95215	YES	YES
178	a	1080.89	25.03434	YES	YES
179	a	1083.74	11.64714	YES	YES
180	a	1084.12	10.18397	YES	YES
181	a	1137.03	0.86265	YES	YES
182	a	1142.48	0.42514	YES	YES
183	a	1142.77	0.35569	YES	YES
184	a	1142.89	0.30158	YES	YES
185	a	1142.96	0.36614	YES	YES
186	a	1143.32	0.29625	YES	YES
187	a	1143.78	0.92477	YES	YES
188	a	1151.08	35.18646	YES	YES
189	a	1167.54	6.77937	YES	YES
190	a	1169.44	1.08252	YES	YES
191	a	1170.16	4.67993	YES	YES
192	a	1170.68	9.15182	YES	YES
193	a	1173.04	1.34322	YES	YES
194	a	1173.36	7.11480	YES	YES
195	a	1179.52	2.88109	YES	YES
196	a	1228.15	5.83340	YES	YES
197	a	1291.86	6.38660	YES	YES
198	a	1292.79	1.17790	YES	YES

* zero point VIBRATIONAL energy : 0.7456086 Hartree *

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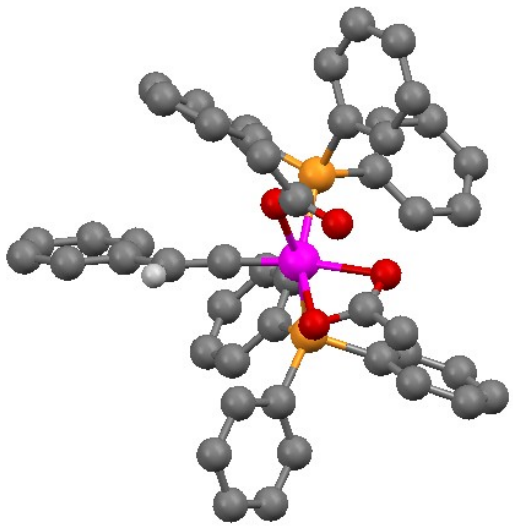


bp86-SVP SCF energy: -2931.4530605770
pbe-TZVPP SCF energy: -2931.000267458

XYZ Coordinates
97

C	-2.42626	0.74898	-1.84076
C	-1.25053	0.36770	-1.32120
C	-3.70391	1.11997	-1.22452
H	-2.38741	0.78550	-2.95129
C	-6.21675	1.87448	-0.11923
C	-6.03657	1.84044	-1.51314
C	-4.79877	1.46889	-2.05789
C	-3.90142	1.15825	0.17986
C	-5.13991	1.52946	0.71947
H	-7.18858	2.16845	0.31106
H	-6.86903	2.10727	-2.18613
H	-4.66772	1.44660	-3.15332
H	-3.06968	0.89172	0.85128
H	-5.26536	1.54966	1.81504
C	2.70364	0.06261	-2.20945
C	3.94661	0.07881	-3.05454
H	3.86168	-0.78039	-3.75462
H	4.84915	-0.06079	-2.42480
H	4.01479	1.01669	-3.64313
C	0.66724	-2.29472	-3.31795
C	-0.14606	-3.28908	-4.15973
H	0.44602	-3.60898	-5.04106
H	-1.10881	-2.84211	-4.48860
H	-0.38735	-4.18318	-3.54259
C	2.41712	2.09171	1.09655
C	3.58375	2.16288	0.29959
H	3.50334	2.11152	-0.79693
C	4.84382	2.33825	0.89103
H	5.74125	2.39314	0.25309
C	4.96077	2.45046	2.28801
H	5.95105	2.59135	2.75221
C	3.80673	2.39313	3.08604
H	3.88408	2.49536	4.18131
C	2.54209	2.21429	2.49592
H	1.64883	2.18424	3.13806
C	-0.47464	2.29041	1.50682
C	-0.69452	1.40311	2.58543
H	-0.12520	0.46251	2.64938
C	-1.62795	1.71280	3.58843
H	-1.77184	1.01674	4.43128
C	-2.37658	2.90063	3.51567
H	-3.11278	3.14198	4.30029
C	-2.18686	3.77259	2.43136
H	-2.78179	4.69731	2.35308
C	-1.24084	3.47384	1.43516
H	-1.10650	4.16845	0.59310
C	0.79515	3.36508	-0.87151
C	1.36422	4.57134	-0.39886
H	1.83141	4.60907	0.59858
C	1.34173	5.73003	-1.19169
H	1.79111	6.66145	-0.80853
C	0.75453	5.69969	-2.46904
H	0.74308	6.60775	-3.09465
C	0.18951	4.50591	-2.94543
H	-0.26647	4.46946	-3.94832
C	0.20900	3.34439	-2.15368
H	-0.22562	2.41317	-2.54092
C	-1.91595	-2.07258	0.86877
C	-2.52894	-1.82639	2.11502
H	-1.92741	-1.50908	2.98009
C	-3.91888	-1.98141	2.26312
H	-4.38597	-1.79095	3.24403
C	-4.70808	-2.36843	1.16864
H	-5.79796	-2.48542	1.28599
C	-4.10530	-2.58980	-0.08217
H	-4.72176	-2.87276	-0.95093
C	-2.71945	-2.43919	-0.23773
H	-2.24829	-2.59353	-1.22275
C	0.41311	-3.55091	-0.08090
C	-0.36117	-4.70481	0.16413
H	-1.35501	-4.62262	0.63204
C	0.12718	-5.97319	-0.19671
H	-0.49014	-6.86716	-0.00625
C	1.38933	-6.09971	-0.79994
H	1.76879	-7.09472	-1.08670
C	2.16201	-4.95040	-1.04279
H	3.14643	-5.03471	-1.53131
C	1.68364	-3.68038	-0.68265
H	2.28936	-2.78679	-0.90339
C	0.77686	-1.93909	2.16618
C	0.37129	-2.80162	3.21171
H	-0.54553	-3.40403	3.11387
C	1.14918	-2.92056	4.37462
H	0.81661	-3.58944	5.18589
C	2.35531	-2.20671	4.49662
H	2.96880	-2.30893	5.40715
C	2.78329	-1.37977	3.44557
H	3.73665	-0.83212	3.51852
C	1.99875	-1.24454	2.28613
H	2.35365	-0.61285	1.45676
O	2.64491	-0.59263	-1.11243
O	1.66450	0.72991	-2.57414
O	1.86961	-2.11715	-3.53412
O	-0.06238	-1.73911	-2.37846
P	0.79058	1.85230	0.21790
P	-0.11398	-1.87363	0.53716
Ru	0.45078	-0.16128	-1.00471

Vibrational Frequencies

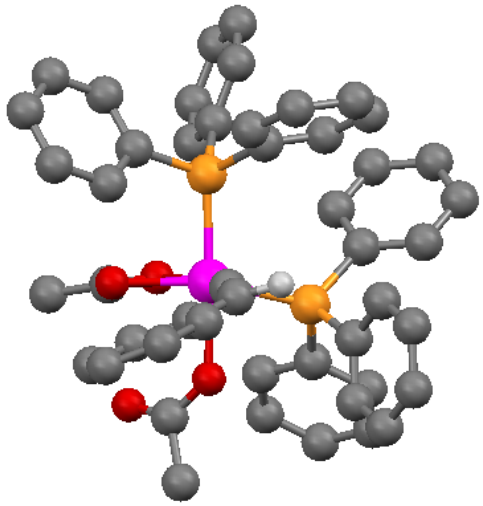
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.15	0.28927	YES	YES
8	a	14.94	0.09077	YES	YES
9	a	17.22	0.13748	YES	YES
10	a	22.79	0.40293	YES	YES
11	a	23.58	0.05264	YES	YES
12	a	28.13	0.27969	YES	YES
13	a	36.26	0.22919	YES	YES
14	a	41.50	0.30217	YES	YES
15	a	43.44	0.21003	YES	YES
16	a	46.28	0.66493	YES	YES

17	a	47.70	0.60324	YES	YES
18	a	51.20	0.23141	YES	YES
19	a	53.38	0.23063	YES	YES
20	a	56.29	0.12698	YES	YES
21	a	60.00	0.00306	YES	YES
22	a	61.91	0.15228	YES	YES
23	a	63.58	1.12172	YES	YES
24	a	67.80	0.15212	YES	YES
25	a	69.71	0.15897	YES	YES
26	a	72.22	0.23153	YES	YES
27	a	78.40	0.31532	YES	YES
28	a	84.91	0.09157	YES	YES
29	a	88.20	0.03095	YES	YES
30	a	92.52	0.35990	YES	YES
31	a	93.06	1.06663	YES	YES
32	a	101.89	3.18846	YES	YES
33	a	105.65	0.34087	YES	YES
34	a	108.73	0.39800	YES	YES
35	a	112.84	3.78589	YES	YES
36	a	113.48	0.97155	YES	YES
37	a	133.11	2.13380	YES	YES
38	a	152.04	7.30262	YES	YES
39	a	169.81	2.05356	YES	YES
40	a	172.24	1.55977	YES	YES
41	a	182.23	3.16177	YES	YES
42	a	187.74	0.82906	YES	YES
43	a	197.59	1.39714	YES	YES
44	a	204.44	1.14509	YES	YES
45	a	207.22	0.33222	YES	YES
46	a	210.56	1.48745	YES	YES
47	a	216.97	1.73469	YES	YES
48	a	221.30	5.84748	YES	YES
49	a	228.89	2.17279	YES	YES
50	a	230.38	3.03550	YES	YES
51	a	245.66	0.66737	YES	YES
52	a	246.84	0.53951	YES	YES
53	a	247.90	1.07611	YES	YES
54	a	250.38	6.11971	YES	YES
55	a	251.92	0.22151	YES	YES
56	a	264.44	7.48530	YES	YES
57	a	267.51	0.00967	YES	YES
58	a	273.33	4.61689	YES	YES
59	a	285.28	8.61858	YES	YES
60	a	328.46	11.46833	YES	YES
61	a	392.75	0.15554	YES	YES
62	a	395.96	0.21180	YES	YES
63	a	399.01	0.99321	YES	YES
64	a	399.42	2.48759	YES	YES
65	a	400.89	1.08320	YES	YES
66	a	404.25	0.11083	YES	YES
67	a	405.54	0.41565	YES	YES
68	a	408.29	11.47595	YES	YES
69	a	409.87	15.64824	YES	YES
70	a	420.56	13.56088	YES	YES
71	a	426.65	4.56421	YES	YES
72	a	429.11	20.37264	YES	YES
73	a	450.37	9.06366	YES	YES
74	a	454.07	14.75224	YES	YES
75	a	465.69	1.99949	YES	YES
76	a	469.29	4.12972	YES	YES
77	a	486.86	11.59390	YES	YES
78	a	493.33	2.98318	YES	YES
79	a	497.45	10.92743	YES	YES
80	a	498.30	35.91103	YES	YES
81	a	509.47	58.84992	YES	YES
82	a	510.76	27.88865	YES	YES
83	a	513.38	137.34452	YES	YES
84	a	524.94	77.09238	YES	YES
85	a	559.04	6.23413	YES	YES
86	a	574.93	23.95545	YES	YES
87	a	583.15	2.75619	YES	YES
88	a	607.26	0.51372	YES	YES
89	a	608.62	0.65055	YES	YES
90	a	609.70	0.15486	YES	YES
91	a	610.23	2.09406	YES	YES
92	a	610.65	0.38624	YES	YES
93	a	611.18	0.42450	YES	YES
94	a	613.37	1.12063	YES	YES
95	a	642.09	8.89126	YES	YES
96	a	651.00	4.82144	YES	YES
97	a	673.65	9.80577	YES	YES
98	a	675.31	18.78269	YES	YES
99	a	676.27	55.74398	YES	YES
100	a	682.26	8.46860	YES	YES
101	a	684.26	8.59321	YES	YES
102	a	688.89	19.25465	YES	YES
103	a	690.79	29.26400	YES	YES
104	a	694.48	38.89070	YES	YES
105	a	695.23	25.56380	YES	YES
106	a	696.29	44.14557	YES	YES
107	a	697.43	36.87823	YES	YES
108	a	698.77	3.70484	YES	YES
109	a	700.21	37.94341	YES	YES
110	a	706.63	6.99201	YES	YES
111	a	736.77	9.99597	YES	YES
112	a	739.02	8.59898	YES	YES
113	a	739.88	12.84741	YES	YES
114	a	743.64	5.55490	YES	YES
115	a	746.44	4.97809	YES	YES
116	a	747.36	2.23006	YES	YES
117	a	754.29	4.01851	YES	YES
118	a	760.51	25.78519	YES	YES
119	a	818.82	5.61162	YES	YES
120	a	823.29	0.02146	YES	YES
121	a	831.58	0.73046	YES	YES
122	a	835.58	0.14932	YES	YES
123	a	836.07	0.26517	YES	YES
124	a	836.60	1.06048	YES	YES
125	a	842.44	1.14116	YES	YES
126	a	844.61	1.62819	YES	YES
127	a	889.20	6.02130	YES	YES
128	a	905.28	0.31699	YES	YES
129	a	907.79	0.42332	YES	YES
130	a	908.55	0.98888	YES	YES
131	a	911.80	0.22814	YES	YES
132	a	912.56	0.54610	YES	YES
133	a	915.01	0.45487	YES	YES
134	a	919.65	0.17611	YES	YES
135	a	938.29	18.25050	YES	YES
136	a	947.30	0.17143	YES	YES
137	a	956.39	0.27607	YES	YES
138	a	959.20	0.09191	YES	YES
139	a	959.67	0.24493	YES	YES
140	a	962.21	0.28781	YES	YES
141	a	963.35	0.44020	YES	YES
142	a	966.73	0.35011	YES	YES
143	a	969.92	0.42433	YES	YES
144	a	979.29	0.91266	YES	YES
145	a	981.39	1.52211	YES	YES
146	a	981.92	0.11534	YES	YES
147	a	983.01	0.49941	YES	YES
148	a	983.21	1.60952	YES	YES
149	a	984.29	0.76647	YES	YES
150	a	984.68	0.85905	YES	YES
151	a	984.85	1.61091	YES	YES
152	a	985.44	2.68676	YES	YES
153	a	985.78	1.55789	YES	YES
154	a	986.34	6.16685	YES	YES
155	a	987.01	0.06164	YES	YES
156	a	987.92	1.34339	YES	YES
157	a	989.65	4.06994	YES	YES
158	a	990.09	0.18577	YES	YES
159	a	1013.20	8.26966	YES	YES
160	a	1013.98	13.82769	YES	YES
161	a	1023.58	1.16274	YES	YES
162	a	1024.30	1.41597	YES	YES
163	a	1024.89	1.33518	YES	YES
164	a	1025.09	1.26518	YES	YES

165	a	1025.77	0.15018	YES	YES
166	a	1026.28	4.28157	YES	YES
167	a	1026.64	0.19506	YES	YES
168	a	1069.77	11.23028	YES	YES
169	a	1071.30	13.17473	YES	YES
170	a	1071.99	13.59472	YES	YES
171	a	1072.32	9.02325	YES	YES
172	a	1075.30	23.21630	YES	YES
173	a	1076.00	5.55242	YES	YES
174	a	1077.46	1.82733	YES	YES
175	a	1078.47	2.32150	YES	YES
176	a	1079.01	2.76926	YES	YES
177	a	1079.63	1.05034	YES	YES
178	a	1082.12	33.09984	YES	YES
179	a	1083.00	9.28841	YES	YES
180	a	1086.56	8.83879	YES	YES
181	a	1133.45	19.05871	YES	YES
182	a	1138.53	9.25733	YES	YES
183	a	1142.32	0.43623	YES	YES
184	a	1142.56	0.47297	YES	YES
185	a	1142.98	0.23752	YES	YES
186	a	1144.38	0.78310	YES	YES
187	a	1144.72	0.17317	YES	YES
188	a	1145.52	0.32451	YES	YES
189	a	1161.87	5.80848	YES	YES
190	a	1170.32	1.31062	YES	YES
191	a	1170.69	5.47529	YES	YES
192	a	1171.10	6.99481	YES	YES
193	a	1173.65	3.30761	YES	YES
194	a	1174.27	0.33227	YES	YES
195	a	1175.99	4.21197	YES	YES
196	a	1233.42	4.66839	YES	YES
197	a	1284.60	307.91082	YES	YES
198	a	1291.95	0.44786	YES	YES

* zero point VIBRATIONAL energy : 0.7452080 Hartree *

Cis 5_afby



bp86-SVP SCF energy: -2931.4622453700
pbe-TZVPP SCF energy: -2931.009836543

XYZ Coordinates
97

C	1.41289	-1.71239	-1.95090
C	0.54915	-1.00178	-1.21655
C	1.09041	-2.85467	-2.82086
H	2.47396	-1.39870	-1.88890
C	0.53049	-5.07661	-4.50697
C	1.85915	-4.68663	-4.26432
C	2.13661	-3.59159	-3.43184
C	-0.24823	-3.25442	-3.08014
C	-0.51849	-4.35192	-3.90873
H	0.31230	-5.93577	-5.16264
H	2.69199	-5.24108	-4.72938
H	3.18309	-3.29358	-3.24805
H	-1.07904	-2.68174	-2.63549
H	-1.56635	-4.64037	-4.09742
C	-3.21871	-0.72938	0.16301
C	-4.67199	-1.09860	0.26346
H	-5.15319	-0.74786	-0.67524
H	-5.14730	-0.58403	1.12340
H	-4.79698	-2.19753	0.34537
C	-2.56375	0.52962	-2.83818
C	-2.51622	0.81883	-4.34597
H	-3.53022	0.71466	-4.78187
H	-1.80792	0.13135	-4.85649
H	-2.15428	1.85685	-4.51876
C	-0.41723	-0.33361	3.33487
C	-1.65307	0.33648	3.47772
H	-2.30500	0.46717	2.59721
C	-2.04588	0.84021	4.73007
H	-3.01343	1.36090	4.82517
C	-1.21335	0.68669	5.85183
H	-1.52394	1.08426	6.83254
C	0.01600	0.01882	5.71754
H	0.67479	-0.11244	6.59226
C	0.41063	-0.49395	4.46993
H	1.37332	-1.02233	4.38443
C	1.88054	-1.23660	1.80495
C	2.65513	-0.10228	2.14018
H	2.16282	0.85173	2.38520
C	4.05698	-0.18074	2.18151
H	4.64211	0.71233	2.45743
C	4.70877	-1.39067	1.88243
H	5.80920	-1.45264	1.91802
C	3.94652	-2.52058	1.54410
H	4.44435	-3.47622	1.30997
C	2.54230	-2.44669	1.50770
H	1.96237	-3.34617	1.25077
C	-0.54785	-2.84048	1.89200
C	-0.94323	-3.36159	3.14295
H	-0.94597	-2.72004	4.03770
C	-1.34404	-4.70393	3.26194
H	-1.65364	-5.09258	4.24653
C	-1.35212	-5.54350	2.13596
H	-1.66753	-6.59598	2.23066
C	-0.96497	-5.03137	0.88564
H	-0.97622	-5.67429	-0.00945
C	-0.57567	-3.68793	0.76097
H	-0.29519	-3.29890	-0.22892
C	1.67832	1.91068	-1.81002
C	2.95704	1.41378	-1.46840
H	3.17728	1.10660	-0.43233
C	3.95233	1.28220	-2.45051
H	4.94819	0.90168	-2.16845
C	3.67799	1.62542	-3.78602
H	4.45888	1.51865	-4.55721
C	2.39960	2.08985	-4.13533
H	2.16924	2.34130	-5.18385
C	1.40252	2.23221	-3.15543
H	0.40004	2.58391	-3.44091
C	-0.80408	3.32239	-1.08254
C	-0.26066	4.55799	-1.50375
H	0.83166	4.69590	-1.55965
C	-1.10643	5.62168	-1.85420
H	-0.67069	6.57803	-2.18844
C	-2.50229	5.46705	-1.77436
H	-3.16741	6.30304	-2.04885
C	-3.04385	4.24511	-1.34460
H	-4.13621	4.11067	-1.28429
C	-2.20336	3.17123	-0.99876
H	-2.64892	2.21754	-0.67445
C	1.10098	2.83768	0.92449
C	2.32876	3.53341	0.88586
H	2.93856	3.53656	-0.03078
C	2.78227	4.23489	2.01758
H	3.74486	4.77150	1.97380
C	2.01394	4.25953	3.19382
H	2.37351	4.80908	4.07957
C	0.77966	3.58681	3.23199
H	0.16218	3.60412	4.14464
C	0.32747	2.88307	2.10482
H	-0.64338	2.36442	2.14311
O	-2.77666	0.39714	0.57830
O	-2.37619	-1.55479	-0.34927
O	-3.64283	0.38754	-2.25376
O	-1.36314	0.49337	-2.30814
P	0.02894	-1.07916	1.68856
P	0.34407	1.96714	-0.53571
Ru	-0.76281	-0.13314	-0.33898

Vibrational Frequencies

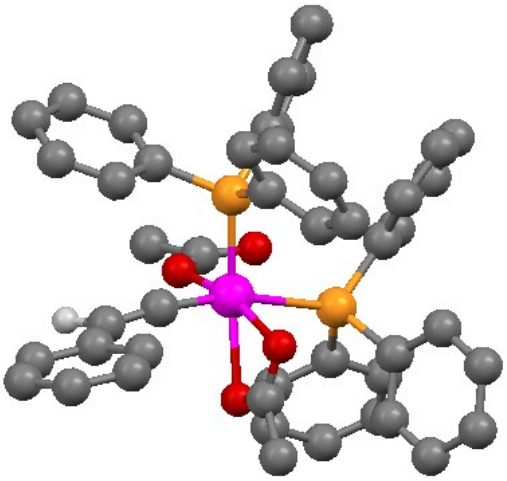
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.08	0.11371	YES	YES
8	a	13.00	0.00397	YES	YES
9	a	15.95	0.07760	YES	YES
10	a	21.43	0.72834	YES	YES
11	a	23.53	0.02097	YES	YES
12	a	29.26	0.06258	YES	YES
13	a	30.64	0.28342	YES	YES
14	a	36.98	0.29870	YES	YES
15	a	39.18	0.72413	YES	YES

16	a	45.08	0.22062	YES	YES
17	a	48.46	0.61244	YES	YES
18	a	50.36	0.31471	YES	YES
19	a	52.85	0.04030	YES	YES
20	a	55.70	0.89640	YES	YES
21	a	58.51	0.10738	YES	YES
22	a	61.67	0.25751	YES	YES
23	a	63.81	0.25552	YES	YES
24	a	67.85	0.08803	YES	YES
25	a	72.03	0.41206	YES	YES
26	a	72.21	0.07741	YES	YES
27	a	76.93	0.17604	YES	YES
28	a	83.01	0.16417	YES	YES
29	a	84.14	0.83672	YES	YES
30	a	90.68	0.08881	YES	YES
31	a	91.71	0.49124	YES	YES
32	a	98.36	0.73879	YES	YES
33	a	100.44	0.34379	YES	YES
34	a	102.62	0.41702	YES	YES
35	a	107.76	1.77023	YES	YES
36	a	113.40	3.48357	YES	YES
37	a	122.82	2.99537	YES	YES
38	a	154.65	10.11719	YES	YES
39	a	164.75	0.89314	YES	YES
40	a	172.42	1.36733	YES	YES
41	a	186.32	2.51113	YES	YES
42	a	188.64	2.22931	YES	YES
43	a	195.43	0.21813	YES	YES
44	a	210.88	1.73397	YES	YES
45	a	211.80	6.67568	YES	YES
46	a	215.54	0.45031	YES	YES
47	a	217.81	4.87267	YES	YES
48	a	223.28	1.96920	YES	YES
49	a	227.53	5.30398	YES	YES
50	a	233.27	3.58654	YES	YES
51	a	241.65	1.45429	YES	YES
52	a	243.27	2.24043	YES	YES
53	a	245.85	0.81707	YES	YES
54	a	247.45	0.99999	YES	YES
55	a	252.69	0.88959	YES	YES
56	a	263.64	0.57178	YES	YES
57	a	265.71	5.73499	YES	YES
58	a	275.39	3.80306	YES	YES
59	a	287.00	0.66321	YES	YES
60	a	317.00	14.18769	YES	YES
61	a	392.56	0.28219	YES	YES
62	a	397.36	0.05797	YES	YES
63	a	398.79	0.09529	YES	YES
64	a	401.43	0.31981	YES	YES
65	a	404.51	0.00466	YES	YES
66	a	405.24	1.08419	YES	YES
67	a	407.74	0.64643	YES	YES
68	a	414.51	41.23807	YES	YES
69	a	420.71	13.14123	YES	YES
70	a	423.08	8.96594	YES	YES
71	a	429.47	11.10313	YES	YES
72	a	436.11	1.37737	YES	YES
73	a	449.04	16.88465	YES	YES
74	a	460.21	5.64611	YES	YES
75	a	463.95	8.16186	YES	YES
76	a	475.38	18.48317	YES	YES
77	a	485.07	6.56666	YES	YES
78	a	491.69	16.46862	YES	YES
79	a	495.38	37.50030	YES	YES
80	a	498.72	17.73725	YES	YES
81	a	509.39	47.84104	YES	YES
82	a	509.86	35.62996	YES	YES
83	a	517.56	114.90354	YES	YES
84	a	526.01	94.00031	YES	YES
85	a	563.09	4.84248	YES	YES
86	a	588.22	1.31682	YES	YES
87	a	592.37	27.87272	YES	YES
88	a	607.92	0.67762	YES	YES
89	a	609.44	2.25700	YES	YES
90	a	609.54	0.13587	YES	YES
91	a	609.90	1.98209	YES	YES
92	a	610.58	0.10483	YES	YES
93	a	611.30	2.12706	YES	YES
94	a	616.12	9.42837	YES	YES
95	a	641.24	6.70263	YES	YES
96	a	644.24	10.02767	YES	YES
97	a	673.01	8.72661	YES	YES
98	a	675.18	20.65010	YES	YES
99	a	676.71	45.64168	YES	YES
100	a	684.08	9.91675	YES	YES
101	a	685.47	14.26095	YES	YES
102	a	688.08	14.46000	YES	YES
103	a	692.21	36.29381	YES	YES
104	a	693.27	36.27531	YES	YES
105	a	695.70	26.45324	YES	YES
106	a	696.37	31.12158	YES	YES
107	a	698.43	18.38831	YES	YES
108	a	698.92	40.28240	YES	YES
109	a	703.58	9.71711	YES	YES
110	a	708.47	26.08414	YES	YES
111	a	709.98	5.11502	YES	YES
112	a	737.24	11.23246	YES	YES
113	a	740.80	7.86848	YES	YES
114	a	742.61	5.50990	YES	YES
115	a	745.91	7.73951	YES	YES
116	a	746.84	1.97417	YES	YES
117	a	749.97	7.43187	YES	YES
118	a	759.72	30.61833	YES	YES
119	a	821.01	2.42258	YES	YES
120	a	824.80	0.17092	YES	YES
121	a	833.57	0.31074	YES	YES
122	a	834.53	0.72165	YES	YES
123	a	837.43	0.43509	YES	YES
124	a	838.31	0.40946	YES	YES
125	a	841.37	2.03737	YES	YES
126	a	854.09	0.92526	YES	YES
127	a	889.84	3.35915	YES	YES
128	a	904.98	0.64335	YES	YES
129	a	906.30	0.67430	YES	YES
130	a	908.31	1.21000	YES	YES
131	a	911.17	1.09806	YES	YES
132	a	914.00	0.23216	YES	YES
133	a	918.70	0.22357	YES	YES
134	a	929.95	0.35211	YES	YES
135	a	940.62	14.83350	YES	YES
136	a	948.50	0.06412	YES	YES
137	a	957.45	0.62254	YES	YES
138	a	958.88	0.42506	YES	YES
139	a	961.32	0.13324	YES	YES
140	a	963.74	0.28882	YES	YES
141	a	964.83	0.39071	YES	YES
142	a	971.66	0.14747	YES	YES
143	a	977.45	0.08536	YES	YES
144	a	980.70	0.53500	YES	YES
145	a	981.58	1.75313	YES	YES
146	a	982.11	0.63760	YES	YES
147	a	982.14	0.63530	YES	YES
148	a	983.09	3.50388	YES	YES
149	a	984.09	0.98073	YES	YES
150	a	984.29	0.87141	YES	YES
151	a	984.67	2.89786	YES	YES
152	a	985.85	0.71954	YES	YES
153	a	986.48	9.29371	YES	YES
154	a	987.15	0.06627	YES	YES
155	a	987.60	0.15739	YES	YES
156	a	988.54	0.53424	YES	YES
157	a	990.41	2.92532	YES	YES
158	a	1012.47	7.00218	YES	YES
159	a	1017.60	4.12423	YES	YES
160	a	1020.11	9.94769	YES	YES
161	a	1022.84	0.82384	YES	YES
162	a	1023.53	1.91001	YES	YES
163	a	1024.31	1.55359	YES	YES

164	a	1024.47	0.74528	YES	YES
165	a	1024.91	0.63107	YES	YES
166	a	1025.50	0.94509	YES	YES
167	a	1026.09	4.92337	YES	YES
168	a	1070.34	17.86791	YES	YES
169	a	1070.52	8.66703	YES	YES
170	a	1071.76	5.55347	YES	YES
171	a	1073.26	12.15121	YES	YES
172	a	1073.82	2.55853	YES	YES
173	a	1075.37	0.53843	YES	YES
174	a	1076.69	15.97036	YES	YES
175	a	1077.50	5.60546	YES	YES
176	a	1079.01	6.92332	YES	YES
177	a	1079.89	4.05528	YES	YES
178	a	1081.97	31.84423	YES	YES
179	a	1083.22	16.03230	YES	YES
180	a	1087.43	7.20015	YES	YES
181	a	1135.54	14.33942	YES	YES
182	a	1139.36	10.48635	YES	YES
183	a	1140.68	0.42712	YES	YES
184	a	1141.27	0.98556	YES	YES
185	a	1142.93	0.38344	YES	YES
186	a	1143.03	0.30288	YES	YES
187	a	1143.19	0.83110	YES	YES
188	a	1143.70	0.33445	YES	YES
189	a	1163.79	1.49671	YES	YES
190	a	1165.91	1.44870	YES	YES
191	a	1167.76	4.07611	YES	YES
192	a	1172.11	1.81662	YES	YES
193	a	1172.80	2.76075	YES	YES
194	a	1174.92	7.33395	YES	YES
195	a	1175.98	8.09162	YES	YES
196	a	1237.22	1.16224	YES	YES
197	a	1285.47	305.75049	YES	YES
198	a	1288.77	3.76461	YES	YES

* zero point VIBRATIONAL energy : 0.7452251 Hartree *

Cis 5_pfbx



bp86-SVP SCF energy: -2931.4361106240
pbe-TZVPP SCF energy: -2930.978771784

XYZ Coordinates
97

C	1.58527	-3.09569	-1.62853
C	1.07426	-1.95992	-1.14425
C	2.30878	-4.13768	-0.88763
H	1.40340	-3.26186	-2.71086
C	3.69519	-6.19437	0.50415
C	3.25385	-5.04422	1.18645
C	2.57048	-4.02834	0.50509
C	2.75783	-5.30155	-1.56129
C	3.44286	-6.31468	-0.87346
H	4.23282	-6.99107	1.04424
H	3.44508	-4.93695	2.26761
H	2.23394	-3.12791	1.04708
H	2.56487	-5.40567	-2.64253
H	3.78372	-7.20940	-1.42150
C	2.95478	-0.12383	0.39832
C	4.32765	-0.25502	1.00280
H	4.66081	-1.31182	0.88878
H	4.30392	-0.01197	2.08419
H	5.05034	0.39649	0.47248
C	-0.77266	1.05207	-2.98997
C	-1.15708	0.95255	-4.46709
H	-1.26287	1.96834	-4.89823
H	-2.13598	0.42942	-4.55360
H	-0.41151	0.36231	-5.03852
C	1.61499	2.70051	1.48817
C	2.99863	2.87229	1.24242
H	3.38343	2.81891	0.21238
C	3.89575	3.13341	2.29168
H	4.96641	3.27433	2.06642
C	3.43437	3.22688	3.61510
H	4.13659	3.43930	4.43836
C	2.06470	3.05875	3.87390
H	1.68090	3.14258	4.90454
C	1.16689	2.79761	2.82390
H	0.09849	2.70162	3.06386
C	-1.08467	3.15882	0.50518
C	-1.82474	2.65708	1.60013
H	-1.50294	1.73672	2.11331
C	-3.00007	3.29480	2.03032
H	-3.55428	2.88827	2.89207
C	-3.47811	4.42381	1.34645
H	-4.40220	4.92488	1.67974
C	-2.78614	4.89050	0.21592
H	-3.17207	5.75434	-0.35117
C	-1.60184	4.26310	-0.20550
H	-1.08888	4.62367	-1.10881
C	1.32097	3.41818	-1.21461
C	1.48693	4.79444	-0.93996
H	1.09280	5.22306	-0.00413
C	2.16701	5.62619	-1.84474
H	2.28015	6.69983	-1.61927
C	2.70993	5.08920	-3.02487
H	3.24955	5.74041	-3.73279
C	2.57122	3.71685	-3.29131
H	3.00555	3.28354	-4.20739
C	1.87857	2.88579	-2.39435
H	1.78567	1.81079	-2.60684
C	-3.01141	-0.26159	0.31278
C	-4.02110	-0.67132	1.21449
H	-3.83188	-1.48372	1.93257
C	-5.28018	-0.04951	1.20529
H	-6.05560	-0.38287	1.91532
C	-5.55269	0.98540	0.29314
H	-6.54461	1.46763	0.28238
C	-4.54913	1.40794	-0.59208
H	-4.73807	2.23367	-1.29698
C	-3.28209	0.79693	-0.57844
H	-2.49735	1.18297	-1.24771
C	-1.97906	-2.68402	-0.79239
C	-2.98132	-2.53215	-1.77473
H	-3.47447	-1.55757	-1.91242
C	-3.36481	-3.61898	-2.57897
H	-4.15033	-3.48034	-3.34025
C	-2.75904	-4.87460	-2.40794
H	-3.06569	-5.72911	-3.03399
C	-1.75854	-5.03507	-1.43390
H	-1.27078	-6.01378	-1.29283
C	-1.36220	-3.94679	-0.63914
H	-0.56746	-4.09378	0.10888
C	-1.23028	-1.86748	1.93163
C	-1.88856	-3.03382	2.38584
H	-2.49571	-3.63457	1.69074
C	-1.77918	-3.43944	3.72703
H	-2.29661	-4.35386	4.06233
C	-1.01712	-2.68550	4.63507
H	-0.93065	-3.00644	5.68652
C	-0.36157	-1.52420	4.19337
H	0.24745	-0.92914	4.89371
C	-0.46389	-1.11863	2.85208
H	0.08475	-0.22639	2.51431
O	1.91545	-0.45065	1.09150
O	2.78179	0.23195	-0.81184
O	-1.03207	2.07973	-2.33705
O	-0.21021	-0.02644	-2.53007
P	0.49063	2.30427	0.02186
P	-1.40770	-1.21472	0.19783
Ru	0.59146	-0.30547	-0.59554

Vibrational Frequencies

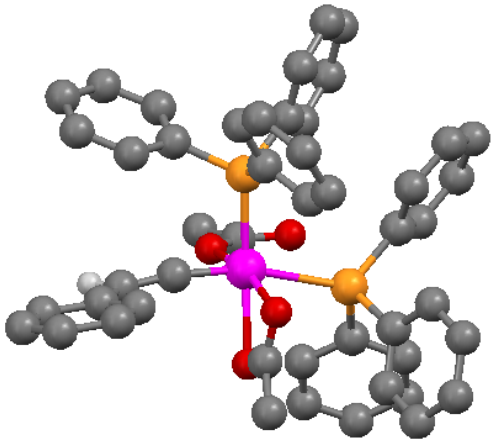
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.61	0.01775	YES	YES
8	a	16.79	0.02259	YES	YES
9	a	18.02	0.01182	YES	YES
10	a	21.60	0.01953	YES	YES
11	a	28.20	0.15122	YES	YES
12	a	32.48	0.09082	YES	YES
13	a	35.51	0.02866	YES	YES
14	a	39.43	0.41095	YES	YES
15	a	42.24	0.06847	YES	YES
16	a	45.23	0.11936	YES	YES
17	a	49.49	0.22382	YES	YES
18	a	53.05	0.06274	YES	YES

19	a	53.41	0.36829	YES	YES
20	a	57.49	0.20633	YES	YES
21	a	58.90	0.64774	YES	YES
22	a	63.20	0.16846	YES	YES
23	a	64.93	0.01380	YES	YES
24	a	68.54	0.31784	YES	YES
25	a	75.92	1.86562	YES	YES
26	a	81.15	0.54168	YES	YES
27	a	81.73	0.37293	YES	YES
28	a	87.08	1.46194	YES	YES
29	a	91.95	0.74784	YES	YES
30	a	96.46	0.20562	YES	YES
31	a	102.13	1.55969	YES	YES
32	a	108.48	1.52297	YES	YES
33	a	111.03	1.01910	YES	YES
34	a	113.11	0.73259	YES	YES
35	a	122.89	1.03383	YES	YES
36	a	130.28	0.85253	YES	YES
37	a	137.54	0.33738	YES	YES
38	a	144.81	5.15202	YES	YES
39	a	149.78	2.61944	YES	YES
40	a	170.78	4.41513	YES	YES
41	a	173.66	1.63032	YES	YES
42	a	187.41	1.85998	YES	YES
43	a	197.10	2.21166	YES	YES
44	a	198.98	0.30685	YES	YES
45	a	201.49	3.55268	YES	YES
46	a	211.41	1.15744	YES	YES
47	a	213.73	2.32929	YES	YES
48	a	220.58	1.13680	YES	YES
49	a	231.75	0.93884	YES	YES
50	a	239.39	6.04785	YES	YES
51	a	246.50	0.19628	YES	YES
52	a	250.25	2.17229	YES	YES
53	a	254.43	0.55615	YES	YES
54	a	256.71	1.17669	YES	YES
55	a	258.99	1.44940	YES	YES
56	a	265.75	0.57152	YES	YES
57	a	267.71	0.64495	YES	YES
58	a	282.98	0.53349	YES	YES
59	a	295.01	22.29711	YES	YES
60	a	326.78	16.25701	YES	YES
61	a	382.62	17.18491	YES	YES
62	a	398.42	0.44096	YES	YES
63	a	399.90	0.62667	YES	YES
64	a	401.91	0.51362	YES	YES
65	a	402.78	0.04249	YES	YES
66	a	405.46	0.02520	YES	YES
67	a	412.35	3.70282	YES	YES
68	a	413.98	1.39464	YES	YES
69	a	417.05	2.29150	YES	YES
70	a	421.14	6.31637	YES	YES
71	a	424.22	14.78863	YES	YES
72	a	432.61	12.85446	YES	YES
73	a	448.97	25.83396	YES	YES
74	a	455.27	8.62843	YES	YES
75	a	471.32	1.18578	YES	YES
76	a	475.95	1.81049	YES	YES
77	a	478.33	16.68276	YES	YES
78	a	488.18	11.33225	YES	YES
79	a	496.90	20.46776	YES	YES
80	a	506.14	24.46698	YES	YES
81	a	507.59	12.05226	YES	YES
82	a	513.54	35.77084	YES	YES
83	a	519.54	110.21874	YES	YES
84	a	522.98	73.30233	YES	YES
85	a	578.59	17.30287	YES	YES
86	a	597.42	7.87398	YES	YES
87	a	598.43	2.61525	YES	YES
88	a	608.41	0.42987	YES	YES
89	a	609.26	0.71477	YES	YES
90	a	609.72	0.56325	YES	YES
91	a	610.53	0.74782	YES	YES
92	a	611.48	1.39005	YES	YES
93	a	612.50	0.41869	YES	YES
94	a	613.33	2.42863	YES	YES
95	a	658.04	9.63684	YES	YES
96	a	663.36	5.19384	YES	YES
97	a	665.44	4.41666	YES	YES
98	a	673.32	10.14182	YES	YES
99	a	674.01	54.03679	YES	YES
100	a	677.31	11.74156	YES	YES
101	a	681.72	9.46460	YES	YES
102	a	688.99	12.44939	YES	YES
103	a	691.63	14.78102	YES	YES
104	a	695.62	29.66412	YES	YES
105	a	696.10	42.67172	YES	YES
106	a	699.40	47.31095	YES	YES
107	a	699.83	42.09411	YES	YES
108	a	702.54	28.33827	YES	YES
109	a	705.78	7.41904	YES	YES
110	a	706.83	14.33724	YES	YES
111	a	723.11	7.82464	YES	YES
112	a	734.08	9.99198	YES	YES
113	a	740.34	4.46497	YES	YES
114	a	742.06	2.10952	YES	YES
115	a	743.59	6.23641	YES	YES
116	a	746.87	6.28036	YES	YES
117	a	749.08	6.94795	YES	YES
118	a	764.03	31.71444	YES	YES
119	a	815.74	0.40050	YES	YES
120	a	828.72	1.02753	YES	YES
121	a	829.91	0.47543	YES	YES
122	a	831.85	0.76580	YES	YES
123	a	836.73	0.11560	YES	YES
124	a	841.18	0.06587	YES	YES
125	a	842.17	0.39472	YES	YES
126	a	845.78	0.90801	YES	YES
127	a	896.14	4.70326	YES	YES
128	a	900.24	0.45280	YES	YES
129	a	904.19	1.18651	YES	YES
130	a	910.49	0.38737	YES	YES
131	a	917.57	0.22154	YES	YES
132	a	918.07	0.61745	YES	YES
133	a	924.67	0.08788	YES	YES
134	a	926.65	3.57638	YES	YES
135	a	942.60	15.32710	YES	YES
136	a	952.56	0.52189	YES	YES
137	a	952.79	0.40123	YES	YES
138	a	955.24	0.18492	YES	YES
139	a	959.45	0.31793	YES	YES
140	a	964.40	0.13423	YES	YES
141	a	965.53	0.04794	YES	YES
142	a	972.12	0.35807	YES	YES
143	a	974.54	0.59085	YES	YES
144	a	977.60	0.40609	YES	YES
145	a	979.46	0.21585	YES	YES
146	a	980.06	0.45463	YES	YES
147	a	981.05	3.32129	YES	YES
148	a	982.42	1.10551	YES	YES
149	a	982.54	0.94936	YES	YES
150	a	983.58	1.09178	YES	YES
151	a	983.95	0.64181	YES	YES
152	a	984.33	2.74825	YES	YES
153	a	984.43	0.98138	YES	YES
154	a	985.09	1.70598	YES	YES
155	a	985.73	1.47789	YES	YES
156	a	988.29	0.87803	YES	YES
157	a	994.02	2.67696	YES	YES
158	a	1004.49	0.07330	YES	YES
159	a	1022.38	5.92147	YES	YES
160	a	1023.35	6.06494	YES	YES
161	a	1024.29	1.81462	YES	YES
162	a	1024.45	2.91417	YES	YES
163	a	1024.87	0.86789	YES	YES
164	a	1025.06	8.99168	YES	YES
165	a	1025.78	0.31408	YES	YES
166	a	1026.53	7.53208	YES	YES

167	a	1026.57	1.41644	YES	YES
168	a	1062.74	10.39338	YES	YES
169	a	1068.78	18.88091	YES	YES
170	a	1069.92	8.37066	YES	YES
171	a	1072.21	2.51527	YES	YES
172	a	1073.83	12.83911	YES	YES
173	a	1075.02	1.31579	YES	YES
174	a	1076.20	14.23732	YES	YES
175	a	1078.31	0.61015	YES	YES
176	a	1079.49	7.07682	YES	YES
177	a	1079.81	8.82966	YES	YES
178	a	1081.49	5.43235	YES	YES
179	a	1081.92	5.97975	YES	YES
180	a	1084.02	9.40480	YES	YES
181	a	1126.45	25.34173	YES	YES
182	a	1138.47	0.58632	YES	YES
183	a	1141.19	0.28526	YES	YES
184	a	1141.50	0.14631	YES	YES
185	a	1141.95	0.31711	YES	YES
186	a	1142.69	0.16469	YES	YES
187	a	1142.84	0.14447	YES	YES
188	a	1143.39	0.82634	YES	YES
189	a	1163.99	2.37276	YES	YES
190	a	1167.89	3.27076	YES	YES
191	a	1169.08	3.16696	YES	YES
192	a	1170.04	5.66418	YES	YES
193	a	1171.93	0.69744	YES	YES
194	a	1175.17	1.31738	YES	YES
195	a	1176.18	2.44759	YES	YES
196	a	1235.50	5.04110	YES	YES
197	a	1286.67	2.12084	YES	YES
198	a	1289.71	2.90645	YES	YES

* zero point VIBRATIONAL energy : 0.7456555 Hartree *

Cis 5_pfby



bp86-SVP SCF energy: -2931.4421210700
pbe-TZVPP SCF energy: -2930.985863222

XYZ Coordinates
97

C	1.26597	-3.09556	-1.80110
C	0.87819	-1.94489	-1.23588
C	0.49656	-3.90309	-2.76011
H	2.26504	-3.47086	-1.49883
C	-0.95501	-5.50063	-4.61022
C	-1.47361	-4.26619	-4.17317
C	-0.76117	-3.47347	-3.26342
C	1.00791	-5.14661	-3.20937
C	0.29067	-5.93371	-4.12321
H	-1.51803	-6.11891	-5.32891
H	-2.44703	-3.91232	-4.55285
H	-1.16904	-2.50299	-2.93257
H	1.98406	-5.49594	-2.83200
H	0.71039	-6.89723	-4.45859
C	2.45617	0.64312	-1.88648
C	3.74442	1.07500	-2.53715
H	4.51100	0.28129	-2.39812
H	4.12296	1.99981	-2.05207
H	3.58935	1.25724	-3.61805
C	-2.56942	-0.11210	-0.44557
C	-3.95491	-0.56395	-0.89857
H	-4.70026	0.22643	-0.67609
H	-4.23197	-1.47580	-0.32261
H	-3.97355	-0.82386	-1.97674
C	1.24497	3.48114	-1.11094
C	1.35954	3.56504	-2.51991
H	0.66978	2.99738	-3.16245
C	2.33755	4.37448	-3.11896
H	2.39601	4.42782	-4.21901
C	3.23142	5.11452	-2.32587
H	3.99736	5.75352	-2.79605
C	3.12875	5.03988	-0.92791
H	3.81263	5.62362	-0.28899
C	2.14648	4.23161	-0.32657
H	2.07739	4.21939	0.77059
C	-0.40491	3.09848	1.25455
C	0.64248	2.99602	2.20041
H	1.55329	2.42507	1.95537
C	0.53323	3.60873	3.45913
H	1.36813	3.53395	4.17457
C	-0.64298	4.29153	3.81120
H	-0.72935	4.77560	4.79829
C	-1.72129	4.32152	2.91128
H	-2.66531	4.81690	3.19418
C	-1.60752	3.72546	1.64348
H	-2.46729	3.74290	0.95732
C	-1.47255	3.02541	-1.52028
C	-1.84759	4.38888	-1.48076
H	-1.38436	5.07006	-0.74872
C	-2.79029	4.89681	-2.38809
H	-3.07631	5.96083	-2.33822
C	-3.35298	4.05822	-3.36686
H	-4.08894	4.45940	-4.08368
C	-2.95858	2.71295	-3.43635
H	-3.37783	2.05178	-4.21299
C	-2.02215	2.19766	-2.52143
H	-1.71403	1.14352	-2.58956
C	-0.00043	-0.33374	3.01682
C	1.02311	-0.39408	3.98846
H	1.95059	-0.95025	3.78452
C	0.85568	0.22843	5.23822
H	1.66132	0.16345	5.98881
C	-0.33762	0.90568	5.53576
H	-0.47692	1.37472	6.52436
C	-1.34908	0.98963	4.56294
H	-2.28247	1.53372	4.78060
C	-1.18105	0.39165	3.30432
H	-1.96864	0.47485	2.53826
C	-1.32840	-2.47609	1.58741
C	-2.01280	-2.67080	2.80893
H	-1.74074	-2.08257	3.69782
C	-3.04617	-3.61892	2.90751
H	-3.56802	-3.75333	3.86973
C	-3.40920	-4.39072	1.79137
H	-4.21994	-5.13429	1.87047
C	-2.72973	-4.20924	0.57494
H	-2.99875	-4.80948	-0.30972
C	-1.69858	-3.26069	0.47236
H	-1.17979	-3.13564	-0.48777
C	1.55898	-2.43310	1.80478
C	1.38812	-3.65834	2.48402
H	0.38089	-3.99177	2.77911
C	2.49724	-4.46845	2.78182
H	2.34564	-5.42732	3.30530
C	3.79070	-4.06306	2.41174
H	4.65974	-4.70050	2.64618
C	3.96842	-2.84330	1.73621
H	4.97912	-2.51826	1.43733
C	2.86147	-2.03304	1.42845
H	3.01090	-1.09096	0.87624
O	2.43943	0.39435	-0.61585
O	1.37780	0.48852	-2.54179
O	-2.42658	0.66170	0.51415
O	-1.59100	-0.62489	-1.14922
P	-0.11967	2.37214	-0.42213
P	0.11767	-1.30423	1.43356
Ru	0.41856	-0.30290	-0.64855

Vibrational Frequencies

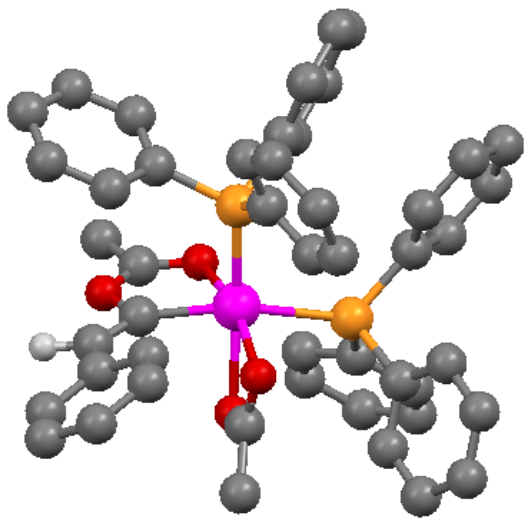
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.92	0.23681	YES	YES
8	a	16.47	0.01700	YES	YES
9	a	19.33	0.06009	YES	YES
10	a	24.47	0.03948	YES	YES
11	a	31.48	0.01519	YES	YES
12	a	34.87	0.09700	YES	YES
13	a	38.77	0.39634	YES	YES
14	a	41.56	0.66807	YES	YES
15	a	42.27	0.08585	YES	YES
16	a	46.52	0.03867	YES	YES
17	a	49.31	0.10927	YES	YES
18	a	52.06	0.16081	YES	YES
19	a	53.69	0.61635	YES	YES

20	a	57.06	0.45610	YES	YES
21	a	57.96	2.26470	YES	YES
22	a	59.47	0.69347	YES	YES
23	a	62.74	0.60777	YES	YES
24	a	66.50	0.32743	YES	YES
25	a	69.12	1.04464	YES	YES
26	a	75.56	3.08645	YES	YES
27	a	79.64	0.09038	YES	YES
28	a	83.01	1.71932	YES	YES
29	a	89.51	1.10005	YES	YES
30	a	91.21	0.23435	YES	YES
31	a	97.28	1.43914	YES	YES
32	a	99.33	1.52238	YES	YES
33	a	104.09	2.68073	YES	YES
34	a	107.88	0.21503	YES	YES
35	a	116.67	1.21297	YES	YES
36	a	120.31	1.87590	YES	YES
37	a	126.42	4.22172	YES	YES
38	a	136.72	0.50387	YES	YES
39	a	154.92	0.75672	YES	YES
40	a	178.48	2.02903	YES	YES
41	a	184.45	1.28095	YES	YES
42	a	191.64	1.29653	YES	YES
43	a	198.67	0.66595	YES	YES
44	a	201.16	1.84535	YES	YES
45	a	209.59	0.11362	YES	YES
46	a	213.32	1.55702	YES	YES
47	a	214.56	1.07947	YES	YES
48	a	219.51	0.68207	YES	YES
49	a	230.29	1.46937	YES	YES
50	a	238.51	1.90926	YES	YES
51	a	249.12	1.45245	YES	YES
52	a	252.00	0.37948	YES	YES
53	a	253.02	0.76550	YES	YES
54	a	256.31	1.42151	YES	YES
55	a	261.57	3.47669	YES	YES
56	a	266.03	1.04223	YES	YES
57	a	267.93	0.64848	YES	YES
58	a	282.53	3.80472	YES	YES
59	a	296.94	28.81226	YES	YES
60	a	326.60	19.73765	YES	YES
61	a	384.65	12.59600	YES	YES
62	a	395.67	0.06960	YES	YES
63	a	396.55	0.19972	YES	YES
64	a	398.84	0.16985	YES	YES
65	a	402.03	0.20877	YES	YES
66	a	404.83	0.60794	YES	YES
67	a	406.00	0.63041	YES	YES
68	a	415.07	14.49158	YES	YES
69	a	415.66	1.93459	YES	YES
70	a	423.96	8.85643	YES	YES
71	a	430.20	1.68909	YES	YES
72	a	436.79	9.90915	YES	YES
73	a	449.32	9.06019	YES	YES
74	a	452.59	25.77687	YES	YES
75	a	467.98	15.00030	YES	YES
76	a	479.35	1.63317	YES	YES
77	a	481.63	15.37156	YES	YES
78	a	484.62	5.97114	YES	YES
79	a	501.18	11.48471	YES	YES
80	a	503.70	7.83164	YES	YES
81	a	505.10	22.64411	YES	YES
82	a	512.38	32.01821	YES	YES
83	a	517.11	109.86116	YES	YES
84	a	522.61	79.10401	YES	YES
85	a	580.39	23.24759	YES	YES
86	a	594.05	7.45430	YES	YES
87	a	598.55	5.94749	YES	YES
88	a	607.80	0.12430	YES	YES
89	a	609.17	1.10412	YES	YES
90	a	609.81	1.02718	YES	YES
91	a	610.63	0.86069	YES	YES
92	a	610.85	1.15084	YES	YES
93	a	612.18	0.15687	YES	YES
94	a	614.53	3.84738	YES	YES
95	a	656.70	4.39431	YES	YES
96	a	664.96	2.97428	YES	YES
97	a	668.54	6.61417	YES	YES
98	a	672.46	64.97768	YES	YES
99	a	674.06	22.74347	YES	YES
100	a	677.20	5.51606	YES	YES
101	a	684.13	11.17903	YES	YES
102	a	684.53	9.34862	YES	YES
103	a	691.51	35.03929	YES	YES
104	a	692.71	23.85767	YES	YES
105	a	692.93	35.14860	YES	YES
106	a	696.66	15.24396	YES	YES
107	a	698.97	45.35271	YES	YES
108	a	701.69	36.96033	YES	YES
109	a	702.29	22.37457	YES	YES
110	a	710.28	13.78519	YES	YES
111	a	713.79	3.65686	YES	YES
112	a	735.62	18.43130	YES	YES
113	a	742.78	8.51336	YES	YES
114	a	744.80	6.00654	YES	YES
115	a	745.87	5.12743	YES	YES
116	a	748.40	4.65066	YES	YES
117	a	749.05	7.18592	YES	YES
118	a	761.45	29.52282	YES	YES
119	a	817.50	1.42004	YES	YES
120	a	828.02	0.64780	YES	YES
121	a	828.45	1.10131	YES	YES
122	a	833.70	0.08887	YES	YES
123	a	835.33	2.28296	YES	YES
124	a	840.59	1.30019	YES	YES
125	a	845.35	1.77792	YES	YES
126	a	847.10	1.14853	YES	YES
127	a	897.66	3.40860	YES	YES
128	a	901.04	0.71226	YES	YES
129	a	906.04	1.33949	YES	YES
130	a	906.98	2.31316	YES	YES
131	a	918.65	0.13254	YES	YES
132	a	920.44	0.89291	YES	YES
133	a	923.52	1.56323	YES	YES
134	a	925.47	0.84197	YES	YES
135	a	940.53	19.52206	YES	YES
136	a	953.66	0.36819	YES	YES
137	a	953.87	0.24758	YES	YES
138	a	957.67	0.28404	YES	YES
139	a	958.51	0.70169	YES	YES
140	a	967.67	0.35751	YES	YES
141	a	968.95	1.73287	YES	YES
142	a	970.17	1.12700	YES	YES
143	a	976.29	0.69199	YES	YES
144	a	978.65	1.61448	YES	YES
145	a	978.98	2.28131	YES	YES
146	a	980.24	0.18986	YES	YES
147	a	981.33	0.31674	YES	YES
148	a	981.59	1.23355	YES	YES
149	a	981.79	2.67758	YES	YES
150	a	982.39	0.98336	YES	YES
151	a	983.11	2.74588	YES	YES
152	a	983.85	1.63866	YES	YES
153	a	985.25	2.10687	YES	YES
154	a	986.03	1.32447	YES	YES
155	a	987.51	4.58788	YES	YES
156	a	988.83	0.38430	YES	YES
157	a	989.13	2.75111	YES	YES
158	a	990.22	0.43265	YES	YES
159	a	1020.22	12.15249	YES	YES
160	a	1023.40	5.93712	YES	YES
161	a	1023.82	1.52048	YES	YES
162	a	1024.15	5.67522	YES	YES
163	a	1024.62	2.60599	YES	YES
164	a	1025.31	0.83336	YES	YES
165	a	1025.64	1.62225	YES	YES
166	a	1026.17	2.35739	YES	YES
167	a	1027.06	5.36036	YES	YES

168	a	1064.21	9.50665	YES	YES
169	a	1069.29	20.78934	YES	YES
170	a	1070.87	0.11504	YES	YES
171	a	1071.98	6.82870	YES	YES
172	a	1072.19	23.38650	YES	YES
173	a	1076.06	1.30934	YES	YES
174	a	1076.54	4.43558	YES	YES
175	a	1078.32	3.76081	YES	YES
176	a	1079.12	1.53011	YES	YES
177	a	1080.32	19.28161	YES	YES
178	a	1081.50	15.12657	YES	YES
179	a	1081.85	1.30536	YES	YES
180	a	1084.95	3.67035	YES	YES
181	a	1135.72	17.80531	YES	YES
182	a	1138.83	10.50435	YES	YES
183	a	1140.40	0.10186	YES	YES
184	a	1141.05	0.55509	YES	YES
185	a	1142.26	0.13216	YES	YES
186	a	1142.46	0.63004	YES	YES
187	a	1142.84	0.36390	YES	YES
188	a	1143.49	0.36268	YES	YES
189	a	1166.71	2.70298	YES	YES
190	a	1167.39	3.89541	YES	YES
191	a	1168.79	3.06377	YES	YES
192	a	1172.35	2.44365	YES	YES
193	a	1175.36	7.95606	YES	YES
194	a	1176.58	8.68691	YES	YES
195	a	1178.89	3.21698	YES	YES
196	a	1237.86	4.84358	YES	YES
197	a	1287.85	4.28995	YES	YES
198	a	1290.27	0.27010	YES	YES

* zero point VIBRATIONAL energy : 0.7455634 Hartree *

Cis 6_pfx



bp86-SVP SCF energy: -2931.4672271700
pbe-TZVPP SCF energy: -2931.016527809

XYZ Coordinates
97

C	1.56461	-3.08321	-1.65149
C	0.82925	-1.92811	-1.69750
C	2.29146	-3.73799	-0.56047
H	1.61001	-3.63718	-2.60960
C	3.72777	-5.17656	1.44641
C	2.78393	-4.19638	1.80368
C	2.07529	-3.48978	0.82126
C	3.23702	-4.74629	-0.89876
C	3.94826	-5.44871	0.08402
H	4.28120	-5.72988	2.22348
H	2.58937	-3.97822	2.86715
H	1.34551	-2.72635	1.12261
H	3.41323	-4.97327	-1.96469
H	4.67843	-6.21975	-0.21585
C	2.97799	-0.19732	-0.20837
C	4.43755	-0.43104	0.07808
H	4.67453	-1.49505	-0.14788
H	4.65855	-0.25185	1.15000
H	5.06983	0.21539	-0.56341
C	-0.48751	-0.80331	-3.32682
C	-1.14543	-0.79331	-4.67748
H	-0.39114	-0.96365	-5.47570
H	-1.65928	0.17350	-4.84258
H	-1.88548	-1.62155	-4.74013
C	1.82365	2.59421	1.26996
C	3.16373	2.70165	0.82918
H	3.39532	2.61646	-0.24384
C	4.20529	2.93284	1.74301
H	5.24109	3.02022	1.37383
C	3.93287	3.05642	3.11592
H	4.75077	3.24064	3.83229
C	2.60606	2.95299	3.56442
H	2.37317	3.06167	4.63712
C	1.56224	2.72399	2.65079
H	0.52996	2.67234	3.02948
C	-0.98333	3.08793	0.75658
C	-1.63941	2.50352	1.86446
H	-1.30859	1.52495	2.24738
C	-2.72586	3.14352	2.48203
H	-3.21393	2.66932	3.34893
C	-3.19923	4.36930	1.98425
H	-4.05661	4.86998	2.46398
C	-2.58106	4.94222	0.86107
H	-2.95233	5.89638	0.45063
C	-1.48221	4.30943	0.25312
H	-1.01329	4.77821	-0.62462
C	0.98317	3.37725	-1.34906
C	1.49686	4.66504	-1.06538
H	1.62560	4.98885	-0.02009
C	1.85099	5.53915	-2.10532
H	2.25188	6.53841	-1.86550
C	1.69957	5.14132	-3.44601
H	1.98382	5.82639	-4.26236
C	1.19029	3.86590	-3.73682
H	1.07396	3.54281	-4.78483
C	0.83545	2.98872	-2.69592
H	0.44241	1.98797	-2.92594
C	-2.95829	-0.01054	0.33246
C	-3.95941	-0.20136	1.30871
H	-3.81052	-0.93090	2.12014
C	-5.15121	0.54133	1.26517
H	-5.92106	0.38198	2.03903
C	-5.36139	1.48250	0.24299
H	-6.29712	2.06530	0.20955
C	-4.36936	1.68092	-0.73151
H	-4.52171	2.42299	-1.53275
C	-3.17313	0.94444	-0.68472
H	-2.39546	1.10663	-1.44721
C	-2.09112	-2.57678	-0.54008
C	-3.20355	-2.50959	-1.40761
H	-3.72994	-1.55381	-1.55612
C	-3.66256	-3.65867	-2.07717
H	-4.53756	-3.58576	-2.74501
C	-3.02236	-4.89366	-1.88288
H	-3.38653	-5.79643	-2.40133
C	-1.91539	-4.97092	-1.01974
H	-1.40136	-5.93324	-0.86015
C	-1.44738	-3.82259	-0.36108
H	-0.57428	-3.90566	0.30485
C	-1.17891	-1.58710	2.04260
C	-1.96518	-2.60241	2.63536
H	-2.71937	-3.13837	2.03686
C	-1.78278	-2.94963	3.98487
H	-2.40237	-3.74517	4.43177
C	-0.81182	-2.29208	4.76040
H	-0.66807	-2.56865	5.81833
C	-0.01595	-1.29239	4.17610
H	0.76180	-0.78312	4.76876
C	-0.19407	-0.94477	2.82564
H	0.46288	-0.19188	2.36159
O	2.08343	-0.55346	0.64239
O	2.57684	0.29950	-1.31758
O	0.22953	-1.86112	-3.05064
O	-0.62031	0.14543	-2.50624
P	0.48540	2.20231	0.01389
P	-1.39516	-1.04146	0.27359
Ru	0.48493	-0.18529	-0.72331

Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	11.13	0.01251	YES	YES
8	a	20.20	0.10303	YES	YES
9	a	24.47	0.01309	YES	YES
10	a	30.64	0.11817	YES	YES
11	a	36.07	0.11660	YES	YES
12	a	36.97	0.04449	YES	YES
13	a	42.85	0.01621	YES	YES
14	a	45.04	0.04868	YES	YES
15	a	45.26	1.51755	YES	YES

16	a	49.68	0.07117	YES	YES
17	a	53.66	0.24066	YES	YES
18	a	54.60	0.13362	YES	YES
19	a	60.60	0.15856	YES	YES
20	a	65.25	0.21062	YES	YES
21	a	65.74	0.19663	YES	YES
22	a	68.05	0.14163	YES	YES
23	a	71.66	0.07108	YES	YES
24	a	75.40	0.59815	YES	YES
25	a	77.48	0.25425	YES	YES
26	a	80.71	0.30156	YES	YES
27	a	83.31	1.13076	YES	YES
28	a	89.22	0.38965	YES	YES
29	a	93.25	0.52955	YES	YES
30	a	100.83	0.56262	YES	YES
31	a	104.20	0.70036	YES	YES
32	a	109.08	0.58550	YES	YES
33	a	112.61	0.96932	YES	YES
34	a	118.69	0.28939	YES	YES
35	a	135.93	0.14319	YES	YES
36	a	141.37	4.53442	YES	YES
37	a	156.90	0.36770	YES	YES
38	a	181.56	1.65866	YES	YES
39	a	183.42	1.77299	YES	YES
40	a	193.82	0.41963	YES	YES
41	a	199.21	1.82950	YES	YES
42	a	199.66	0.80713	YES	YES
43	a	205.57	0.63509	YES	YES
44	a	212.01	2.11229	YES	YES
45	a	215.70	3.37628	YES	YES
46	a	221.32	2.06589	YES	YES
47	a	226.84	1.17437	YES	YES
48	a	227.65	1.69503	YES	YES
49	a	240.44	2.56746	YES	YES
50	a	244.34	0.45285	YES	YES
51	a	248.57	0.07058	YES	YES
52	a	249.54	0.08330	YES	YES
53	a	253.00	1.06434	YES	YES
54	a	264.55	0.16666	YES	YES
55	a	265.73	0.59102	YES	YES
56	a	300.44	4.15783	YES	YES
57	a	315.54	5.64818	YES	YES
58	a	318.97	6.83596	YES	YES
59	a	324.31	0.95401	YES	YES
60	a	356.36	7.98941	YES	YES
61	a	396.61	0.65817	YES	YES
62	a	398.79	0.18933	YES	YES
63	a	399.31	0.14911	YES	YES
64	a	403.49	27.54593	YES	YES
65	a	404.02	2.20399	YES	YES
66	a	410.82	2.21597	YES	YES
67	a	411.47	0.49409	YES	YES
68	a	415.28	1.34575	YES	YES
69	a	418.53	5.87093	YES	YES
70	a	420.36	21.91116	YES	YES
71	a	436.45	16.88668	YES	YES
72	a	445.84	19.82347	YES	YES
73	a	453.62	9.91464	YES	YES
74	a	470.21	1.79173	YES	YES
75	a	480.73	16.64243	YES	YES
76	a	482.58	7.97259	YES	YES
77	a	497.75	4.54703	YES	YES
78	a	502.14	37.85452	YES	YES
79	a	511.27	53.98459	YES	YES
80	a	512.41	29.22050	YES	YES
81	a	515.71	102.58606	YES	YES
82	a	523.35	27.37249	YES	YES
83	a	527.43	74.48333	YES	YES
84	a	562.12	6.24389	YES	YES
85	a	599.18	1.44825	YES	YES
86	a	601.33	4.88395	YES	YES
87	a	608.59	0.64321	YES	YES
88	a	610.18	0.67630	YES	YES
89	a	610.25	0.22233	YES	YES
90	a	610.66	0.78354	YES	YES
91	a	611.32	1.55781	YES	YES
92	a	611.74	6.90185	YES	YES
93	a	612.76	0.75035	YES	YES
94	a	615.32	0.52457	YES	YES
95	a	667.72	10.07167	YES	YES
96	a	670.00	24.82305	YES	YES
97	a	672.54	26.56795	YES	YES
98	a	676.92	8.60544	YES	YES
99	a	678.48	13.91720	YES	YES
100	a	684.01	9.32680	YES	YES
101	a	686.06	10.95932	YES	YES
102	a	692.51	0.30237	YES	YES
103	a	696.88	47.17939	YES	YES
104	a	698.67	65.23168	YES	YES
105	a	698.86	16.81903	YES	YES
106	a	699.97	17.64205	YES	YES
107	a	701.03	32.01561	YES	YES
108	a	705.44	10.51073	YES	YES
109	a	707.00	16.00353	YES	YES
110	a	736.44	10.58414	YES	YES
111	a	739.57	3.27351	YES	YES
112	a	741.41	1.40072	YES	YES
113	a	744.05	4.34225	YES	YES
114	a	747.22	5.94647	YES	YES
115	a	747.96	5.71992	YES	YES
116	a	751.02	6.92841	YES	YES
117	a	774.00	60.13881	YES	YES
118	a	821.97	10.30918	YES	YES
119	a	833.78	1.03891	YES	YES
120	a	835.60	4.61335	YES	YES
121	a	837.63	0.95790	YES	YES
122	a	838.16	2.40582	YES	YES
123	a	841.10	0.58887	YES	YES
124	a	844.41	0.29016	YES	YES
125	a	845.18	0.37532	YES	YES
126	a	849.28	12.43277	YES	YES
127	a	901.13	7.05210	YES	YES
128	a	903.17	0.32625	YES	YES
129	a	909.68	1.22108	YES	YES
130	a	911.40	0.50897	YES	YES
131	a	915.83	3.03312	YES	YES
132	a	918.83	0.92605	YES	YES
133	a	921.49	0.66624	YES	YES
134	a	943.43	12.38791	YES	YES
135	a	952.35	0.18305	YES	YES
136	a	956.09	0.41032	YES	YES
137	a	959.56	0.09695	YES	YES
138	a	962.07	0.05414	YES	YES
139	a	964.22	0.57631	YES	YES
140	a	966.54	0.03352	YES	YES
141	a	968.99	0.06338	YES	YES
142	a	973.85	0.62425	YES	YES
143	a	979.99	12.37997	YES	YES
144	a	980.97	0.20191	YES	YES
145	a	981.66	0.20936	YES	YES
146	a	981.83	1.64372	YES	YES
147	a	982.03	0.17915	YES	YES
148	a	983.09	2.39973	YES	YES
149	a	983.47	1.36101	YES	YES
150	a	983.75	1.73082	YES	YES
151	a	984.03	2.41784	YES	YES
152	a	984.27	0.58780	YES	YES
153	a	984.47	0.55330	YES	YES
154	a	985.25	1.26606	YES	YES
155	a	985.39	0.44805	YES	YES
156	a	988.52	0.11539	YES	YES
157	a	990.04	1.64125	YES	YES
158	a	1008.87	26.06058	YES	YES
159	a	1019.22	7.41971	YES	YES
160	a	1021.78	13.71917	YES	YES
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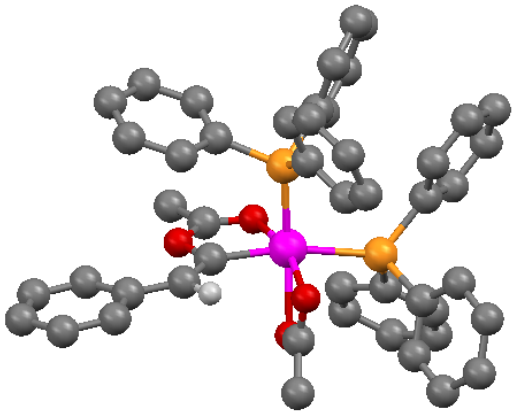
162	a	1023.94	1.64163	YES	YES
163	a	1024.17	1.35049	YES	YES

164	a	1024.60	0.60337	YES	YES
165	a	1025.14	1.90545	YES	YES
166	a	1026.16	1.57391	YES	YES
167	a	1028.03	2.71316	YES	YES
168	a	1067.06	10.60767	YES	YES
169	a	1069.66	8.50750	YES	YES
170	a	1071.10	23.85157	YES	YES
171	a	1071.34	17.10869	YES	YES
172	a	1072.57	2.73616	YES	YES
173	a	1073.05	13.37977	YES	YES
174	a	1074.38	2.89335	YES	YES
175	a	1074.53	5.57396	YES	YES
176	a	1076.23	1.47252	YES	YES
177	a	1078.01	0.99011	YES	YES
178	a	1078.67	2.15032	YES	YES
179	a	1079.52	14.66460	YES	YES
180	a	1080.99	15.26246	YES	YES
181	a	1136.19	0.20372	YES	YES
182	a	1139.52	0.20095	YES	YES
183	a	1140.84	0.38896	YES	YES
184	a	1140.99	0.25579	YES	YES
185	a	1141.29	0.47741	YES	YES
186	a	1141.39	0.61738	YES	YES
187	a	1141.67	0.20169	YES	YES
188	a	1162.47	2.40131	YES	YES
189	a	1163.83	1.14817	YES	YES
190	a	1168.44	5.12371	YES	YES
191	a	1169.43	5.60586	YES	YES
192	a	1171.06	10.11731	YES	YES
193	a	1172.93	2.03071	YES	YES
194	a	1173.53	0.94620	YES	YES
195	a	1214.47	1.67175	YES	YES
196	a	1279.06	7.65087	YES	YES
197	a	1284.16	3.62883	YES	YES
198	a	1289.90	3.02152	YES	YES

* zero point VIBRATIONAL energy : 0.7483016 Hartree *

Cis 6_pfy



bp86-SVP SCF energy: -2931.4715120890
pbe-TZVPP SCF energy: -2931.020259722

XYZ Coordinates
97

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C	-0.43805	-2.17098	-1.03809
C	0.22312	-4.54643	-1.88678
H	1.44407	-2.77993	-1.59377
C	0.08153	-7.29417	-2.67332
C	-1.06717	-6.61321	-2.23064
C	-1.00357	-5.26700	-1.84350
C	1.37158	-5.25833	-2.33577
C	1.30549	-6.60355	-2.72212
H	0.02315	-8.35262	-2.97696
H	-2.03498	-7.14186	-2.18551
H	-1.91521	-4.76020	-1.50085
H	2.33861	-4.72784	-2.37919
H	2.21896	-7.11831	-3.06564
C	1.23430	-0.20593	-2.76338
C	2.11023	-0.40796	-3.97387
H	2.17669	-1.49810	-4.19084
H	3.13467	-0.02714	-3.78431
H	1.66905	0.09079	-4.86031
C	-2.65963	-1.63151	-0.50846
C	-4.09142	-2.05489	-0.35350
H	-4.48026	-2.45621	-1.31492
H	-4.70775	-1.19337	-0.03201
H	-4.16474	-2.86929	0.40007
C	1.37146	2.97043	-1.60316
C	1.43186	2.88308	-3.01425
H	0.57569	2.47512	-3.57377
C	2.56599	3.32617	-3.71507
H	2.58508	3.25546	-4.81565
C	3.66549	3.86132	-3.02301
H	4.55438	4.21176	-3.57359
C	3.61567	3.95452	-1.62262
H	4.46448	4.38561	-1.06533
C	2.48051	3.51371	-0.91964
H	2.46066	3.62254	0.17544
C	-0.22027	3.38636	0.78228
C	0.69340	3.16576	1.83832
H	1.41311	2.33327	1.77917
C	0.69004	3.98280	2.97994
H	1.41941	3.79429	3.78449
C	-0.25000	5.01982	3.10339
H	-0.25831	5.65760	4.00290
C	-1.18767	5.22573	2.07893
H	-1.94100	6.02631	2.17045
C	-1.17240	4.41913	0.92740
H	-1.91516	4.60259	0.13622
C	-1.48307	2.99239	-1.79568
C	-1.38129	4.28865	-2.35411
H	-0.48234	4.89877	-2.16995
C	-2.41566	4.80856	-3.14857
H	-2.31910	5.82011	-3.57764
C	-3.56794	4.04176	-3.39966
H	-4.37740	4.44824	-4.02897
C	-3.67789	2.75491	-2.84931
H	-4.57464	2.14386	-3.04584
C	-2.64207	2.23245	-2.05346
H	-2.72780	1.22105	-1.62943
C	-0.54333	0.36209	2.89042
C	0.00657	0.49045	4.18374
H	0.97463	0.02332	4.42469
C	-0.66522	1.22345	5.17615
H	-0.21830	1.31767	6.18032
C	-1.89819	1.83513	4.89197
H	-2.42422	2.41155	5.67121
C	-2.45180	1.71484	3.60664
H	-3.41408	2.19864	3.37059
C	-1.77707	0.98816	2.61063
H	-2.21005	0.90294	1.60126
C	-0.33723	-2.37017	2.11257
C	-1.55802	-2.53280	2.80379
H	-2.14115	-1.64913	3.10818
C	-2.03362	-3.81659	3.12892
H	-2.98385	-3.92146	3.67950
C	-1.29574	-4.95598	2.76872
H	-1.66629	-5.96256	3.02473
C	-0.07763	-4.80511	2.08302
H	0.50880	-5.69201	1.79245
C	0.39689	-3.52510	1.75452
H	1.35185	-3.42565	1.21643
C	2.04683	-0.71001	2.02028
C	2.54339	-1.47965	3.09812
H	1.86392	-2.12858	3.67415
C	3.90706	-1.44100	3.43479
H	4.27815	-2.04922	4.27684
C	4.79493	-0.63780	2.69812
H	5.86588	-0.61240	2.96035
C	4.31293	0.11892	1.61732
H	5.00347	0.73705	1.01999
C	2.94965	0.08057	1.27648
H	2.58689	0.64188	0.40148
O	1.73066	-0.29679	-1.57990
O	-0.02237	0.00123	-2.86916
O	-1.82509	-2.57709	-0.89119
O	-2.27390	-0.45192	-0.29766
P	-0.13387	2.27952	-0.71964
P	0.24456	-0.68392	1.55207
Ru	-0.18692	-0.20919	-0.64946

Vibrational Frequencies

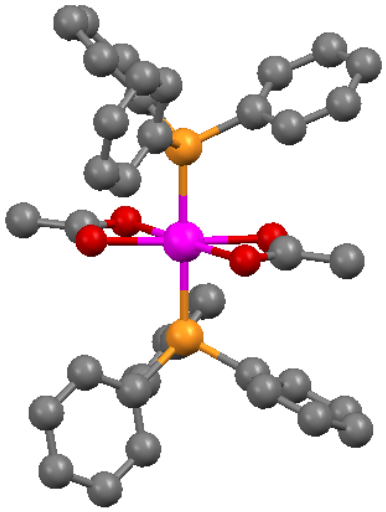
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.29	0.01314	YES	YES
8	a	18.59	0.05282	YES	YES
9	a	22.50	0.02170	YES	YES
10	a	27.21	0.08145	YES	YES
11	a	30.23	0.07658	YES	YES
12	a	36.20	0.31492	YES	YES
13	a	40.05	0.63062	YES	YES
14	a	40.57	0.69717	YES	YES
15	a	44.59	0.19878	YES	YES
16	a	46.41	0.13772	YES	YES
17	a	50.85	0.23019	YES	YES
18	a	53.54	0.03001	YES	YES
19	a	56.17	0.14188	YES	YES

20	a	60.99	0.11299	YES	YES
21	a	66.24	0.08047	YES	YES
22	a	67.51	0.14748	YES	YES
23	a	72.11	0.52655	YES	YES
24	a	74.03	0.08463	YES	YES
25	a	77.16	0.40847	YES	YES
26	a	80.53	0.12145	YES	YES
27	a	84.67	1.52556	YES	YES
28	a	91.23	0.55546	YES	YES
29	a	96.56	0.10127	YES	YES
30	a	99.43	1.21741	YES	YES
31	a	102.95	0.17618	YES	YES
32	a	108.85	0.93869	YES	YES
33	a	114.64	0.48148	YES	YES
34	a	115.38	0.08071	YES	YES
35	a	121.43	0.37116	YES	YES
36	a	131.77	2.02358	YES	YES
37	a	152.76	0.09543	YES	YES
38	a	174.54	2.53136	YES	YES
39	a	186.63	0.28266	YES	YES
40	a	186.80	2.34464	YES	YES
41	a	199.48	0.57650	YES	YES
42	a	200.07	0.52926	YES	YES
43	a	203.26	1.06175	YES	YES
44	a	210.94	0.23049	YES	YES
45	a	215.75	5.52426	YES	YES
46	a	222.21	2.04554	YES	YES
47	a	226.98	1.55894	YES	YES
48	a	228.71	1.67863	YES	YES
49	a	244.48	0.54533	YES	YES
50	a	247.92	0.16582	YES	YES
51	a	248.28	0.37227	YES	YES
52	a	249.98	2.93502	YES	YES
53	a	251.51	1.53938	YES	YES
54	a	265.09	0.18386	YES	YES
55	a	266.22	0.60801	YES	YES
56	a	286.13	4.70629	YES	YES
57	a	299.10	1.86293	YES	YES
58	a	315.58	10.29894	YES	YES
59	a	326.06	5.12399	YES	YES
60	a	349.59	6.91469	YES	YES
61	a	397.87	0.60619	YES	YES
62	a	398.50	0.09659	YES	YES
63	a	399.39	0.39887	YES	YES
64	a	402.83	1.31167	YES	YES
65	a	403.16	36.50406	YES	YES
66	a	405.23	0.04210	YES	YES
67	a	410.20	0.58137	YES	YES
68	a	411.98	0.50216	YES	YES
69	a	418.89	7.19275	YES	YES
70	a	420.86	24.75626	YES	YES
71	a	436.91	12.87545	YES	YES
72	a	448.41	18.54508	YES	YES
73	a	454.05	9.52445	YES	YES
74	a	473.47	2.94067	YES	YES
75	a	480.59	14.14703	YES	YES
76	a	484.47	7.82322	YES	YES
77	a	496.55	6.69207	YES	YES
78	a	500.34	29.51183	YES	YES
79	a	506.35	27.58500	YES	YES
80	a	512.40	56.22939	YES	YES
81	a	516.39	145.15681	YES	YES
82	a	526.37	102.57183	YES	YES
83	a	550.97	14.75519	YES	YES
84	a	574.55	1.57550	YES	YES
85	a	596.56	1.55009	YES	YES
86	a	608.57	0.43109	YES	YES
87	a	609.32	0.41617	YES	YES
88	a	610.20	0.17390	YES	YES
89	a	610.71	1.48127	YES	YES
90	a	611.08	1.69002	YES	YES
91	a	612.08	0.36336	YES	YES
92	a	612.42	0.68170	YES	YES
93	a	617.53	1.77531	YES	YES
94	a	661.12	21.51462	YES	YES
95	a	668.07	4.64521	YES	YES
96	a	670.55	6.10281	YES	YES
97	a	672.98	28.95904	YES	YES
98	a	678.04	5.87187	YES	YES
99	a	678.65	19.64252	YES	YES
100	a	684.96	8.40592	YES	YES
101	a	687.76	13.53516	YES	YES
102	a	690.65	29.94278	YES	YES
103	a	696.88	29.56600	YES	YES
104	a	697.86	77.65364	YES	YES
105	a	698.52	15.52667	YES	YES
106	a	700.72	32.05545	YES	YES
107	a	705.38	9.82891	YES	YES
108	a	707.17	14.61463	YES	YES
109	a	717.32	6.66938	YES	YES
110	a	736.72	9.53969	YES	YES
111	a	739.12	2.70380	YES	YES
112	a	741.33	2.13829	YES	YES
113	a	744.89	3.25219	YES	YES
114	a	747.39	6.65942	YES	YES
115	a	748.51	6.84472	YES	YES
116	a	756.70	14.15212	YES	YES
117	a	800.46	4.97880	YES	YES
118	a	822.08	0.90732	YES	YES
119	a	832.02	0.83490	YES	YES
120	a	833.94	1.02241	YES	YES
121	a	838.43	0.22609	YES	YES
122	a	840.34	1.08188	YES	YES
123	a	844.35	0.48935	YES	YES
124	a	845.92	0.47374	YES	YES
125	a	859.57	10.22815	YES	YES
126	a	861.63	40.78909	YES	YES
127	a	901.21	3.04713	YES	YES
128	a	902.04	6.04009	YES	YES
129	a	903.25	0.11849	YES	YES
130	a	911.09	0.07003	YES	YES
131	a	914.02	3.74305	YES	YES
132	a	919.24	0.49427	YES	YES
133	a	920.01	0.16256	YES	YES
134	a	941.24	14.22659	YES	YES
135	a	951.33	0.11501	YES	YES
136	a	952.78	0.64733	YES	YES
137	a	956.38	0.44533	YES	YES
138	a	961.69	0.24252	YES	YES
139	a	963.35	0.18617	YES	YES
140	a	966.97	0.08029	YES	YES
141	a	967.51	0.05852	YES	YES
142	a	972.95	0.16117	YES	YES
143	a	979.52	5.82302	YES	YES
144	a	979.65	6.06824	YES	YES
145	a	980.78	1.17361	YES	YES
146	a	980.98	3.44033	YES	YES
147	a	981.47	2.22875	YES	YES
148	a	981.64	1.11342	YES	YES
149	a	982.39	2.33824	YES	YES
150	a	982.63	0.50100	YES	YES
151	a	983.07	3.27784	YES	YES
152	a	983.49	0.57682	YES	YES
153	a	983.87	0.93600	YES	YES
154	a	984.91	0.14840	YES	YES
155	a	985.88	0.54998	YES	YES
156	a	987.90	0.05763	YES	YES
157	a	989.58	1.58794	YES	YES
158	a	1005.57	22.85591	YES	YES
159	a	1017.53	9.92115	YES	YES
160	a	1021.14	12.26897	YES	YES
161	a	1023.29	2.14715	YES	YES
162	a	1023.61	1.36248	YES	YES
163	a	1024.28	0.40089	YES	YES
164	a	1024.43	1.32230	YES	YES
165	a	1025.01	1.99051	YES	YES
166	a	1026.05	1.93202	YES	YES
167	a	1029.23	8.27704	YES	YES

168	a	1068.01	10.89257	YES	YES
169	a	1069.85	18.48532	YES	YES
170	a	1071.23	11.37501	YES	YES
171	a	1072.66	13.48671	YES	YES
172	a	1073.75	5.72745	YES	YES
173	a	1074.17	7.23040	YES	YES
174	a	1074.90	14.33684	YES	YES
175	a	1075.24	3.67529	YES	YES
176	a	1076.36	1.14458	YES	YES
177	a	1077.92	8.46554	YES	YES
178	a	1079.60	0.10508	YES	YES
179	a	1079.78	15.49916	YES	YES
180	a	1081.18	15.25800	YES	YES
181	a	1136.91	0.19336	YES	YES
182	a	1139.77	0.16430	YES	YES
183	a	1141.09	0.64058	YES	YES
184	a	1141.37	0.17137	YES	YES
185	a	1141.75	0.60128	YES	YES
186	a	1141.94	0.23173	YES	YES
187	a	1141.96	0.24030	YES	YES
188	a	1163.78	0.90977	YES	YES
189	a	1166.04	2.58111	YES	YES
190	a	1168.39	3.91658	YES	YES
191	a	1168.88	3.37150	YES	YES
192	a	1169.95	5.29748	YES	YES
193	a	1170.76	10.41933	YES	YES
194	a	1175.56	1.35657	YES	YES
195	a	1203.57	6.89349	YES	YES
196	a	1235.09	34.37948	YES	YES
197	a	1287.74	3.99643	YES	YES
198	a	1290.47	2.80760	YES	YES

* zero point VIBRATIONAL energy : 0.7483399 Hartree *

Trans 1



bp86-SVP SCF energy: -2623.2601605370
pbe-TZVPP SCF energy: -2622.860836864

XYZ Coordinates
83

C	-2.60563	-0.08249	-0.26680
C	-4.10851	-0.08126	-0.37639
H	-4.47717	0.96926	-0.38954
H	-4.55792	-0.58934	0.50118
H	-4.42957	-0.57759	-1.31446
C	2.45466	0.03896	0.33669
C	3.93606	0.12146	0.59120
H	4.21419	-0.53427	1.44272
H	4.20445	1.16753	0.85959
H	4.50167	-0.17031	-0.31608
C	0.07372	-3.16014	-1.72456
C	-0.19894	-2.38170	-2.86920
H	-0.46741	-1.32189	-2.74463
C	-0.12887	-2.95695	-4.15042
H	-0.34095	-2.33705	-5.03738
C	0.21478	-4.31036	-4.30245
H	0.27266	-4.75856	-5.30870
C	0.49252	-5.09180	-3.16630
H	0.76904	-6.15380	-3.27789
C	0.42541	-4.52067	-1.88509
H	0.65787	-5.13927	-1.00237
C	-1.49393	-3.17103	0.75403
C	-2.25929	-4.18434	0.13813
H	-1.98838	-4.54600	-0.86590
C	-3.37361	-4.73586	0.79536
H	-3.96229	-5.52500	0.29829
C	-3.73498	-4.28591	2.07623
H	-4.60718	-4.72213	2.59133
C	-2.98674	-3.26671	2.69199
H	-3.27310	-2.89506	3.69000
C	-1.88335	-2.70213	2.03118
H	-1.32800	-1.87406	2.49917
C	1.42824	-3.17652	0.80226
C	1.34768	-3.73955	2.09316
H	0.38465	-3.76581	2.62684
C	2.48809	-4.28685	2.70651
H	2.40428	-4.72825	3.71373
C	3.72490	-4.27998	2.04052
H	4.61735	-4.71422	2.52134
C	3.81500	-3.72028	0.75396
H	4.77942	-3.71433	0.21861
C	2.67820	-3.16962	0.13994
H	2.76086	-2.73628	-0.86976
C	-0.98122	3.04999	1.42592
C	-1.86899	4.14355	1.35399
H	-2.04263	4.65350	0.39327
C	-2.54717	4.58627	2.50416
H	-3.24256	5.43936	2.43135
C	-2.34149	3.94668	3.73756
H	-2.87274	4.29656	4.63861
C	-1.46401	2.85014	3.81503
H	-1.30718	2.33387	4.77691
C	-0.79778	2.39472	2.66623
H	-0.13673	1.51400	2.71991
C	1.63950	3.12178	0.13850
C	2.11214	3.69851	1.33537
H	1.45793	3.74833	2.22016
C	3.41556	4.22331	1.40766
H	3.76745	4.67719	2.34930
C	4.26139	4.17797	0.28659
H	5.28069	4.59526	0.34315
C	3.79932	3.59779	-0.90884
H	4.45589	3.55396	-1.79377
C	2.50149	3.06730	-0.98160
H	2.15219	2.60880	-1.92066
C	-0.69380	3.34234	-1.48196
C	-0.38556	4.71601	-1.62703
H	0.24575	5.22195	-0.87817
C	-0.86661	5.44246	-2.72807
H	-0.61614	6.51197	-2.82867
C	-1.65671	4.80669	-3.70273
H	-2.02908	5.37647	-4.57069
C	-1.96073	3.44220	-3.56930
H	-2.57168	2.93444	-4.33443
C	-1.48250	2.71031	-2.46687
H	-1.71691	1.63809	-2.36651
O	-2.01691	0.03932	0.86047
O	-1.85473	-0.16755	-1.30410
O	1.61093	0.09222	1.30212
O	1.96688	-0.05927	-0.84450
P	-0.02062	-2.36757	-0.04535
P	-0.05464	2.36356	-0.03186
Ru	-0.05742	-0.00876	-0.03795

Vibrational Frequencies

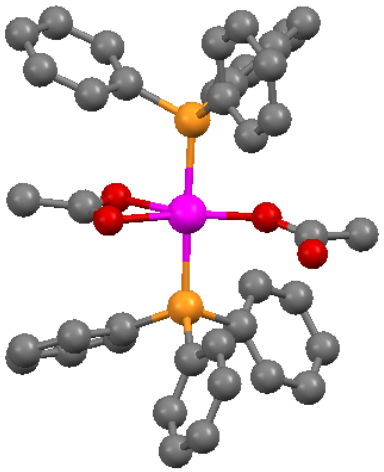
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	1.33	0.05030	YES	YES
8	a	11.04	0.02501	YES	YES
9	a	19.82	0.21452	YES	YES
10	a	26.13	0.32027	YES	YES
11	a	30.16	0.02033	YES	YES
12	a	31.76	0.33531	YES	YES
13	a	33.24	0.26828	YES	YES
14	a	40.02	0.06613	YES	YES
15	a	40.73	0.24668	YES	YES
16	a	43.43	0.11023	YES	YES
17	a	55.07	0.18686	YES	YES
18	a	56.07	0.02358	YES	YES
19	a	59.94	0.10915	YES	YES
20	a	63.09	0.37726	YES	YES
21	a	67.22	1.29497	YES	YES
22	a	69.53	0.53741	YES	YES
23	a	71.54	0.61093	YES	YES
24	a	77.40	0.14206	YES	YES
25	a	79.02	0.81746	YES	YES
26	a	81.81	0.16033	YES	YES
27	a	85.41	0.10629	YES	YES
28	a	94.83	0.33334	YES	YES
29	a	109.29	2.16924	YES	YES
30	a	110.34	2.12401	YES	YES

31	a	132.64	4.91348	YES	YES
32	a	144.60	0.16848	YES	YES
33	a	157.92	0.06404	YES	YES
34	a	167.50	4.89193	YES	YES
35	a	187.54	0.33306	YES	YES
36	a	191.04	1.99578	YES	YES
37	a	193.87	0.23883	YES	YES
38	a	200.35	0.47079	YES	YES
39	a	205.17	4.12213	YES	YES
40	a	213.07	0.40186	YES	YES
41	a	219.54	0.48526	YES	YES
42	a	225.47	1.37822	YES	YES
43	a	240.97	1.26400	YES	YES
44	a	242.82	0.98006	YES	YES
45	a	246.13	0.41247	YES	YES
46	a	248.08	0.36545	YES	YES
47	a	260.33	1.53292	YES	YES
48	a	264.97	1.22994	YES	YES
49	a	266.05	0.18044	YES	YES
50	a	266.40	0.40102	YES	YES
51	a	278.47	0.01246	YES	YES
52	a	335.62	4.07112	YES	YES
53	a	368.86	38.94628	YES	YES
54	a	395.25	0.28985	YES	YES
55	a	395.63	0.90833	YES	YES
56	a	397.09	0.33883	YES	YES
57	a	398.86	0.21515	YES	YES
58	a	404.63	2.49346	YES	YES
59	a	405.13	2.72864	YES	YES
60	a	406.97	85.66670	YES	YES
61	a	420.54	0.61933	YES	YES
62	a	425.83	12.38306	YES	YES
63	a	433.55	3.42898	YES	YES
64	a	443.91	6.37913	YES	YES
65	a	455.71	23.07861	YES	YES
66	a	477.68	2.28893	YES	YES
67	a	485.88	15.63610	YES	YES
68	a	489.34	0.64796	YES	YES
69	a	493.95	47.83710	YES	YES
70	a	501.73	82.04641	YES	YES
71	a	510.07	81.35648	YES	YES
72	a	514.13	161.73384	YES	YES
73	a	529.44	5.01529	YES	YES
74	a	593.52	2.08233	YES	YES
75	a	601.67	3.42352	YES	YES
76	a	609.16	0.07010	YES	YES
77	a	609.41	0.15621	YES	YES
78	a	609.91	2.45898	YES	YES
79	a	610.20	0.06556	YES	YES
80	a	610.82	2.18225	YES	YES
81	a	611.18	0.13292	YES	YES
82	a	659.23	79.78515	YES	YES
83	a	671.37	18.22222	YES	YES
84	a	673.14	0.56459	YES	YES
85	a	673.87	0.52207	YES	YES
86	a	683.40	3.49360	YES	YES
87	a	685.14	20.80773	YES	YES
88	a	688.29	4.71906	YES	YES
89	a	690.14	21.37496	YES	YES
90	a	694.16	45.97641	YES	YES
91	a	695.50	34.16257	YES	YES
92	a	696.49	32.80116	YES	YES
93	a	698.90	32.51334	YES	YES
94	a	701.39	20.63532	YES	YES
95	a	706.43	26.14252	YES	YES
96	a	738.10	2.36934	YES	YES
97	a	739.67	13.41047	YES	YES
98	a	742.93	1.72482	YES	YES
99	a	744.09	2.38307	YES	YES
100	a	747.20	1.67970	YES	YES
101	a	748.18	9.64203	YES	YES
102	a	832.47	0.57853	YES	YES
103	a	832.91	0.91848	YES	YES
104	a	835.08	0.45021	YES	YES
105	a	838.41	0.70664	YES	YES
106	a	839.63	0.77968	YES	YES
107	a	848.69	0.12782	YES	YES
108	a	902.59	0.77300	YES	YES
109	a	903.20	0.28472	YES	YES
110	a	908.76	0.40813	YES	YES
111	a	910.70	0.50024	YES	YES
112	a	912.03	0.55663	YES	YES
113	a	926.26	0.69785	YES	YES
114	a	944.66	0.55560	YES	YES
115	a	950.53	23.57454	YES	YES
116	a	955.11	0.42963	YES	YES
117	a	956.03	0.16804	YES	YES
118	a	958.27	0.49677	YES	YES
119	a	960.15	0.59408	YES	YES
120	a	960.72	0.31686	YES	YES
121	a	973.84	0.20062	YES	YES
122	a	979.56	0.12595	YES	YES
123	a	980.48	0.03495	YES	YES
124	a	981.59	2.03101	YES	YES
125	a	982.09	0.27142	YES	YES
126	a	982.44	0.02580	YES	YES
127	a	982.84	0.94831	YES	YES
128	a	983.05	0.09448	YES	YES
129	a	983.11	2.04809	YES	YES
130	a	983.63	3.57478	YES	YES
131	a	984.10	1.94100	YES	YES
132	a	984.51	1.65487	YES	YES
133	a	984.90	0.40908	YES	YES
134	a	985.55	0.71899	YES	YES
135	a	999.26	1.17266	YES	YES
136	a	1020.95	17.87988	YES	YES
137	a	1023.18	2.15845	YES	YES
138	a	1023.39	1.72793	YES	YES
139	a	1023.76	2.00234	YES	YES
140	a	1024.09	3.27147	YES	YES
141	a	1024.46	2.21032	YES	YES
142	a	1024.58	2.07278	YES	YES
143	a	1026.85	12.45798	YES	YES
144	a	1070.53	7.05496	YES	YES
145	a	1072.25	1.90220	YES	YES
146	a	1072.47	9.73799	YES	YES
147	a	1073.24	6.84285	YES	YES
148	a	1073.53	4.73865	YES	YES
149	a	1074.43	16.38665	YES	YES
150	a	1074.93	5.20759	YES	YES
151	a	1076.09	13.25434	YES	YES
152	a	1077.13	7.93265	YES	YES
153	a	1077.55	30.92761	YES	YES
154	a	1081.87	21.92459	YES	YES
155	a	1083.08	4.53719	YES	YES
156	a	1140.80	0.13890	YES	YES
157	a	1140.95	0.30324	YES	YES
158	a	1141.17	0.20036	YES	YES
159	a	1141.19	0.17586	YES	YES
160	a	1141.51	0.25185	YES	YES
161	a	1141.91	0.29375	YES	YES
162	a	1165.43	9.44204	YES	YES
163	a	1167.20	3.40053	YES	YES
164	a	1168.70	6.39141	YES	YES
165	a	1169.22	4.96942	YES	YES
166	a	1169.47	8.38711	YES	YES
167	a	1171.53	4.19440	YES	YES
168	a	1289.53	6.32862	YES	YES
169	a	1291.07	1.56623	YES	YES
170	a	1292.88	6.34307	YES	YES
171	a	1295.03	1.55798	YES	YES
172	a	1296.54	3.69622	YES	YES
173	a	1300.03	2.68086	YES	YES
174	a	1324.50	0.63229	YES	YES
175	a	1328.50	0.44252	YES	YES
176	a	1356.50	2.56403	YES	YES
177	a	1357.03	0.91544	YES	YES
178	a	1358.02	1.45131	YES	YES

179	a	1359.94	2.09434	YES	YES
180	a	1361.47	3.32731	YES	YES
181	a	1361.90	2.77051	YES	YES
182	a	1394.56	33.22153	YES	YES
183	a	1397.55	31.00079	YES	YES
184	a	1409.05	14.85741	YES	YES
185	a	1411.00	19.93823	YES	YES
186	a	1426.86	15.46517	YES	YES
187	a	1426.97	15.85065	YES	YES
188	a	1427.31	15.92783	YES	YES
189	a	1427.64	9.67025	YES	YES
190	a	1431.13	25.44016	YES	YES
191	a	1431.62	11.66905	YES	YES
192	a	1461.03	314.12280	YES	YES
193	a	1463.05	12.53365	YES	YES
194	a	1470.34	14.99465	YES	YES
195	a	1471.28	6.57433	YES	YES
196	a	1471.61	7.96603	YES	YES
197	a	1471.71	9.81730	YES	YES
198	a	1472.86	9.44000	YES	YES

* zero point VIBRATIONAL energy : 0.6365325 Hartree *

Trans I_{12}



bp86-SVP SCF energy: -2623.2288208430
pbe-TZVPP SCF energy: -2622.828918495

XYZ Coordinates
83

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C	-0.65811	-2.95693	-1.64675
C	1.63148	-3.23623	0.16386
C	-0.39960	3.25885	1.57689
C	1.70721	3.10207	-0.39131
C	-1.07432	3.03946	-1.26828
C	2.58771	-0.09192	0.27669
C	4.07644	-0.20329	0.42876
H	4.38200	0.08139	1.45514
H	4.58379	0.44529	-0.31530
H	4.38635	-1.25585	0.24226
C	-3.12316	0.25180	0.45766
C	-4.16806	0.38959	-0.64354
H	-5.18228	0.41084	-0.19692
H	-3.99665	1.33632	-1.20279
H	-4.08661	-0.44427	-1.37281
O	2.00798	-0.08561	-0.86461
O	1.79004	-0.03099	1.28339
O	-1.92003	-0.05082	0.01516
O	-3.38588	0.38995	1.65565
P	-0.01265	-2.38488	-0.00555
P	0.06223	2.34542	0.02736
Ru	0.06482	-0.01864	0.04972
C	4.17592	-4.41130	0.55435
C	3.50523	-3.80362	1.63141
C	2.24519	-3.21568	1.43833
C	2.30965	-3.84817	-0.91090
C	3.57459	-4.43129	-0.71519
H	5.16567	-4.87319	0.70663
H	3.96728	-3.78569	2.63277
H	1.73067	-2.73835	2.28836
H	1.84698	-3.87839	-1.91009
H	4.08932	-4.91132	-1.56432
C	-1.60527	-3.64610	-4.22102
C	-2.16519	-4.24130	-3.07865
C	-1.69360	-3.90261	-1.79735
C	-0.11513	-2.34248	-2.80097
C	-0.57762	-2.69595	-4.07877
H	-1.97640	-3.91476	-5.22411
H	-2.97994	-4.97743	-3.18165
H	-2.14400	-4.37461	-0.90982
H	0.66918	-1.57447	-2.68900
H	-0.13966	-2.21607	-4.97008
C	-2.51535	-4.68629	3.21024
C	-1.63843	-5.39187	2.36565
C	-0.88872	-4.70476	1.39777
C	-1.88649	-2.59854	2.11537
C	-2.63545	-3.29321	3.08284
H	-3.10141	-5.22704	3.97225
H	-1.53294	-6.48545	2.46404
H	-0.19439	-5.26555	0.75030
H	-1.99230	-1.50438	2.03554
H	-3.31644	-2.72820	3.74002
C	-1.15970	4.60547	3.94223
C	-0.31787	5.23943	3.01107
C	0.05893	4.57257	1.83382
C	-1.24703	2.62901	2.51415
C	-1.62622	3.30566	3.68679
H	-1.45275	5.12882	4.86804
H	0.05107	6.26136	3.20222
H	0.72335	5.07885	1.11493
H	-1.63994	1.61496	2.32476
H	-2.29350	2.80204	4.40549
C	-2.76282	3.98224	-3.33030
C	-2.65119	4.69741	-2.12518
C	-1.81047	4.23149	-1.09904
C	-1.20651	2.31559	-2.47518
C	-2.03922	2.78881	-3.50318
H	-3.42326	4.35028	-4.13318
H	-3.22546	5.62746	-1.97912
H	-1.73458	4.79834	-0.15735
H	-0.65853	1.36499	-2.59623
H	-2.13099	2.21504	-4.44032
C	4.28638	4.10959	-0.98299
C	3.99676	3.61903	0.30264
C	2.71938	3.11422	0.59693
C	2.00739	3.59322	-1.67918
C	3.28812	4.09369	-1.97149
H	5.28875	4.50802	-1.21231
H	4.77174	3.63152	1.08753
H	2.50338	2.73633	1.60977
H	1.23349	3.59289	-2.46351
H	3.50347	4.47970	-2.98217

Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	9.06	0.05648	YES	YES
8	a	11.24	0.21937	YES	YES
9	a	18.22	0.27444	YES	YES
10	a	21.00	0.05851	YES	YES
11	a	26.31	0.12604	YES	YES
12	a	30.01	0.26954	YES	YES
13	a	34.03	0.31426	YES	YES
14	a	39.42	0.14996	YES	YES
15	a	41.26	0.05734	YES	YES
16	a	45.80	0.83752	YES	YES
17	a	48.27	0.06977	YES	YES
18	a	50.74	0.29215	YES	YES
19	a	53.71	0.13355	YES	YES
20	a	57.34	0.26806	YES	YES
21	a	58.77	0.13225	YES	YES
22	a	61.87	0.28280	YES	YES
23	a	65.98	0.58585	YES	YES
24	a	69.11	0.14836	YES	YES
25	a	72.22	0.47230	YES	YES
26	a	80.29	0.34603	YES	YES
27	a	82.79	0.17127	YES	YES
28	a	87.16	0.06718	YES	YES
29	a	101.65	6.18356	YES	YES
30	a	108.40	3.96095	YES	YES
31	a	110.69	5.03933	YES	YES
32	a	114.03	2.11627	YES	YES

33	a	141.72	0.27135	YES	YES
34	a	145.26	0.14789	YES	YES
35	a	155.18	0.20373	YES	YES
36	a	167.27	0.40138	YES	YES
37	a	170.72	0.51426	YES	YES
38	a	189.03	2.10063	YES	YES
39	a	190.47	1.22628	YES	YES
40	a	200.57	0.60985	YES	YES
41	a	205.46	5.05317	YES	YES
42	a	215.93	0.51457	YES	YES
43	a	225.56	1.00266	YES	YES
44	a	239.39	1.58273	YES	YES
45	a	240.82	0.74672	YES	YES
46	a	246.15	1.45641	YES	YES
47	a	247.74	0.08051	YES	YES
48	a	248.99	0.33793	YES	YES
49	a	258.23	0.92182	YES	YES
50	a	265.49	0.12403	YES	YES
51	a	267.31	0.21889	YES	YES
52	a	296.26	3.37287	YES	YES
53	a	362.61	21.81226	YES	YES
54	a	395.83	0.38961	YES	YES
55	a	396.22	0.68737	YES	YES
56	a	398.04	0.12753	YES	YES
57	a	398.46	0.36898	YES	YES
58	a	404.06	0.12676	YES	YES
59	a	405.47	2.34920	YES	YES
60	a	408.31	69.34860	YES	YES
61	a	423.51	0.45202	YES	YES
62	a	427.88	8.43404	YES	YES
63	a	433.91	5.91503	YES	YES
64	a	443.46	9.65269	YES	YES
65	a	452.51	18.34819	YES	YES
66	a	488.57	14.01841	YES	YES
67	a	493.11	4.51667	YES	YES
68	a	495.52	54.48271	YES	YES
69	a	496.38	7.10215	YES	YES
70	a	501.69	78.61988	YES	YES
71	a	510.59	79.51108	YES	YES
72	a	513.96	148.07417	YES	YES
73	a	528.07	2.92926	YES	YES
74	a	571.36	11.47630	YES	YES
75	a	597.95	4.28204	YES	YES
76	a	607.94	1.77902	YES	YES
77	a	608.81	0.31797	YES	YES
78	a	609.57	1.16470	YES	YES
79	a	609.96	0.89024	YES	YES
80	a	610.13	0.68584	YES	YES
81	a	610.49	0.26275	YES	YES
82	a	618.79	28.42253	YES	YES
83	a	667.71	38.41750	YES	YES
84	a	672.38	14.38252	YES	YES
85	a	674.70	0.33539	YES	YES
86	a	686.01	2.86133	YES	YES
87	a	687.80	20.12108	YES	YES
88	a	690.14	7.51027	YES	YES
89	a	692.86	14.89019	YES	YES
90	a	696.15	51.53541	YES	YES
91	a	698.16	29.37676	YES	YES
92	a	698.82	23.00948	YES	YES
93	a	700.97	37.42043	YES	YES
94	a	702.42	19.92498	YES	YES
95	a	705.61	26.48257	YES	YES
96	a	740.09	1.59568	YES	YES
97	a	741.39	14.38529	YES	YES
98	a	742.96	4.47041	YES	YES
99	a	744.67	4.57354	YES	YES
100	a	747.84	3.09329	YES	YES
101	a	748.70	9.21688	YES	YES
102	a	835.52	0.54142	YES	YES
103	a	836.74	0.93662	YES	YES
104	a	839.95	1.65109	YES	YES
105	a	840.39	0.34874	YES	YES
106	a	844.36	0.66908	YES	YES
107	a	848.75	0.41949	YES	YES
108	a	905.07	0.41216	YES	YES
109	a	905.72	0.22886	YES	YES
110	a	911.33	0.14364	YES	YES
111	a	913.09	0.23319	YES	YES
112	a	919.26	2.20439	YES	YES
113	a	923.88	5.81831	YES	YES
114	a	929.04	4.23267	YES	YES
115	a	951.55	18.44318	YES	YES
116	a	957.95	0.08972	YES	YES
117	a	958.35	0.54710	YES	YES
118	a	961.95	1.48574	YES	YES
119	a	962.67	0.43651	YES	YES
120	a	966.04	0.65968	YES	YES
121	a	972.54	0.30784	YES	YES
122	a	980.38	0.48791	YES	YES
123	a	980.70	0.95922	YES	YES
124	a	981.78	0.56016	YES	YES
125	a	981.92	0.65271	YES	YES
126	a	982.26	1.62210	YES	YES
127	a	982.70	2.37687	YES	YES
128	a	983.06	1.46407	YES	YES
129	a	983.43	2.08376	YES	YES
130	a	983.71	0.29730	YES	YES
131	a	984.55	0.19617	YES	YES
132	a	985.47	0.53960	YES	YES
133	a	992.04	2.19399	YES	YES
134	a	996.71	18.53621	YES	YES
135	a	999.71	4.67138	YES	YES
136	a	1018.91	10.29146	YES	YES
137	a	1022.56	1.50559	YES	YES
138	a	1022.87	0.65929	YES	YES
139	a	1023.56	3.03173	YES	YES
140	a	1023.95	3.02931	YES	YES
141	a	1024.34	2.27059	YES	YES
142	a	1024.43	1.12844	YES	YES
143	a	1025.60	19.71276	YES	YES
144	a	1069.56	2.84915	YES	YES
145	a	1072.76	2.17923	YES	YES
146	a	1073.61	6.23614	YES	YES
147	a	1074.11	7.92525	YES	YES
148	a	1074.69	12.49211	YES	YES
149	a	1075.04	5.78799	YES	YES
150	a	1076.21	17.25672	YES	YES
151	a	1076.99	9.86427	YES	YES
152	a	1078.10	24.38731	YES	YES
153	a	1080.27	11.08096	YES	YES
154	a	1082.90	16.10389	YES	YES
155	a	1083.63	0.26611	YES	YES
156	a	1141.08	0.74631	YES	YES
157	a	1141.29	0.13924	YES	YES
158	a	1141.86	0.13877	YES	YES
159	a	1141.94	0.19842	YES	YES
160	a	1142.35	0.50563	YES	YES
161	a	1142.55	0.45588	YES	YES
162	a	1163.69	3.50180	YES	YES
163	a	1166.28	3.01646	YES	YES
164	a	1168.91	5.56423	YES	YES
165	a	1170.25	1.55851	YES	YES
166	a	1170.83	4.85561	YES	YES
167	a	1174.78	2.93118	YES	YES
168	a	1286.29	115.97634	YES	YES
169	a	1288.19	5.05756	YES	YES
170	a	1293.21	52.68191	YES	YES
171	a	1293.63	67.50589	YES	YES
172	a	1295.70	117.97121	YES	YES
173	a	1298.59	22.92222	YES	YES
174	a	1302.19	41.15922	YES	YES
175	a	1334.03	0.23614	YES	YES
176	a	1342.70	152.88942	YES	YES
177	a	1357.38	1.49336	YES	YES
178	a	1357.87	2.16677	YES	YES
179	a	1358.41	5.03434	YES	YES
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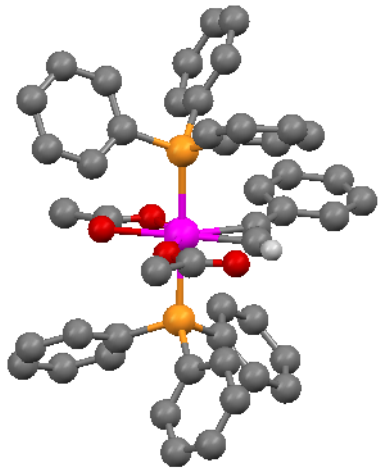
181	a	1361.79	1.89403	YES	YES
182	a	1362.25	3.56425	YES	YES
183	a	1393.35	26.75955	YES	YES
184	a	1406.07	7.29413	YES	YES
185	a	1409.01	12.42221	YES	YES
186	a	1417.65	6.75202	YES	YES
187	a	1426.46	14.41384	YES	YES
188	a	1427.13	18.20724	YES	YES
189	a	1427.67	21.16861	YES	YES
190	a	1428.31	14.10207	YES	YES
191	a	1431.23	19.29184	YES	YES
192	a	1431.52	14.39536	YES	YES
193	a	1468.60	9.84735	YES	YES
194	a	1470.48	5.73379	YES	YES
195	a	1471.94	17.63074	YES	YES
196	a	1472.49	1.91821	YES	YES
197	a	1473.14	4.39664	YES	YES
198	a	1474.04	3.90109	YES	YES

* zero point VIBRATIONAL energy : 0.6354927 Hartree *

Trans 2_ax



bp86-SVP SCF energy: -2931.4450563130
pbe-TZVPP SCF energy: -2930.993158956

XYZ Coordinates
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C	1.28427	3.34749	1.21102
C	0.88255	3.17223	-1.62564
C	2.54198	-0.18774	2.09221
C	4.07325	-0.28413	2.09055
H	4.44623	-0.25949	3.13393
H	4.52203	0.54951	1.50872
H	4.39669	-1.23544	1.61261
C	0.22894	0.16280	-2.64535
C	0.21684	0.29576	-4.14511
H	0.86381	-0.48411	-4.60014
H	-0.81475	0.21529	-4.54283
H	0.63739	1.28694	-4.42622
O	2.06182	-0.04530	0.87622
O	1.90198	-0.23842	3.14859
O	-0.86799	0.18880	-1.96611
O	1.31373	0.03838	-1.99286
P	0.30646	-2.40764	-0.08048
P	0.23879	2.44941	-0.03630
Ru	0.21741	0.02709	-0.06899
C	3.90016	-4.12563	-2.55519
C	4.01561	-2.90206	-1.87294
C	2.92727	-2.38576	-1.14933
C	1.59871	-4.32814	-1.77980
C	2.68851	-4.83575	-2.50799
H	4.75431	-4.52491	-3.12759
H	4.96030	-2.33434	-1.91073
H	3.00956	-1.42002	-0.62628
H	0.65610	-4.89691	-1.75163
H	2.58670	-5.79524	-3.04221
C	-3.24867	-4.89423	-1.85915
C	-2.59547	-5.35475	-0.70387
C	-1.54492	-4.61111	-0.13867
C	-1.80570	-2.93100	-1.87660
C	-2.84790	-3.68139	-2.44485
H	-4.07260	-5.47881	-2.30133
H	-2.90227	-6.30514	-0.23583
H	-1.03664	-4.99253	0.76077
H	-1.51223	-1.97103	-2.32787
H	-3.35748	-3.30786	-3.34868
C	1.00030	-4.13019	4.21575
C	2.03745	-4.18074	3.27086
C	1.83511	-3.69183	1.96881
C	-0.44964	-3.09163	2.55530
C	-0.24459	-3.58844	3.85201
H	1.16078	-4.51349	5.23717
H	3.01676	-4.60697	3.54519
H	2.65570	-3.74757	1.23606
H	-1.43132	-2.67214	2.28550
H	-1.06661	-3.54640	4.58587
C	-3.97508	4.43822	0.41639
C	-2.93302	4.82746	1.27411
C	-1.65935	4.24550	1.15154
C	-2.47457	2.86228	-0.67950
C	-3.74159	3.45575	-0.56127
H	-4.97417	4.89450	0.51522
H	-3.10897	5.59223	2.04893
H	-0.85064	4.56237	1.82782
H	-2.30190	2.07840	-1.43352
H	-4.55784	3.13112	-1.22700
C	2.00757	4.20543	-4.00747
C	0.68931	4.53182	-3.64910
C	0.12962	4.02132	-2.46278
C	2.20731	2.84189	-1.99741
C	2.76623	3.36147	-3.17509
H	2.44658	4.61051	-4.93454
H	0.08800	5.19674	-4.29151
H	-0.89990	4.29785	-2.18677
H	2.80251	2.17117	-1.35792
H	3.80160	3.09860	-3.44833
C	2.76761	4.74521	3.17389
C	2.15614	3.52049	3.48792
C	1.41761	2.82598	2.51421
C	1.89974	4.58270	0.90229
C	2.63537	5.27499	1.87834
H	3.35154	5.28687	3.93683
H	2.26019	3.08423	4.49491
H	0.96762	1.85820	2.77713
H	1.80420	5.01224	-0.10735
H	3.11011	6.23665	1.62067
C	-0.66129	-0.01402	1.85751
C	-1.64796	-0.03810	1.03957
H	-0.11471	-0.10066	2.80051
C	-3.07597	-0.12358	0.82217
C	-5.89684	-0.32132	0.53324
C	-5.05731	-0.41425	-0.59051
C	-3.66442	-0.31583	-0.45296
C	-3.93766	-0.02776	1.95159
C	-5.32645	-0.12685	1.80614
H	-6.99101	-0.39973	0.42008
H	-5.49386	-0.56947	-1.59179
H	-3.01007	-0.38066	-1.33259
H	-3.49326	0.13173	2.94737
H	-5.97373	-0.04965	2.69611

Vibrational Frequencies

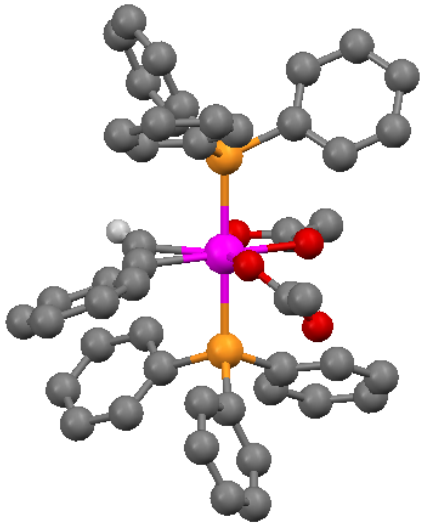
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.26	0.00370	YES	YES
8	a	13.91	0.19865	YES	YES
9	a	18.06	0.07975	YES	YES
10	a	20.99	0.00119	YES	YES
11	a	24.15	0.31183	YES	YES
12	a	29.42	0.02775	YES	YES
13	a	35.94	0.17709	YES	YES
14	a	38.33	0.32657	YES	YES
15	a	40.76	0.17316	YES	YES
16	a	42.26	0.19948	YES	YES
17	a	45.62	0.64815	YES	YES

18	a	47.18	0.77542	YES	YES
19	a	49.83	0.11862	YES	YES
20	a	53.87	0.35641	YES	YES
21	a	57.73	0.28990	YES	YES
22	a	60.17	0.62999	YES	YES
23	a	60.76	0.27652	YES	YES
24	a	62.77	0.10706	YES	YES
25	a	69.86	0.80284	YES	YES
26	a	76.13	0.14736	YES	YES
27	a	77.98	1.04230	YES	YES
28	a	79.79	0.05874	YES	YES
29	a	81.20	0.47047	YES	YES
30	a	84.06	0.66273	YES	YES
31	a	87.94	1.59367	YES	YES
32	a	89.94	0.48550	YES	YES
33	a	98.63	3.04891	YES	YES
34	a	102.85	1.67617	YES	YES
35	a	115.96	1.44428	YES	YES
36	a	135.72	0.29925	YES	YES
37	a	138.20	0.01361	YES	YES
38	a	148.14	2.12188	YES	YES
39	a	154.72	1.09088	YES	YES
40	a	164.97	0.78734	YES	YES
41	a	184.18	1.58924	YES	YES
42	a	192.52	2.22127	YES	YES
43	a	193.61	0.39316	YES	YES
44	a	195.73	1.45648	YES	YES
45	a	197.78	2.74288	YES	YES
46	a	202.34	2.19441	YES	YES
47	a	211.55	0.41717	YES	YES
48	a	218.94	4.30439	YES	YES
49	a	226.03	1.54497	YES	YES
50	a	228.06	1.66899	YES	YES
51	a	242.04	3.56835	YES	YES
52	a	243.07	0.12131	YES	YES
53	a	248.11	0.74481	YES	YES
54	a	252.52	0.06223	YES	YES
55	a	252.85	0.73945	YES	YES
56	a	255.33	0.49538	YES	YES
57	a	263.33	0.68699	YES	YES
58	a	263.97	0.24200	YES	YES
59	a	307.14	14.12170	YES	YES
60	a	318.38	1.46687	YES	YES
61	a	367.76	2.00273	YES	YES
62	a	395.75	0.90255	YES	YES
63	a	397.92	0.23843	YES	YES
64	a	399.54	2.50481	YES	YES
65	a	400.93	1.89316	YES	YES
66	a	402.04	21.16228	YES	YES
67	a	404.62	5.52131	YES	YES
68	a	405.59	2.60718	YES	YES
69	a	411.79	1.23049	YES	YES
70	a	415.19	6.46639	YES	YES
71	a	431.86	1.74229	YES	YES
72	a	435.33	7.93844	YES	YES
73	a	444.27	8.49862	YES	YES
74	a	448.12	13.23993	YES	YES
75	a	457.02	3.45442	YES	YES
76	a	465.75	13.39638	YES	YES
77	a	490.18	43.61414	YES	YES
78	a	492.49	6.30984	YES	YES
79	a	496.18	17.77231	YES	YES
80	a	504.91	51.29827	YES	YES
81	a	506.01	80.75167	YES	YES
82	a	512.10	144.09453	YES	YES
83	a	514.16	9.77956	YES	YES
84	a	524.31	1.83230	YES	YES
85	a	533.70	0.28460	YES	YES
86	a	568.85	16.51778	YES	YES
87	a	581.71	6.08850	YES	YES
88	a	603.05	3.39769	YES	YES
89	a	609.17	0.72905	YES	YES
90	a	609.45	0.74224	YES	YES
91	a	609.97	0.11395	YES	YES
92	a	610.09	1.69900	YES	YES
93	a	610.33	0.78410	YES	YES
94	a	610.61	0.58490	YES	YES
95	a	613.39	1.41024	YES	YES
96	a	638.17	28.82358	YES	YES
97	a	667.16	35.39550	YES	YES
98	a	672.31	12.85839	YES	YES
99	a	674.07	1.60396	YES	YES
100	a	680.84	4.21124	YES	YES
101	a	686.21	1.43192	YES	YES
102	a	687.26	8.49753	YES	YES
103	a	688.46	10.80923	YES	YES
104	a	689.45	18.24879	YES	YES
105	a	692.49	61.96878	YES	YES
106	a	695.03	22.08613	YES	YES
107	a	698.36	29.85975	YES	YES
108	a	701.10	18.80733	YES	YES
109	a	701.18	43.38568	YES	YES
110	a	702.32	29.65839	YES	YES
111	a	704.08	17.22687	YES	YES
112	a	737.70	3.93372	YES	YES
113	a	740.60	7.82896	YES	YES
114	a	743.08	9.92707	YES	YES
115	a	744.11	0.29266	YES	YES
116	a	746.00	7.44113	YES	YES
117	a	747.75	9.08531	YES	YES
118	a	753.67	41.82608	YES	YES
119	a	772.61	15.36941	YES	YES
120	a	785.92	2.05565	YES	YES
121	a	829.21	0.75751	YES	YES
122	a	830.60	0.90732	YES	YES
123	a	836.30	0.93221	YES	YES
124	a	839.27	0.95552	YES	YES
125	a	841.28	1.89407	YES	YES
126	a	842.40	0.90110	YES	YES
127	a	845.31	0.64275	YES	YES
128	a	902.11	0.31755	YES	YES
129	a	903.34	2.38328	YES	YES
130	a	910.19	2.12229	YES	YES
131	a	910.94	3.27397	YES	YES
132	a	913.64	0.18557	YES	YES
133	a	917.10	0.16272	YES	YES
134	a	919.99	0.57733	YES	YES
135	a	921.88	1.08064	YES	YES
136	a	946.11	12.37762	YES	YES
137	a	952.78	0.00963	YES	YES
138	a	955.71	0.94336	YES	YES
139	a	959.80	0.17126	YES	YES
140	a	962.56	0.88283	YES	YES
141	a	963.22	0.14387	YES	YES
142	a	964.73	0.32224	YES	YES
143	a	971.25	0.08815	YES	YES
144	a	976.96	0.86367	YES	YES
145	a	979.01	0.04641	YES	YES
146	a	981.84	0.85915	YES	YES
147	a	982.15	1.79691	YES	YES
148	a	982.57	1.19054	YES	YES
149	a	982.74	0.93611	YES	YES
150	a	983.14	0.43085	YES	YES
151	a	984.00	2.01064	YES	YES
152	a	984.20	0.76797	YES	YES
153	a	984.56	0.65512	YES	YES
154	a	984.86	1.75396	YES	YES
155	a	985.64	0.32038	YES	YES
156	a	988.05	4.90662	YES	YES
157	a	988.41	0.43303	YES	YES
158	a	988.79	2.24262	YES	YES
159	a	993.94	1.97017	YES	YES
160	a	1014.42	7.58079	YES	YES
161	a	1023.20	1.47654	YES	YES
162	a	1024.03	0.76138	YES	YES
163	a	1024.59	5.87826	YES	YES
164	a	1024.77	4.90635	YES	YES
165	a	1025.04	9.06675	YES	YES

166	a	1025.21	4.01825	YES	YES
167	a	1025.74	3.00087	YES	YES
168	a	1026.33	1.66417	YES	YES
169	a	1069.36	3.62625	YES	YES
170	a	1072.77	2.05955	YES	YES
171	a	1073.22	8.98610	YES	YES
172	a	1073.93	2.26729	YES	YES
173	a	1074.12	21.72588	YES	YES
174	a	1075.20	6.34750	YES	YES
175	a	1075.64	24.64516	YES	YES
176	a	1076.14	1.99389	YES	YES
177	a	1076.74	4.19749	YES	YES
178	a	1078.36	9.57528	YES	YES
179	a	1079.06	12.80635	YES	YES
180	a	1083.61	16.27248	YES	YES
181	a	1084.10	2.28453	YES	YES
182	a	1137.80	0.07637	YES	YES
183	a	1141.28	0.50010	YES	YES
184	a	1141.43	0.46538	YES	YES
185	a	1141.80	0.85614	YES	YES
186	a	1142.35	0.47883	YES	YES
187	a	1142.62	0.37453	YES	YES
188	a	1143.84	0.50362	YES	YES
189	a	1154.13	1.34468	YES	YES
190	a	1168.52	3.46697	YES	YES
191	a	1169.97	3.42468	YES	YES
192	a	1170.18	2.15706	YES	YES
193	a	1170.76	7.75473	YES	YES
194	a	1171.42	3.99046	YES	YES
195	a	1173.26	5.77086	YES	YES
196	a	1191.14	0.32255	YES	YES
197	a	1282.90	222.85129	YES	YES
198	a	1289.02	3.04837	YES	YES

* zero point VIBRATIONAL energy : 0.7443429 Hartree *

Trans 2_ay



bp86-SVP SCF energy: -2931.4478592710
pbe-TZVPP SCF energy: -2930.994898683

XYZ Coordinates
97

C	1.01490	-3.40283	0.65812
C	-1.77760	-3.02226	0.02191
C	0.20973	-3.06464	-2.10564
C	-1.71667	3.35352	-0.52711
C	0.53584	3.25492	1.28541
C	0.98755	3.27563	-1.59110
C	2.79233	-0.36125	0.40458
C	4.01860	-0.00905	1.25210
H	4.94344	-0.22568	0.67923
H	4.02000	-0.65203	2.16079
H	4.00451	1.05002	1.58319
C	-0.31704	0.03774	-2.87362
C	-0.47682	-0.03876	-4.36673
H	-0.28037	-1.08361	-4.69726
H	-1.50565	0.24367	-4.66841
H	0.26527	0.61994	-4.86331
O	1.71971	0.31148	0.75787
O	2.85628	-1.21609	-0.48422
O	-1.34049	-0.02111	-2.08760
O	0.82442	0.13112	-2.31953
P	-0.08918	-2.35854	-0.40616
P	-0.08406	2.49389	-0.28806
Ru	-0.06791	0.07396	-0.31857
C	0.77242	-4.09208	-4.68233
C	1.73516	-3.33071	-3.99526
C	1.46100	-2.81401	-2.71829
C	-0.75066	-3.83580	-2.79673
C	-0.47044	-4.34370	-4.07826
H	0.99348	-4.49373	-5.68574
H	2.71624	-3.13173	-4.45859
H	2.21186	-2.21823	-2.17602
H	-1.72542	-4.05499	-2.33447
H	-1.23101	-4.94720	-4.60168
C	-4.38680	-3.93785	0.63780
C	-3.27651	-4.44533	1.33108
C	-1.97960	-3.99394	1.02393
C	-2.90373	-2.50577	-0.66334
C	-4.19515	-2.96760	-0.36278
H	-5.40222	-4.29572	0.87698
H	-3.41514	-5.20397	2.11950
H	-1.11937	-4.40541	1.57420
H	-2.76063	-1.73501	-1.43825
H	-5.06111	-2.56153	-0.91247
C	2.60590	-5.00402	2.36113
C	2.27796	-5.45420	1.07086
C	1.48493	-4.66118	0.22415
C	1.35164	-2.95512	1.95232
C	2.13787	-3.75342	2.79976
H	3.22862	-5.62780	3.02417
H	2.64230	-6.43268	0.71569
H	1.23446	-5.02676	-0.78395
H	1.00405	-1.97175	2.30164
H	2.38832	-3.38804	3.80942
C	-4.18596	4.64909	-1.01478
C	-3.20517	5.27262	-0.22435
C	-1.97824	4.63201	0.01744
C	-2.70658	2.73551	-1.32352
C	-3.93139	3.38171	-1.56491
H	-5.14939	5.15265	-1.20101
H	-3.39449	6.26859	0.21013
H	-1.21976	5.13408	0.63878
H	-2.51044	1.74152	-1.75791
H	-4.69461	2.88533	-2.18730
C	2.70399	4.41449	-3.53046
C	1.44214	4.98047	-3.28430
C	0.58897	4.41736	-2.31937
C	2.25242	2.70236	-1.85626
C	3.10634	3.27507	-2.81260
H	3.37187	4.85748	-4.28818
H	1.11407	5.87071	-3.84685
H	-0.39625	4.87475	-2.13713
H	2.56301	1.79115	-1.32423
H	4.08931	2.81484	-3.00663
C	1.43921	4.32948	3.74197
C	0.14789	3.78360	3.64180
C	-0.30006	3.24428	2.42550
C	1.83168	3.80169	1.39457
C	2.27964	4.33385	2.61613
H	1.79019	4.75154	4.69838
H	-0.51764	3.76781	4.52038
H	-1.31188	2.81389	2.36385
H	2.49727	3.82383	0.51787
H	3.29390	4.76180	2.68282
C	-1.84103	0.11528	0.77406
C	-0.97286	0.00241	1.71014
H	-2.86655	0.24294	0.41665
C	-0.65417	-0.15730	3.11077
C	-0.14262	-0.47889	5.88703
C	0.85409	0.02687	5.03343
C	0.60827	0.18809	3.66126
C	-1.65319	-0.67304	3.98470
C	-1.39837	-0.82736	5.35332
H	0.05691	-0.60361	6.96449
H	1.83923	0.30715	5.44292
H	1.38043	0.58213	2.98535
H	-2.63154	-0.95867	3.56599
H	-2.18672	-1.22943	6.01210

Vibrational Frequencies

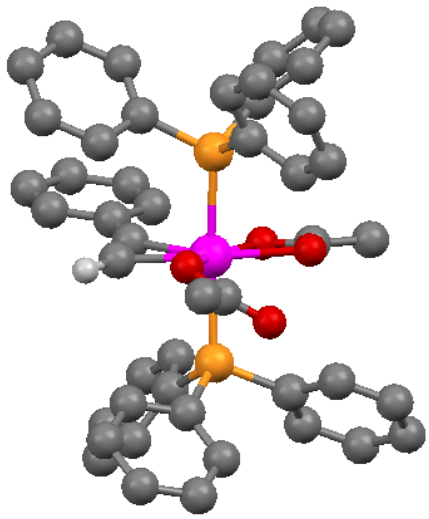
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.37	0.03826	YES	YES
8	a	13.16	0.32550	YES	YES
9	a	18.60	0.64044	YES	YES
10	a	23.08	0.01080	YES	YES
11	a	26.15	0.15568	YES	YES
12	a	29.66	0.03120	YES	YES
13	a	35.52	0.00152	YES	YES
14	a	38.52	0.04800	YES	YES
15	a	39.44	0.37116	YES	YES
16	a	46.21	0.18538	YES	YES

17	a	50.27	0.02290	YES	YES
18	a	52.30	0.10460	YES	YES
19	a	55.90	0.04853	YES	YES
20	a	58.76	0.41377	YES	YES
21	a	60.15	0.26969	YES	YES
22	a	63.19	0.82993	YES	YES
23	a	65.29	0.24707	YES	YES
24	a	69.94	0.32806	YES	YES
25	a	71.25	1.81325	YES	YES
26	a	73.70	0.83795	YES	YES
27	a	75.23	0.21639	YES	YES
28	a	78.59	1.53868	YES	YES
29	a	79.58	0.15893	YES	YES
30	a	84.57	0.51964	YES	YES
31	a	89.67	0.98687	YES	YES
32	a	92.66	0.94557	YES	YES
33	a	101.27	0.55665	YES	YES
34	a	109.59	4.11395	YES	YES
35	a	111.78	2.00737	YES	YES
36	a	135.96	0.58461	YES	YES
37	a	137.98	0.44657	YES	YES
38	a	141.01	2.35899	YES	YES
39	a	151.54	0.69599	YES	YES
40	a	165.34	1.37708	YES	YES
41	a	179.95	1.32422	YES	YES
42	a	184.70	1.83230	YES	YES
43	a	193.14	0.43405	YES	YES
44	a	196.06	1.87410	YES	YES
45	a	199.86	0.89224	YES	YES
46	a	201.96	2.73098	YES	YES
47	a	208.16	2.00382	YES	YES
48	a	220.95	1.00466	YES	YES
49	a	222.74	1.90867	YES	YES
50	a	228.41	1.67813	YES	YES
51	a	241.70	2.56248	YES	YES
52	a	243.82	2.05311	YES	YES
53	a	248.42	0.23789	YES	YES
54	a	251.95	0.56101	YES	YES
55	a	255.12	0.98645	YES	YES
56	a	262.43	0.21784	YES	YES
57	a	264.64	0.29650	YES	YES
58	a	269.62	3.95066	YES	YES
59	a	299.51	6.22390	YES	YES
60	a	337.16	10.79284	YES	YES
61	a	351.89	1.81785	YES	YES
62	a	397.66	0.30400	YES	YES
63	a	398.19	0.42146	YES	YES
64	a	399.55	0.12480	YES	YES
65	a	399.81	0.12400	YES	YES
66	a	402.95	29.83885	YES	YES
67	a	405.57	7.40951	YES	YES
68	a	406.55	0.10935	YES	YES
69	a	406.85	0.03573	YES	YES
70	a	416.08	5.22421	YES	YES
71	a	430.46	3.96546	YES	YES
72	a	434.87	8.94160	YES	YES
73	a	447.74	8.72471	YES	YES
74	a	450.33	19.35560	YES	YES
75	a	464.86	0.39512	YES	YES
76	a	476.72	7.61430	YES	YES
77	a	489.96	20.69276	YES	YES
78	a	498.32	6.82370	YES	YES
79	a	499.69	12.10589	YES	YES
80	a	503.74	24.19971	YES	YES
81	a	506.69	86.35485	YES	YES
82	a	512.31	32.86235	YES	YES
83	a	515.81	145.71248	YES	YES
84	a	523.12	12.85405	YES	YES
85	a	533.29	15.03288	YES	YES
86	a	549.73	5.87188	YES	YES
87	a	594.43	4.25196	YES	YES
88	a	600.69	2.25322	YES	YES
89	a	609.33	0.17609	YES	YES
90	a	609.92	2.95858	YES	YES
91	a	610.25	0.33991	YES	YES
92	a	610.89	0.30236	YES	YES
93	a	611.03	0.24636	YES	YES
94	a	611.22	1.92880	YES	YES
95	a	613.11	2.02629	YES	YES
96	a	644.49	40.99826	YES	YES
97	a	668.58	31.07029	YES	YES
98	a	671.18	18.81130	YES	YES
99	a	672.08	13.84733	YES	YES
100	a	673.76	1.95841	YES	YES
101	a	684.58	5.73337	YES	YES
102	a	687.69	9.21915	YES	YES
103	a	688.63	7.86103	YES	YES
104	a	690.85	15.22632	YES	YES
105	a	694.00	34.77947	YES	YES
106	a	696.84	37.33226	YES	YES
107	a	697.50	23.63160	YES	YES
108	a	699.88	31.19366	YES	YES
109	a	700.99	36.98827	YES	YES
110	a	704.57	18.13491	YES	YES
111	a	706.86	27.00299	YES	YES
112	a	740.03	5.84527	YES	YES
113	a	743.63	8.04687	YES	YES
114	a	744.62	3.58110	YES	YES
115	a	746.07	1.35433	YES	YES
116	a	748.19	10.24352	YES	YES
117	a	748.71	6.55049	YES	YES
118	a	758.95	13.66314	YES	YES
119	a	773.98	0.36955	YES	YES
120	a	831.57	0.32153	YES	YES
121	a	834.21	0.80945	YES	YES
122	a	837.73	1.80627	YES	YES
123	a	839.42	3.04114	YES	YES
124	a	840.00	4.19202	YES	YES
125	a	843.65	2.67880	YES	YES
126	a	848.30	0.71754	YES	YES
127	a	851.03	2.00659	YES	YES
128	a	904.63	3.12755	YES	YES
129	a	908.65	0.92592	YES	YES
130	a	909.90	1.25952	YES	YES
131	a	911.34	0.33229	YES	YES
132	a	915.63	0.21458	YES	YES
133	a	918.38	0.94134	YES	YES
134	a	924.08	0.09114	YES	YES
135	a	926.83	0.39700	YES	YES
136	a	947.78	17.14592	YES	YES
137	a	957.41	0.54375	YES	YES
138	a	958.05	0.01171	YES	YES
139	a	962.14	0.46737	YES	YES
140	a	962.38	0.16494	YES	YES
141	a	966.84	0.49035	YES	YES
142	a	972.36	0.22988	YES	YES
143	a	975.11	0.10993	YES	YES
144	a	977.97	1.19693	YES	YES
145	a	981.42	1.06500	YES	YES
146	a	982.03	0.32731	YES	YES
147	a	982.29	0.23944	YES	YES
148	a	982.55	0.67794	YES	YES
149	a	983.22	1.27762	YES	YES
150	a	983.60	0.15431	YES	YES
151	a	984.79	0.68619	YES	YES
152	a	984.89	0.58566	YES	YES
153	a	985.28	0.92178	YES	YES
154	a	985.50	3.46564	YES	YES
155	a	985.68	1.38681	YES	YES
156	a	987.25	4.91607	YES	YES
157	a	987.43	0.07147	YES	YES
158	a	1000.39	0.21270	YES	YES
159	a	1002.30	0.89306	YES	YES
160	a	1017.63	7.56372	YES	YES
161	a	1023.79	1.62148	YES	YES
162	a	1024.17	7.35182	YES	YES
163	a	1024.28	0.10613	YES	YES
164	a	1024.65	2.91331	YES	YES

165	a	1024.83	2.70939	YES	YES
166	a	1025.10	1.40074	YES	YES
167	a	1025.74	2.27333	YES	YES
168	a	1026.13	16.87166	YES	YES
169	a	1066.77	2.38884	YES	YES
170	a	1073.21	0.52468	YES	YES
171	a	1073.49	17.20045	YES	YES
172	a	1074.00	1.46452	YES	YES
173	a	1074.73	3.53742	YES	YES
174	a	1074.99	13.98565	YES	YES
175	a	1075.44	21.76114	YES	YES
176	a	1077.13	0.80279	YES	YES
177	a	1077.31	18.73242	YES	YES
178	a	1079.02	13.46247	YES	YES
179	a	1079.47	5.02790	YES	YES
180	a	1083.88	12.05742	YES	YES
181	a	1084.87	6.73894	YES	YES
182	a	1137.49	0.37136	YES	YES
183	a	1141.32	0.77510	YES	YES
184	a	1141.34	0.24693	YES	YES
185	a	1141.44	0.50099	YES	YES
186	a	1141.61	0.67777	YES	YES
187	a	1142.27	0.51086	YES	YES
188	a	1143.19	0.27515	YES	YES
189	a	1152.39	3.51603	YES	YES
190	a	1168.02	3.65875	YES	YES
191	a	1169.99	1.43724	YES	YES
192	a	1170.44	8.53865	YES	YES
193	a	1171.76	7.84062	YES	YES
194	a	1174.69	2.85728	YES	YES
195	a	1177.41	13.95674	YES	YES
196	a	1188.45	0.84330	YES	YES
197	a	1283.60	53.09457	YES	YES
198	a	1290.42	37.47970	YES	YES

* zero point VIBRATIONAL energy : 0.7449341 Hartree *

Trans 2_bx



bp86-SVP SCF energy: -2931.4488160390
pbe-TZVPP SCF energy: -2930.996613787

XYZ Coordinates
97

C	3.22522	1.56317	0.71750
C	3.28374	-1.33144	1.17231
C	3.24898	-0.27735	-1.51852
C	-2.92769	-0.04536	2.19942
C	-3.27273	1.48566	-0.23177
C	-3.27339	-1.44783	-0.30319
C	0.04241	2.55404	0.17974
C	0.12443	4.05564	0.14879
H	1.18839	4.36107	0.26675
H	-0.45168	4.48718	0.99249
H	-0.25329	4.45001	-0.81612
C	0.43726	-1.20559	2.85166
C	0.15083	-2.28090	3.90118
H	0.32208	-3.29713	3.48724
H	0.79623	-2.12007	4.78773
H	-0.91557	-2.21927	4.21237
O	0.10121	1.86513	-0.90660
O	-0.04386	1.90350	1.27123
O	-0.10598	-1.47286	1.68851
O	1.09945	-0.19612	3.12067
P	2.45150	-0.02966	0.14282
P	-2.37271	-0.00043	0.42402
Ru	0.02542	-0.02491	0.14298
C	4.40747	-0.53353	-4.08737
C	3.34137	0.35882	-3.87900
C	2.76342	0.48359	-2.60547
C	4.32549	-1.16485	-1.73402
C	4.89768	-1.29306	-3.01201
H	4.85516	-0.63803	-5.08984
H	2.94391	0.95444	-4.71702
H	1.93022	1.18482	-2.44611
H	4.72614	-1.76047	-0.89941
H	5.73626	-1.99299	-3.16437
C	4.51124	-3.39614	2.67076
C	4.84326	-2.05240	2.91070
C	4.23461	-1.02623	2.16807
C	2.95373	-2.68514	0.93861
C	3.56543	-3.70958	1.67929
H	4.98904	-4.19967	3.25567
H	5.58401	-1.79489	3.68603
H	4.50311	0.02158	2.37155
H	2.22225	-2.94224	0.15781
H	3.29840	-4.76089	1.47996
C	4.33772	3.99251	1.65023
C	3.42174	3.28042	2.44481
C	2.86008	2.07694	1.98535
C	4.15130	2.27918	-0.07386
C	4.70047	3.48772	0.39008
H	4.77189	4.93893	2.01440
H	3.13398	3.66487	3.43775
H	2.14268	1.51480	2.60337
H	4.45433	1.89448	-1.05951
H	5.42300	4.03340	-0.23985
C	-3.80779	-0.00496	4.88785
C	-2.64019	0.68194	4.51384
C	-2.19873	0.66511	3.17942
C	-4.10274	-0.73132	2.58072
C	-4.53808	-0.71121	3.91677
H	-4.14842	0.00790	5.93682
H	-2.05502	1.23385	5.26804
H	-1.27922	1.20082	2.89977
H	-4.68707	-1.28793	1.83100
H	-5.45618	-1.25387	4.19831
C	-4.52645	-3.76354	-1.33052
C	-3.49949	-3.88066	-0.37576
C	-2.87075	-2.73306	0.13142
C	-4.30396	-1.33663	-1.25796
C	-4.92500	-2.49099	-1.76969
H	-5.01690	-4.66666	-1.73065
H	-3.18282	-4.87675	-0.02352
H	-2.06683	-2.82240	0.88173
H	-4.63471	-0.34478	-1.60444
H	-5.73091	-2.38868	-2.51543
C	-4.57647	3.75805	-1.30742
C	-4.72050	3.43741	0.05268
C	-4.07700	2.30779	0.58812
C	-3.12100	1.82531	-1.59551
C	-3.77652	2.94612	-2.13057
H	-5.08552	4.64218	-1.72624
H	-5.34398	4.06867	0.70771
H	-4.20451	2.06624	1.65463
H	-2.48774	1.20635	-2.25001
H	-3.65423	3.18762	-3.19959
C	-0.15344	-1.00310	-1.80168
C	0.03721	-1.86356	-0.87287
C	-0.42980	-0.69741	-3.18784
H	0.10573	-2.88246	-0.48871
C	-0.98079	-0.25404	-5.94300
C	-0.92066	-1.56554	-5.43283
C	-0.65102	-1.78709	-4.07774
C	-0.49213	0.61865	-3.71538
C	-0.76554	0.83100	-5.07634
H	-1.19461	-0.08172	-7.01101
H	-1.08961	-2.42678	-6.10111
H	-0.61009	-2.81427	-3.68156
H	-0.31958	1.46957	-3.04077
H	-0.80849	1.86267	-5.46515

Vibrational Frequencies

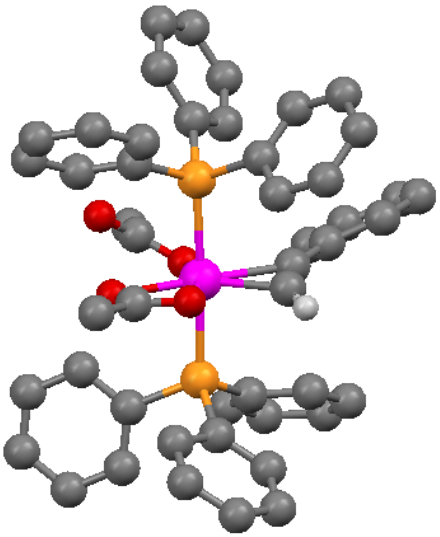
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.09	0.04175	YES	YES
8	a	12.18	0.08030	YES	YES
9	a	15.83	0.36148	YES	YES
10	a	17.79	0.39612	YES	YES
11	a	23.38	0.02215	YES	YES
12	a	24.67	0.09947	YES	YES
13	a	29.55	0.15022	YES	YES
14	a	36.15	0.09520	YES	YES
15	a	41.43	0.13271	YES	YES
16	a	44.23	0.04768	YES	YES

17	a	48.62	0.01209	YES	YES
18	a	49.95	0.03802	YES	YES
19	a	52.52	0.18147	YES	YES
20	a	56.29	0.08252	YES	YES
21	a	59.13	0.34432	YES	YES
22	a	61.88	0.13302	YES	YES
23	a	64.31	0.05570	YES	YES
24	a	65.61	0.32066	YES	YES
25	a	70.43	1.21135	YES	YES
26	a	73.77	1.58318	YES	YES
27	a	77.36	0.01339	YES	YES
28	a	78.97	2.56753	YES	YES
29	a	80.54	0.62562	YES	YES
30	a	84.44	0.79415	YES	YES
31	a	86.19	0.31569	YES	YES
32	a	96.03	3.51349	YES	YES
33	a	98.87	3.26182	YES	YES
34	a	103.79	1.42423	YES	YES
35	a	116.58	2.98048	YES	YES
36	a	129.61	3.50340	YES	YES
37	a	140.44	0.17277	YES	YES
38	a	142.84	0.74753	YES	YES
39	a	146.87	2.91384	YES	YES
40	a	155.25	0.04783	YES	YES
41	a	172.43	2.15238	YES	YES
42	a	187.52	1.16442	YES	YES
43	a	192.72	0.26293	YES	YES
44	a	195.77	1.18377	YES	YES
45	a	198.79	0.10982	YES	YES
46	a	209.21	3.04038	YES	YES
47	a	214.13	0.93449	YES	YES
48	a	218.06	1.11413	YES	YES
49	a	221.99	2.59620	YES	YES
50	a	229.24	4.28661	YES	YES
51	a	240.88	2.76683	YES	YES
52	a	242.03	0.50159	YES	YES
53	a	252.71	0.95423	YES	YES
54	a	254.58	0.22113	YES	YES
55	a	258.31	0.95055	YES	YES
56	a	260.55	1.19134	YES	YES
57	a	262.46	1.15689	YES	YES
58	a	265.55	2.29359	YES	YES
59	a	311.43	4.05506	YES	YES
60	a	323.62	8.38204	YES	YES
61	a	361.33	1.02089	YES	YES
62	a	395.20	4.07127	YES	YES
63	a	396.72	19.32583	YES	YES
64	a	397.47	4.33434	YES	YES
65	a	398.36	4.81223	YES	YES
66	a	402.57	1.59581	YES	YES
67	a	404.27	1.70541	YES	YES
68	a	407.69	0.62009	YES	YES
69	a	412.36	0.56956	YES	YES
70	a	414.27	4.83911	YES	YES
71	a	435.93	3.47523	YES	YES
72	a	439.43	0.57301	YES	YES
73	a	444.89	16.04753	YES	YES
74	a	448.86	18.16667	YES	YES
75	a	465.51	0.97884	YES	YES
76	a	468.28	10.68866	YES	YES
77	a	493.64	3.49419	YES	YES
78	a	496.46	6.05503	YES	YES
79	a	498.22	52.70314	YES	YES
80	a	502.12	44.14114	YES	YES
81	a	504.82	6.61311	YES	YES
82	a	507.60	49.12214	YES	YES
83	a	513.58	191.34192	YES	YES
84	a	526.43	1.50965	YES	YES
85	a	530.55	1.41193	YES	YES
86	a	559.78	28.44287	YES	YES
87	a	590.48	4.55890	YES	YES
88	a	598.10	2.95197	YES	YES
89	a	609.31	1.10506	YES	YES
90	a	609.94	3.63116	YES	YES
91	a	610.19	0.66144	YES	YES
92	a	610.65	0.28356	YES	YES
93	a	610.77	1.12405	YES	YES
94	a	611.15	0.25586	YES	YES
95	a	614.10	4.81173	YES	YES
96	a	663.69	17.96639	YES	YES
97	a	668.98	45.56807	YES	YES
98	a	671.88	4.61524	YES	YES
99	a	673.02	29.15394	YES	YES
100	a	673.63	1.18370	YES	YES
101	a	686.14	4.44133	YES	YES
102	a	687.93	6.49786	YES	YES
103	a	689.27	9.75669	YES	YES
104	a	690.19	17.25895	YES	YES
105	a	694.74	53.69394	YES	YES
106	a	695.97	51.47167	YES	YES
107	a	697.58	27.61699	YES	YES
108	a	700.86	1.14587	YES	YES
109	a	703.38	24.33877	YES	YES
110	a	704.62	24.29317	YES	YES
111	a	705.45	24.14456	YES	YES
112	a	741.48	4.55617	YES	YES
113	a	742.20	3.96429	YES	YES
114	a	743.13	8.58898	YES	YES
115	a	745.62	2.68958	YES	YES
116	a	746.46	6.92413	YES	YES
117	a	748.22	5.08264	YES	YES
118	a	756.03	17.32560	YES	YES
119	a	774.95	3.92061	YES	YES
120	a	790.80	2.10654	YES	YES
121	a	834.15	0.37414	YES	YES
122	a	834.83	1.14272	YES	YES
123	a	839.27	0.31362	YES	YES
124	a	840.44	0.75746	YES	YES
125	a	842.14	0.44199	YES	YES
126	a	845.56	0.90648	YES	YES
127	a	849.31	1.01519	YES	YES
128	a	906.40	0.19005	YES	YES
129	a	907.61	1.66397	YES	YES
130	a	913.38	1.23930	YES	YES
131	a	913.45	0.64794	YES	YES
132	a	915.93	1.90178	YES	YES
133	a	917.88	0.07639	YES	YES
134	a	921.97	1.75012	YES	YES
135	a	925.69	0.14162	YES	YES
136	a	952.47	9.88025	YES	YES
137	a	957.58	0.04571	YES	YES
138	a	959.62	1.07021	YES	YES
139	a	963.12	0.44652	YES	YES
140	a	963.60	0.19538	YES	YES
141	a	965.25	0.29149	YES	YES
142	a	967.42	0.15968	YES	YES
143	a	973.38	0.26970	YES	YES
144	a	980.51	0.39882	YES	YES
145	a	981.40	0.60667	YES	YES
146	a	982.05	0.13360	YES	YES
147	a	982.62	0.71141	YES	YES
148	a	983.04	0.51169	YES	YES
149	a	983.58	0.71608	YES	YES
150	a	984.54	1.20843	YES	YES
151	a	985.18	0.22610	YES	YES
152	a	985.61	1.36873	YES	YES
153	a	986.00	1.28429	YES	YES
154	a	986.41	0.01641	YES	YES
155	a	986.72	2.56712	YES	YES
156	a	987.16	3.60653	YES	YES
157	a	988.41	1.87471	YES	YES
158	a	991.28	1.68522	YES	YES
159	a	1002.01	0.33486	YES	YES
160	a	1017.96	9.67724	YES	YES
161	a	1024.03	2.61347	YES	YES
162	a	1024.40	1.64474	YES	YES
163	a	1024.54	0.81281	YES	YES
164	a	1024.72	2.09592	YES	YES

165	a	1025.09	1.19663	YES	YES
166	a	1025.40	1.93713	YES	YES
167	a	1026.34	5.85414	YES	YES
168	a	1027.34	19.16288	YES	YES
169	a	1070.93	3.89088	YES	YES
170	a	1071.90	2.74250	YES	YES
171	a	1072.63	14.67967	YES	YES
172	a	1073.68	3.43853	YES	YES
173	a	1074.84	14.29321	YES	YES
174	a	1075.22	5.15127	YES	YES
175	a	1075.56	9.20205	YES	YES
176	a	1076.13	1.53106	YES	YES
177	a	1077.15	13.26905	YES	YES
178	a	1078.03	22.17042	YES	YES
179	a	1078.56	9.80418	YES	YES
180	a	1083.11	14.28137	YES	YES
181	a	1083.73	3.96713	YES	YES
182	a	1138.38	0.14217	YES	YES
183	a	1141.28	0.77317	YES	YES
184	a	1141.35	0.14856	YES	YES
185	a	1141.40	0.54797	YES	YES
186	a	1141.50	0.29295	YES	YES
187	a	1141.61	0.53144	YES	YES
188	a	1141.88	0.54890	YES	YES
189	a	1158.20	1.69895	YES	YES
190	a	1167.87	3.75802	YES	YES
191	a	1169.14	3.08425	YES	YES
192	a	1170.14	4.64421	YES	YES
193	a	1170.46	4.02769	YES	YES
194	a	1172.04	7.46679	YES	YES
195	a	1176.58	11.42369	YES	YES
196	a	1189.02	0.12241	YES	YES
197	a	1291.67	11.91875	YES	YES
198	a	1292.41	3.44235	YES	YES

* zero point VIBRATIONAL energy : 0.7448612 Hartree *

Trans 2_by



bp86-SVP SCF energy: -2931.4445618840
pbe-TZVPP SCF energy: -2930.992301324

XYZ Coordinates
97

C	3.34789	1.05207	1.29575
C	3.19208	-1.53432	-0.01381
C	3.35639	0.98658	-1.55673
C	-2.94968	2.20852	0.26502
C	-3.13893	0.02715	-1.65549
C	-3.30199	-0.51410	1.18669
C	0.12529	2.84206	-0.54294
C	0.03502	4.31807	-0.82316
H	0.63853	4.88736	-0.08679
H	-1.02585	4.63880	-0.71606
H	0.36688	4.54315	-1.85733
C	-0.19529	-0.40152	2.74540
C	0.04299	-1.33797	3.93192
H	-0.19869	-0.81321	4.87788
H	-0.61567	-2.22961	3.83859
H	1.09349	-1.69803	3.95135
O	-0.00122	1.98000	-1.49100
O	0.28752	2.38568	0.63472
O	0.28795	-0.86682	1.61938
O	-0.79085	0.67534	2.87996
P	2.49867	0.18270	-0.11245
P	-2.33028	0.48057	-0.04189
Ru	0.08709	0.30252	-0.12774
C	4.52318	2.38778	-3.72903
C	3.85500	3.09055	-2.71067
C	3.27663	2.39727	-1.63735
C	4.04201	0.29271	-2.57540
C	4.61856	0.98945	-3.65336
H	4.97711	2.93140	-4.57420
H	3.78692	4.19052	-2.74886
H	2.78151	2.96315	-0.83178
H	4.15493	-0.80041	-2.52619
H	5.15567	0.42754	-4.43580
C	4.13235	-4.20296	0.18546
C	4.29174	-3.31331	1.26094
C	3.82628	-1.99122	1.16395
C	3.01147	-2.44796	-1.08041
C	3.48784	-3.76587	-0.98342
H	4.50041	-5.23956	0.26186
H	4.78536	-3.64788	2.18868
H	3.95997	-1.30920	2.01701
H	2.47208	-2.14151	-1.98840
H	3.33665	-4.45962	-1.82642
C	4.69206	2.33122	3.42723
C	5.41960	1.85690	2.32018
C	4.75243	1.22291	1.26127
C	2.62326	1.53419	2.40516
C	3.29815	2.16939	3.46449
H	5.21519	2.83256	4.25891
H	6.51446	1.98303	2.27914
H	5.33154	0.85658	0.39718
H	1.52818	1.44327	2.44116
H	2.71826	2.54556	4.32346
C	-3.83769	4.82968	0.84594
C	-4.22000	4.20508	-0.35311
C	-3.78117	2.90019	-0.64250
C	-2.56205	2.84294	1.46948
C	-3.01253	4.14241	1.75454
H	-4.18601	5.85116	1.07467
H	-4.87204	4.73125	-1.07055
H	-4.10077	2.42027	-1.58044
H	-1.91067	2.30293	2.17543
H	-2.70883	4.62365	2.69937
C	-4.80570	-2.12109	2.96331
C	-5.20422	-0.80029	2.69521
C	-4.46011	-0.00132	1.81086
C	-2.90504	-1.83960	1.46346
C	-3.65584	-2.63826	2.34270
H	-5.39151	-2.74671	3.65748
H	-6.10434	-0.38373	3.17746
H	-4.78495	1.03115	1.60942
H	-1.99996	-2.25277	0.99565
H	-3.33242	-3.67308	2.54346
C	-4.28364	-0.61564	-4.16361
C	-3.23690	0.32092	-4.08317
C	-2.66148	0.63466	-2.84139
C	-4.18822	-0.91094	-1.74476
C	-4.75390	-1.23141	-2.99260
H	-4.73040	-0.86619	-5.14036
H	-2.85910	0.80884	-4.99751
H	-1.83357	1.36072	-2.78493
H	-4.57093	-1.39948	-0.83518
H	-5.57270	-1.96852	-3.04471
C	-0.12107	-1.71478	-1.06379
C	0.05695	-0.76631	-1.90489
C	-0.35735	-3.10659	-0.75955
H	0.21973	-0.36912	-2.91108
C	-0.82210	-5.86688	-0.27905
C	-1.26392	-5.27291	-1.47654
C	-1.03929	-3.91094	-1.71606
C	0.07978	-3.71651	0.44606
C	-0.15240	-5.08099	0.67602
H	-1.00136	-6.93883	-0.09168
H	-1.79420	-5.87824	-2.23121
H	-1.39633	-3.44396	-2.64798
H	0.59684	-3.09197	1.18819
H	0.20152	-5.53897	1.61513

Vibrational Frequencies

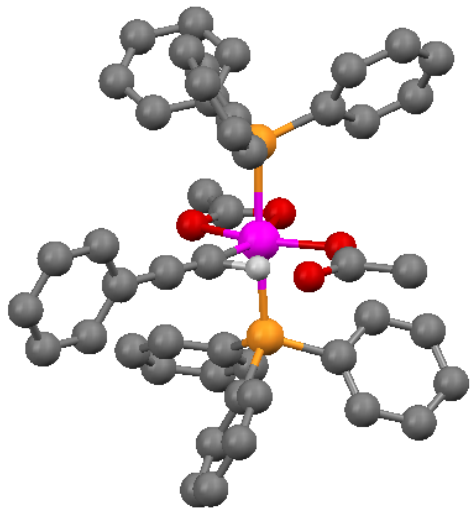
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.62	0.04281	YES	YES
8	a	16.21	0.11333	YES	YES
9	a	20.66	0.05555	YES	YES
10	a	24.57	0.06999	YES	YES
11	a	28.83	0.00160	YES	YES
12	a	31.50	0.10345	YES	YES
13	a	38.41	0.27731	YES	YES
14	a	39.49	0.09256	YES	YES
15	a	46.29	0.10189	YES	YES

16	a	48.90	0.10307	YES	YES
17	a	53.22	0.42135	YES	YES
18	a	55.87	1.17341	YES	YES
19	a	56.94	1.05557	YES	YES
20	a	59.07	0.25565	YES	YES
21	a	60.11	0.48083	YES	YES
22	a	61.86	0.68856	YES	YES
23	a	63.18	0.09534	YES	YES
24	a	68.58	2.71732	YES	YES
25	a	72.69	0.57133	YES	YES
26	a	76.42	0.69729	YES	YES
27	a	79.90	1.03948	YES	YES
28	a	82.39	0.23133	YES	YES
29	a	85.10	1.96331	YES	YES
30	a	89.99	1.44387	YES	YES
31	a	96.88	0.41358	YES	YES
32	a	99.41	1.71602	YES	YES
33	a	99.89	0.04831	YES	YES
34	a	104.78	2.45545	YES	YES
35	a	113.42	3.57953	YES	YES
36	a	132.10	1.04598	YES	YES
37	a	138.74	0.93739	YES	YES
38	a	141.44	1.15258	YES	YES
39	a	147.40	0.18836	YES	YES
40	a	155.38	1.89895	YES	YES
41	a	171.82	2.45019	YES	YES
42	a	177.52	1.81481	YES	YES
43	a	188.47	0.62544	YES	YES
44	a	192.08	2.42968	YES	YES
45	a	196.92	1.15996	YES	YES
46	a	197.68	1.37591	YES	YES
47	a	209.84	0.80036	YES	YES
48	a	216.23	1.41572	YES	YES
49	a	221.13	1.51125	YES	YES
50	a	223.84	3.68043	YES	YES
51	a	241.55	2.58587	YES	YES
52	a	245.26	1.18435	YES	YES
53	a	246.76	0.76644	YES	YES
54	a	248.88	0.06614	YES	YES
55	a	255.32	0.65616	YES	YES
56	a	261.63	0.31372	YES	YES
57	a	267.06	2.99282	YES	YES
58	a	267.93	0.18120	YES	YES
59	a	292.04	8.74225	YES	YES
60	a	334.25	9.76651	YES	YES
61	a	354.90	1.17365	YES	YES
62	a	396.15	1.09018	YES	YES
63	a	397.77	0.44113	YES	YES
64	a	399.40	29.29524	YES	YES
65	a	400.08	1.63062	YES	YES
66	a	402.68	1.57441	YES	YES
67	a	405.16	2.22992	YES	YES
68	a	406.31	0.10887	YES	YES
69	a	409.48	0.83731	YES	YES
70	a	415.77	4.05315	YES	YES
71	a	428.00	5.34006	YES	YES
72	a	435.35	5.03117	YES	YES
73	a	447.20	13.40134	YES	YES
74	a	454.78	14.74056	YES	YES
75	a	467.98	0.50334	YES	YES
76	a	478.25	13.86786	YES	YES
77	a	486.49	14.17176	YES	YES
78	a	498.74	0.92352	YES	YES
79	a	498.96	18.87902	YES	YES
80	a	502.12	23.78875	YES	YES
81	a	508.05	56.87973	YES	YES
82	a	513.15	135.08759	YES	YES
83	a	514.11	84.82441	YES	YES
84	a	525.53	7.08453	YES	YES
85	a	534.67	22.09061	YES	YES
86	a	544.10	1.16729	YES	YES
87	a	586.66	5.60570	YES	YES
88	a	599.72	3.75545	YES	YES
89	a	608.94	1.34776	YES	YES
90	a	609.57	1.79455	YES	YES
91	a	609.89	0.35784	YES	YES
92	a	610.19	0.18006	YES	YES
93	a	610.52	1.73467	YES	YES
94	a	611.98	0.00819	YES	YES
95	a	613.16	1.42823	YES	YES
96	a	664.15	32.35098	YES	YES
97	a	667.58	24.86950	YES	YES
98	a	671.07	21.34469	YES	YES
99	a	671.53	19.44507	YES	YES
100	a	673.31	2.75819	YES	YES
101	a	685.74	4.64407	YES	YES
102	a	686.41	7.08313	YES	YES
103	a	689.59	8.05234	YES	YES
104	a	690.24	24.24699	YES	YES
105	a	693.12	34.84793	YES	YES
106	a	695.66	31.14103	YES	YES
107	a	697.46	44.55152	YES	YES
108	a	701.29	30.48639	YES	YES
109	a	702.34	37.81365	YES	YES
110	a	704.34	5.40558	YES	YES
111	a	706.14	23.92225	YES	YES
112	a	735.75	6.59005	YES	YES
113	a	741.39	4.35752	YES	YES
114	a	743.75	7.53777	YES	YES
115	a	745.33	2.07487	YES	YES
116	a	746.62	5.88440	YES	YES
117	a	748.04	7.55660	YES	YES
118	a	757.86	14.82619	YES	YES
119	a	769.76	0.28490	YES	YES
120	a	831.32	0.19634	YES	YES
121	a	832.16	0.99322	YES	YES
122	a	835.32	0.18349	YES	YES
123	a	839.54	1.75443	YES	YES
124	a	840.58	8.45558	YES	YES
125	a	842.51	0.19965	YES	YES
126	a	846.98	1.12373	YES	YES
127	a	850.18	0.80546	YES	YES
128	a	903.20	0.71178	YES	YES
129	a	904.65	1.17107	YES	YES
130	a	907.47	3.50444	YES	YES
131	a	911.27	0.48561	YES	YES
132	a	918.85	1.45945	YES	YES
133	a	920.56	0.46223	YES	YES
134	a	921.30	0.23771	YES	YES
135	a	925.00	0.07421	YES	YES
136	a	949.10	16.61406	YES	YES
137	a	955.17	0.57363	YES	YES
138	a	957.33	0.20618	YES	YES
139	a	959.69	0.64920	YES	YES
140	a	961.55	0.77883	YES	YES
141	a	967.90	0.04199	YES	YES
142	a	970.47	0.15535	YES	YES
143	a	972.51	0.28356	YES	YES
144	a	978.15	1.58329	YES	YES
145	a	980.39	0.64016	YES	YES
146	a	981.72	0.77926	YES	YES
147	a	981.95	0.07795	YES	YES
148	a	982.22	0.07542	YES	YES
149	a	982.76	0.80149	YES	YES
150	a	983.15	0.61437	YES	YES
151	a	983.25	1.64838	YES	YES
152	a	984.47	0.11197	YES	YES
153	a	985.12	2.54965	YES	YES
154	a	985.83	2.98529	YES	YES
155	a	986.87	0.84164	YES	YES
156	a	987.73	6.17013	YES	YES
157	a	991.20	0.17697	YES	YES
158	a	991.24	0.10628	YES	YES
159	a	999.40	0.08091	YES	YES
160	a	1016.37	8.70637	YES	YES
161	a	1023.38	0.89556	YES	YES
162	a	1023.79	1.93919	YES	YES
163	a	1024.27	1.75398	YES	YES

164	a	1024.52	1.17775	YES	YES
165	a	1025.03	20.80608	YES	YES
166	a	1025.25	2.88969	YES	YES
167	a	1025.45	5.89193	YES	YES
168	a	1026.11	1.03140	YES	YES
169	a	1069.04	2.14739	YES	YES
170	a	1072.82	6.30726	YES	YES
171	a	1072.96	1.20649	YES	YES
172	a	1073.96	2.30807	YES	YES
173	a	1074.37	18.11329	YES	YES
174	a	1075.71	1.41120	YES	YES
175	a	1076.38	15.04587	YES	YES
176	a	1076.57	24.60517	YES	YES
177	a	1076.92	5.64150	YES	YES
178	a	1078.61	11.43948	YES	YES
179	a	1080.39	4.57709	YES	YES
180	a	1082.26	8.15735	YES	YES
181	a	1083.15	5.86933	YES	YES
182	a	1137.99	0.17673	YES	YES
183	a	1140.56	0.44099	YES	YES
184	a	1141.78	0.48867	YES	YES
185	a	1142.13	0.41844	YES	YES
186	a	1142.55	0.19825	YES	YES
187	a	1142.70	0.67942	YES	YES
188	a	1143.06	0.38069	YES	YES
189	a	1155.36	2.49190	YES	YES
190	a	1166.58	1.12861	YES	YES
191	a	1169.40	3.75139	YES	YES
192	a	1169.65	3.23211	YES	YES
193	a	1171.59	6.34758	YES	YES
194	a	1175.16	2.17112	YES	YES
195	a	1178.76	12.38244	YES	YES
196	a	1187.60	0.75098	YES	YES
197	a	1288.31	12.11793	YES	YES
198	a	1290.46	9.96027	YES	YES

* zero point VIBRATIONAL energy : 0.7448881 Hartree *

Trans TS_{34}*_s*



bp86-SVP SCF energy: -2931.4461375830
pbe-TZVPP SCF energy: -2930.989367005

XYZ Coordinates
97

C	-1.12136	-3.40321	0.26675
C	0.43324	-3.07760	-2.16001
C	1.74625	-3.14898	0.44834
C	-0.92247	3.44729	0.34361
C	1.93586	3.05757	0.38391
C	0.49852	3.04370	-2.15709
C	2.80017	-0.06702	0.09883
C	4.27014	-0.09316	0.42403
H	4.54607	0.83699	0.96800
H	4.87128	-0.17166	-0.50326
H	4.49092	-0.95333	1.09222
C	-2.05565	0.08436	-2.21340
C	-2.70807	0.17613	-3.57849
H	-3.71062	-0.29690	-3.55856
H	-2.83983	1.25007	-3.83969
H	-2.06825	-0.29275	-4.35225
O	2.37914	-0.05386	-1.11495
O	1.92129	-0.05070	1.02942
O	-0.77932	0.01554	-2.17295
O	-2.78963	0.11088	-1.17244
P	0.28822	-2.40878	-0.43219
P	0.40230	2.38738	-0.42198
Ru	0.28210	-0.01173	-0.36530
C	3.93253	-4.19475	1.90313
C	2.95216	-3.42468	2.55660
C	1.87089	-2.89659	1.83468
C	2.73196	-3.92049	-0.20086
C	3.82129	-4.43821	0.52439
H	4.78452	-4.60470	2.47108
H	3.03366	-3.22522	3.63805
H	1.11585	-2.28065	2.34913
H	2.65009	-4.12579	-1.28009
H	4.58443	-5.04100	0.00418
C	0.72629	-4.02029	-4.80968
C	-0.17335	-4.64812	-3.93251
C	-0.31848	-4.18283	-2.61363
C	1.32920	-2.44239	-3.05119
C	1.47846	-2.91909	-4.36369
H	0.83928	-4.38713	-5.84368
H	-0.77027	-5.51051	-4.27406
H	-1.02631	-4.68637	-1.93634
H	1.91182	-1.57290	-2.70623
H	2.18413	-2.41767	-5.04708
C	-3.30186	-4.94923	1.20205
C	-1.98376	-5.39138	1.40560
C	-0.90076	-4.62594	0.93987
C	-2.44930	-2.96320	0.07091
C	-3.52962	-3.73490	0.53231
H	-4.15123	-5.55048	1.56742
H	-1.79183	-6.34247	1.92997
H	0.12558	-4.98986	1.10278
H	-2.65502	-2.01017	-0.43968
H	-4.55869	-3.37332	0.37164
C	-2.97796	5.07756	1.41095
C	-1.63140	5.44783	1.56465
C	-0.61031	4.64051	1.03367
C	-2.27928	3.08256	0.19325
C	-3.29680	3.89547	0.72137
H	-3.77868	5.70928	1.83048
H	-1.36761	6.37465	2.10115
H	0.43916	4.94861	1.15876
H	-2.55718	2.15851	-0.33623
H	-4.34905	3.59006	0.59919
C	0.70866	3.95590	-4.82451
C	-0.12909	4.62216	-3.91485
C	-0.23241	4.17212	-2.58652
C	1.33174	2.37019	-3.08044
C	1.44075	2.83196	-4.40204
H	0.78899	4.31068	-5.86574
H	-0.70896	5.50315	-4.23782
H	-0.89044	4.70556	-1.88224
H	1.89660	1.48220	-2.75353
H	2.09741	2.30085	-5.11128
C	4.23705	4.00544	1.72549
C	3.25404	3.28587	2.43020
C	2.11525	2.80673	1.76448
C	2.92492	3.77834	-0.31653
C	4.07084	4.24741	0.35201
H	5.13364	4.37750	2.24912
H	3.37785	3.08822	3.50799
H	1.35738	2.23101	2.31922
H	2.80128	3.98240	-1.39194
H	4.83522	4.81131	-0.20844
C	-1.79444	0.02064	2.10280
C	-1.16417	0.01331	1.01317
C	-2.54136	0.03612	3.31002
H	-1.86746	0.06113	-0.06956
C	-4.02572	0.06727	5.73763
C	-3.37218	1.23171	5.29091
C	-2.64335	1.22231	4.09531
C	-3.20913	-1.13398	3.77900
C	-3.94136	-1.11137	4.97235
H	-4.60006	0.07945	6.67892
H	-3.43272	2.15962	5.88432
H	-2.13586	2.13505	3.74287
H	-3.14265	-2.05620	3.18038
H	-4.45309	-2.02714	5.31370

Vibrational Frequencies

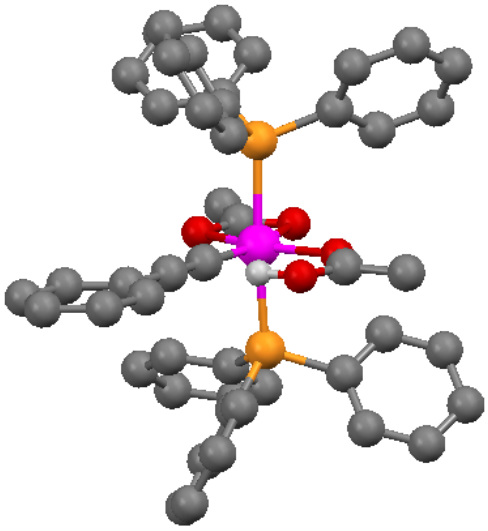
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-215.98	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	9.12	0.01210	YES	YES
9	a	12.50	0.03028	YES	YES
10	a	17.45	0.06769	YES	YES
11	a	20.17	0.02084	YES	YES
12	a	23.16	0.08591	YES	YES
13	a	27.86	0.19657	YES	YES
14	a	34.76	0.03866	YES	YES
15	a	36.40	0.04749	YES	YES
16	a	38.36	0.02025	YES	YES

17	a	42.26	0.07467	YES	YES
18	a	44.09	0.15272	YES	YES
19	a	49.83	0.21148	YES	YES
20	a	51.27	0.16758	YES	YES
21	a	54.12	0.31364	YES	YES
22	a	56.26	0.53171	YES	YES
23	a	57.87	0.14963	YES	YES
24	a	58.59	0.95926	YES	YES
25	a	60.01	0.45914	YES	YES
26	a	63.96	2.05779	YES	YES
27	a	65.24	0.20240	YES	YES
28	a	72.94	1.41244	YES	YES
29	a	74.03	0.69294	YES	YES
30	a	78.52	0.66074	YES	YES
31	a	81.10	0.66264	YES	YES
32	a	86.21	0.37549	YES	YES
33	a	93.18	0.19115	YES	YES
34	a	98.25	0.10353	YES	YES
35	a	106.46	3.16825	YES	YES
36	a	117.06	6.29375	YES	YES
37	a	132.77	3.88951	YES	YES
38	a	141.55	0.63330	YES	YES
39	a	161.30	2.14876	YES	YES
40	a	175.67	66.85095	YES	YES
41	a	182.79	10.99971	YES	YES
42	a	185.38	0.58326	YES	YES
43	a	190.99	0.85199	YES	YES
44	a	193.98	1.46259	YES	YES
45	a	195.89	0.68715	YES	YES
46	a	209.89	0.07957	YES	YES
47	a	216.86	5.36329	YES	YES
48	a	221.80	0.27557	YES	YES
49	a	226.54	5.84464	YES	YES
50	a	229.70	21.99726	YES	YES
51	a	240.34	3.04424	YES	YES
52	a	240.98	0.80684	YES	YES
53	a	253.48	0.10105	YES	YES
54	a	255.64	0.99151	YES	YES
55	a	256.58	1.82913	YES	YES
56	a	258.54	2.37914	YES	YES
57	a	262.22	0.36866	YES	YES
58	a	263.71	0.12363	YES	YES
59	a	318.49	1.87228	YES	YES
60	a	340.35	33.05098	YES	YES
61	a	360.88	5.53170	YES	YES
62	a	388.32	18.93072	YES	YES
63	a	397.74	0.26371	YES	YES
64	a	398.17	1.12933	YES	YES
65	a	398.80	0.21348	YES	YES
66	a	399.99	0.86737	YES	YES
67	a	402.64	0.48289	YES	YES
68	a	403.36	14.22082	YES	YES
69	a	404.87	2.61644	YES	YES
70	a	406.29	30.72733	YES	YES
71	a	423.91	13.05908	YES	YES
72	a	432.71	0.32730	YES	YES
73	a	440.13	2.92077	YES	YES
74	a	442.19	24.41918	YES	YES
75	a	449.39	11.84734	YES	YES
76	a	469.15	20.33426	YES	YES
77	a	492.20	75.44934	YES	YES
78	a	494.02	2.28197	YES	YES
79	a	500.14	21.93591	YES	YES
80	a	502.98	59.64576	YES	YES
81	a	504.46	0.73163	YES	YES
82	a	509.02	81.90505	YES	YES
83	a	511.88	198.27029	YES	YES
84	a	520.21	59.19459	YES	YES
85	a	527.16	0.37854	YES	YES
86	a	556.76	35.33952	YES	YES
87	a	604.52	1.34635	YES	YES
88	a	608.22	2.89435	YES	YES
89	a	609.06	1.17735	YES	YES
90	a	609.25	0.15740	YES	YES
91	a	609.54	0.96657	YES	YES
92	a	609.97	1.42604	YES	YES
93	a	610.17	2.72792	YES	YES
94	a	610.53	0.44024	YES	YES
95	a	612.84	0.06568	YES	YES
96	a	663.97	113.38897	YES	YES
97	a	667.81	56.89501	YES	YES
98	a	672.69	16.59040	YES	YES
99	a	674.43	1.65692	YES	YES
100	a	686.84	1.36210	YES	YES
101	a	687.48	0.81504	YES	YES
102	a	688.01	16.73088	YES	YES
103	a	688.23	23.15721	YES	YES
104	a	689.21	20.41986	YES	YES
105	a	697.13	47.06429	YES	YES
106	a	698.28	24.38434	YES	YES
107	a	700.56	5.09200	YES	YES
108	a	701.45	27.32912	YES	YES
109	a	702.44	46.60239	YES	YES
110	a	702.74	33.87646	YES	YES
111	a	742.50	1.95227	YES	YES
112	a	743.91	13.23077	YES	YES
113	a	744.83	1.89971	YES	YES
114	a	745.73	4.31201	YES	YES
115	a	746.39	1.89464	YES	YES
116	a	747.39	9.06397	YES	YES
117	a	754.86	57.59437	YES	YES
118	a	769.30	53.88768	YES	YES
119	a	825.77	0.09129	YES	YES
120	a	836.53	0.05739	YES	YES
121	a	837.81	0.27110	YES	YES
122	a	841.11	1.88874	YES	YES
123	a	842.02	3.54077	YES	YES
124	a	843.76	2.45891	YES	YES
125	a	845.89	0.58095	YES	YES
126	a	864.62	106.98163	YES	YES
127	a	899.20	1.17408	YES	YES
128	a	908.37	0.80078	YES	YES
129	a	910.19	0.67722	YES	YES
130	a	915.07	11.77067	YES	YES
131	a	918.39	0.32645	YES	YES
132	a	919.28	6.63407	YES	YES
133	a	920.45	5.17970	YES	YES
134	a	924.05	238.80345	YES	YES
135	a	945.30	19.46352	YES	YES
136	a	954.29	0.10671	YES	YES
137	a	959.34	0.12793	YES	YES
138	a	960.34	0.40555	YES	YES
139	a	960.72	8.59836	YES	YES
140	a	967.64	1.37960	YES	YES
141	a	967.95	0.47592	YES	YES
142	a	969.97	0.20437	YES	YES
143	a	974.10	0.00280	YES	YES
144	a	979.06	2.24563	YES	YES
145	a	980.11	2.71299	YES	YES
146	a	981.88	0.19621	YES	YES
147	a	981.99	0.93157	YES	YES
148	a	982.11	0.41784	YES	YES
149	a	982.70	0.26101	YES	YES
150	a	983.16	5.78849	YES	YES
151	a	983.62	0.08608	YES	YES
152	a	983.92	0.43956	YES	YES
153	a	984.96	2.74718	YES	YES
154	a	985.59	4.98938	YES	YES
155	a	988.52	0.00133	YES	YES
156	a	991.13	1.78247	YES	YES
157	a	991.29	1.08926	YES	YES
158	a	1000.56	4.10004	YES	YES
159	a	1013.29	39.28544	YES	YES
160	a	1022.34	4.20622	YES	YES
161	a	1022.96	1.25609	YES	YES
162	a	1023.20	2.20469	YES	YES
163	a	1024.51	0.30498	YES	YES
164	a	1025.20	0.59059	YES	YES

165	a	1025.51	2.78707	YES	YES
166	a	1027.04	1.59169	YES	YES
167	a	1028.07	2.32786	YES	YES
168	a	1028.43	28.52893	YES	YES
169	a	1067.15	2.99593	YES	YES
170	a	1073.24	4.36074	YES	YES
171	a	1073.50	8.09112	YES	YES
172	a	1075.25	3.69099	YES	YES
173	a	1075.70	12.61587	YES	YES
174	a	1075.98	8.15569	YES	YES
175	a	1076.20	45.91377	YES	YES
176	a	1077.03	23.63594	YES	YES
177	a	1077.32	9.11089	YES	YES
178	a	1078.22	12.83663	YES	YES
179	a	1080.70	15.81188	YES	YES
180	a	1083.59	10.19204	YES	YES
181	a	1084.09	29.91772	YES	YES
182	a	1101.46	1072.68929	YES	YES
183	a	1136.64	0.05740	YES	YES
184	a	1141.52	0.19520	YES	YES
185	a	1141.80	0.29922	YES	YES
186	a	1142.11	0.32982	YES	YES
187	a	1142.33	0.40853	YES	YES
188	a	1142.57	0.32076	YES	YES
189	a	1142.61	0.87398	YES	YES
190	a	1155.70	48.09182	YES	YES
191	a	1168.50	0.90879	YES	YES
192	a	1169.04	8.63036	YES	YES
193	a	1172.35	3.65116	YES	YES
194	a	1173.53	5.93123	YES	YES
195	a	1175.90	19.09178	YES	YES
196	a	1176.58	2.83808	YES	YES
197	a	1229.39	103.04199	YES	YES
198	a	1282.67	0.00780	YES	YES

* zero point VIBRATIONAL energy : 0.7405991 Hartree *

Trans 4



bp86-SVP SCF energy: -2931.4513639140
pbe-TZVPP SCF energy: -2931.005785750

XYZ Coordinates
97

C	-0.06838	-3.47372	1.03629
C	-1.40694	-3.03991	-1.50184
C	1.50848	-3.09926	-1.34147
C	-0.07260	3.48027	1.00535
C	1.52456	3.08074	-1.35297
C	-1.39065	3.02570	-1.53809
C	1.76707	-0.01969	-2.26683
C	2.87244	-0.07645	-3.28993
H	3.76688	0.46888	-2.92640
H	2.52578	0.35006	-4.25281
H	3.15845	-1.13948	-3.45642
C	-2.91498	0.01513	0.59883
C	-4.39788	0.07433	0.34041
H	-4.94962	-0.51198	1.10352
H	-4.73619	1.13247	0.41419
H	-4.62221	-0.29629	-0.67836
O	0.53541	-0.01753	-2.60866
O	2.04809	-0.00601	-1.01207
O	-2.09985	-0.00020	-0.34770
O	-2.56463	0.01143	1.87184
P	0.01377	-2.40458	-0.48324
P	0.02109	2.39542	-0.50308
Ru	0.02190	-0.00431	-0.36786
C	3.86139	-4.09706	-2.54937
C	3.93813	-3.36827	-1.34797
C	2.77219	-2.86454	-0.75112
C	1.43842	-3.82806	-2.54634
C	2.61061	-4.32243	-3.14777
H	4.77926	-4.48847	-3.01933
H	4.91633	-3.18277	-0.87411
H	2.84046	-2.28409	0.18255
H	0.46237	-4.01852	-3.01973
H	2.54082	-4.89371	-4.08860
C	-3.56662	-3.90312	-3.10955
C	-3.25543	-4.58347	-1.92075
C	-2.17966	-4.15802	-1.12143
C	-1.72883	-2.35481	-2.69675
C	-2.79741	-2.79125	-3.49639
H	-4.41021	-4.23916	-3.73580
H	-3.85277	-5.45708	-1.60958
H	-1.94373	-4.70357	-0.19371
H	-1.12768	-1.48104	-2.99820
H	-3.03483	-2.25164	-4.42866
C	-0.29334	-5.10284	3.34301
C	0.56624	-5.47504	2.29594
C	0.67794	-4.66818	1.15016
C	-0.93267	-3.11204	2.09252
C	-1.04542	-3.92089	3.23541
H	-0.37446	-5.73174	4.24510
H	1.15946	-6.40193	2.36731
H	1.35368	-4.97677	0.33812
H	-1.52100	-2.18678	2.03170
H	-1.71617	-3.61233	4.05374
C	-0.31588	5.13772	3.29013
C	0.53835	5.50620	2.23726
C	0.65931	4.68523	1.10256
C	-0.93174	3.12263	2.06697
C	-1.05343	3.94534	3.19915
H	-0.40404	5.77771	4.18372
H	1.12019	6.44120	2.29556
H	1.33130	4.99064	0.28616
H	-1.50873	2.18955	2.01945
H	-1.71966	3.63938	4.02215
C	-3.53695	3.88105	-3.16851
C	-3.23723	4.56595	-1.97935
C	-2.16804	4.14457	-1.16890
C	-1.70173	2.33583	-2.73313
C	-2.76347	2.76832	-3.54388
H	-4.37520	4.21384	-3.80358
H	-3.83767	5.44065	-1.67722
H	-1.94065	4.69458	-0.24168
H	-1.09849	1.46026	-3.02490
H	-2.99242	2.22450	-4.47580
C	3.88923	4.08038	-2.53581
C	3.95299	3.35950	-1.32894
C	2.78123	2.85446	-0.74467
C	1.46778	3.80108	-2.56353
C	2.64595	4.29648	-3.15216
H	4.81156	4.47302	-2.99588
H	4.92546	3.18208	-0.84024
H	2.83914	2.28060	0.19386
H	0.49733	3.98543	-3.05074
H	2.58658	4.86061	-4.09799
C	0.32571	0.00882	2.81286
C	0.21986	0.00407	1.55986
C	0.52650	0.01686	4.22618
H	-1.51440	0.00651	1.97076
C	0.94056	0.03389	7.04986
C	2.03732	0.04930	6.16754
C	1.83885	0.04089	4.78083
C	-0.57085	0.00204	5.13568
C	-0.36317	0.01031	6.52210
H	1.10162	0.04048	8.14077
H	3.06546	0.06796	6.56808
H	2.70140	0.05276	4.09556
H	-1.59656	-0.01584	4.73202
H	-1.23292	-0.00161	7.20123

Vibrational Frequencies

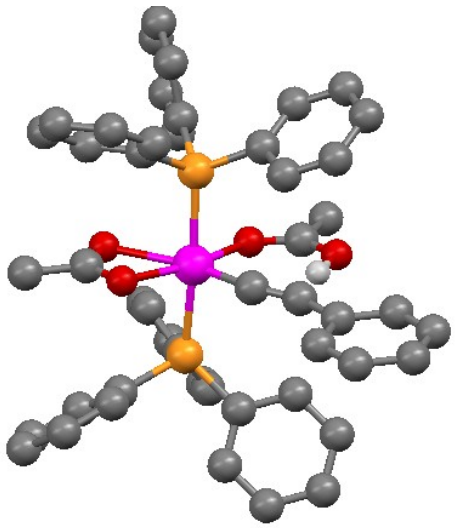
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.95	0.00560	YES	YES
8	a	12.54	0.03311	YES	YES
9	a	15.24	0.05082	YES	YES
10	a	16.98	0.02983	YES	YES
11	a	18.55	0.17774	YES	YES
12	a	22.24	0.05882	YES	YES
13	a	29.48	0.10825	YES	YES
14	a	34.86	0.19289	YES	YES
15	a	36.54	0.06604	YES	YES

16	a	39.85	0.42072	YES	YES
17	a	42.78	0.43284	YES	YES
18	a	45.33	0.00949	YES	YES
19	a	46.84	0.12298	YES	YES
20	a	48.92	0.22536	YES	YES
21	a	52.08	0.32216	YES	YES
22	a	52.95	0.24673	YES	YES
23	a	57.53	0.07308	YES	YES
24	a	60.04	0.48389	YES	YES
25	a	60.60	0.46828	YES	YES
26	a	61.79	0.49911	YES	YES
27	a	71.31	0.01856	YES	YES
28	a	73.77	3.09500	YES	YES
29	a	77.47	0.26690	YES	YES
30	a	79.04	0.00573	YES	YES
31	a	80.75	0.54577	YES	YES
32	a	83.32	0.84637	YES	YES
33	a	90.58	1.16372	YES	YES
34	a	106.74	3.08006	YES	YES
35	a	111.99	0.61077	YES	YES
36	a	117.40	0.79325	YES	YES
37	a	126.28	1.41547	YES	YES
38	a	140.70	0.35557	YES	YES
39	a	156.70	2.57895	YES	YES
40	a	167.26	0.02508	YES	YES
41	a	190.02	1.28100	YES	YES
42	a	191.37	1.63807	YES	YES
43	a	192.87	1.37412	YES	YES
44	a	194.52	1.35508	YES	YES
45	a	208.80	0.26324	YES	YES
46	a	210.77	8.77555	YES	YES
47	a	215.12	0.82269	YES	YES
48	a	221.09	0.06031	YES	YES
49	a	226.21	5.61998	YES	YES
50	a	239.32	1.76971	YES	YES
51	a	239.76	0.77802	YES	YES
52	a	243.22	2.79613	YES	YES
53	a	252.02	0.09328	YES	YES
54	a	253.71	1.07384	YES	YES
55	a	257.01	0.04709	YES	YES
56	a	261.04	1.49372	YES	YES
57	a	263.50	0.08508	YES	YES
58	a	291.36	0.17864	YES	YES
59	a	297.28	2.70345	YES	YES
60	a	324.58	11.30613	YES	YES
61	a	397.42	0.61462	YES	YES
62	a	397.68	0.55339	YES	YES
63	a	398.17	0.15454	YES	YES
64	a	398.99	0.23586	YES	YES
65	a	401.49	30.09070	YES	YES
66	a	403.96	3.04724	YES	YES
67	a	404.22	0.08161	YES	YES
68	a	404.71	18.66015	YES	YES
69	a	414.29	19.39701	YES	YES
70	a	419.73	8.60919	YES	YES
71	a	430.50	0.18338	YES	YES
72	a	434.07	2.60754	YES	YES
73	a	441.85	20.17143	YES	YES
74	a	448.96	20.77062	YES	YES
75	a	458.37	11.23899	YES	YES
76	a	464.91	3.16773	YES	YES
77	a	487.75	1.38289	YES	YES
78	a	497.05	1.73921	YES	YES
79	a	500.81	12.60320	YES	YES
80	a	500.95	11.41845	YES	YES
81	a	504.18	73.73980	YES	YES
82	a	507.90	60.09875	YES	YES
83	a	511.41	205.34985	YES	YES
84	a	522.53	15.87264	YES	YES
85	a	533.75	0.76366	YES	YES
86	a	559.83	25.52429	YES	YES
87	a	586.44	0.05698	YES	YES
88	a	600.21	3.18208	YES	YES
89	a	609.24	2.15097	YES	YES
90	a	609.47	0.47665	YES	YES
91	a	609.72	0.23178	YES	YES
92	a	610.02	0.23163	YES	YES
93	a	610.34	2.56365	YES	YES
94	a	610.74	0.24983	YES	YES
95	a	613.50	0.18125	YES	YES
96	a	644.84	5.13731	YES	YES
97	a	671.85	37.69367	YES	YES
98	a	672.43	22.13481	YES	YES
99	a	674.00	2.01581	YES	YES
100	a	686.28	1.16245	YES	YES
101	a	687.43	1.23894	YES	YES
102	a	687.69	13.36478	YES	YES
103	a	689.05	21.25352	YES	YES
104	a	691.92	28.43192	YES	YES
105	a	697.25	50.66822	YES	YES
106	a	697.90	6.54908	YES	YES
107	a	698.09	44.48544	YES	YES
108	a	698.90	27.16847	YES	YES
109	a	701.05	9.73041	YES	YES
110	a	703.20	40.81247	YES	YES
111	a	741.64	1.32237	YES	YES
112	a	742.88	8.90947	YES	YES
113	a	743.25	0.76782	YES	YES
114	a	744.30	11.74565	YES	YES
115	a	745.90	2.43424	YES	YES
116	a	747.54	6.59543	YES	YES
117	a	753.77	25.25199	YES	YES
118	a	796.06	6.11174	YES	YES
119	a	823.43	0.00372	YES	YES
120	a	832.54	1.02385	YES	YES
121	a	833.58	0.30173	YES	YES
122	a	838.74	0.09948	YES	YES
123	a	839.17	0.21978	YES	YES
124	a	844.10	0.97791	YES	YES
125	a	846.82	0.75111	YES	YES
126	a	888.70	2.79701	YES	YES
127	a	894.36	8.44396	YES	YES
128	a	908.90	0.00672	YES	YES
129	a	910.61	0.06451	YES	YES
130	a	911.24	1.15837	YES	YES
131	a	911.49	0.22317	YES	YES
132	a	918.49	0.21955	YES	YES
133	a	920.99	0.36589	YES	YES
134	a	944.05	12.75199	YES	YES
135	a	948.56	0.25519	YES	YES
136	a	955.56	5.67019	YES	YES
137	a	958.19	0.30523	YES	YES
138	a	961.17	0.04216	YES	YES
139	a	961.60	0.07712	YES	YES
140	a	967.87	0.29370	YES	YES
141	a	969.19	0.13904	YES	YES
142	a	970.22	0.11222	YES	YES
143	a	974.51	27.21657	YES	YES
144	a	978.13	2.33864	YES	YES
145	a	979.28	0.08876	YES	YES
146	a	980.22	0.77551	YES	YES
147	a	981.98	0.26201	YES	YES
148	a	982.87	0.31023	YES	YES
149	a	984.08	1.69473	YES	YES
150	a	984.21	0.36799	YES	YES
151	a	984.35	1.03730	YES	YES
152	a	985.32	0.52256	YES	YES
153	a	985.72	2.49143	YES	YES
154	a	985.96	2.29606	YES	YES
155	a	988.49	0.00733	YES	YES
156	a	991.91	0.15764	YES	YES
157	a	996.80	30.82693	YES	YES
158	a	1006.76	40.43929	YES	YES
159	a	1023.39	0.70129	YES	YES
160	a	1023.52	0.99660	YES	YES
161	a	1023.57	2.94718	YES	YES
162	a	1023.81	4.08739	YES	YES
163	a	1024.52	5.40885	YES	YES

164	a	1024.96	0.26051	YES	YES
165	a	1025.15	0.24248	YES	YES
166	a	1026.02	20.32839	YES	YES
167	a	1028.19	3.52696	YES	YES
168	a	1067.28	6.94580	YES	YES
169	a	1071.20	0.83392	YES	YES
170	a	1071.95	9.55478	YES	YES
171	a	1072.26	13.63273	YES	YES
172	a	1072.40	4.28001	YES	YES
173	a	1075.00	0.77446	YES	YES
174	a	1075.46	4.90643	YES	YES
175	a	1075.96	3.18112	YES	YES
176	a	1076.47	29.91211	YES	YES
177	a	1078.76	9.70369	YES	YES
178	a	1078.95	13.90409	YES	YES
179	a	1082.64	16.03929	YES	YES
180	a	1083.14	2.64969	YES	YES
181	a	1136.31	0.02196	YES	YES
182	a	1139.69	0.22763	YES	YES
183	a	1140.16	0.51637	YES	YES
184	a	1141.71	0.06114	YES	YES
185	a	1141.80	0.52367	YES	YES
186	a	1142.74	0.82465	YES	YES
187	a	1142.95	0.66006	YES	YES
188	a	1157.57	1.99517	YES	YES
189	a	1166.30	2.47815	YES	YES
190	a	1168.78	9.62641	YES	YES
191	a	1169.39	4.49463	YES	YES
192	a	1169.64	3.85807	YES	YES
193	a	1170.85	5.48614	YES	YES
194	a	1171.33	3.66464	YES	YES
195	a	1211.98	49.11300	YES	YES
196	a	1240.50	36.27655	YES	YES
197	a	1284.66	4.34460	YES	YES
198	a	1292.08	16.57060	YES	YES

* zero point VIBRATIONAL energy : 0.7445910 Hartree **

Trans TS_{45}



bp86-SVP SCF energy: -2931.4458422710
pbe-TZVPP SCF energy: -2930.993170855

XYZ Coordinates
97

C	-2.57461	-1.95427	-1.00433
C	-1.57491	-0.45730	-3.30202
C	-0.15132	-2.77570	-2.46169
C	1.45236	1.96913	2.71923
C	3.50909	1.30308	0.80558
C	1.56378	3.39598	0.19543
C	2.42390	-0.47396	-1.71002
C	3.72921	-0.86079	-2.36136
H	4.56199	-0.34601	-1.83063
H	3.74335	-0.54299	-3.42361
H	3.89561	-1.95432	-2.28093
C	-2.26120	1.78862	0.27293
C	-3.14037	2.94728	-0.16194
H	-2.60921	3.90519	0.03575
H	-3.32760	2.89391	-1.25513
H	-4.09898	2.93803	0.39105
O	1.71723	0.49722	-2.14165
O	2.02492	-1.10586	-0.66336
O	-1.21136	1.57562	-0.40395
O	-2.64674	1.13306	1.31483
P	-1.00856	-1.28777	-1.73490
P	1.69518	1.68074	0.90102
Ru	0.32700	0.11671	-0.30771
C	1.27714	-4.93221	-3.61991
C	0.33894	-5.16767	-2.60215
C	-0.37103	-4.09882	-2.02626
C	0.79346	-2.54780	-3.48985
C	1.49936	-3.61684	-4.06387
H	1.82970	-5.77264	-4.07193
H	0.14710	-6.19578	-2.25218
H	-1.11506	-4.31233	-1.24405
H	0.96617	-1.52310	-3.85668
H	2.22593	-3.41869	-4.86964
C	-2.41618	0.78628	-5.69791
C	-1.83702	1.54877	-4.67112
C	-1.41770	0.93291	-3.47734
C	-2.15295	-1.22049	-4.34378
C	-2.57419	-0.60173	-5.53101
H	-2.74181	1.27101	-6.63360
H	-1.70316	2.63603	-4.79749
H	-0.97086	1.53553	-2.67287
H	-2.27157	-2.31030	-4.22769
H	-3.02442	-1.20941	-6.33378
C	-4.92779	-2.93214	0.23088
C	-3.66654	-3.26666	0.75142
C	-2.49818	-2.77241	0.14833
C	-3.84837	-1.61169	-1.51030
C	-5.01498	-2.09827	-0.89600
H	-5.84405	-3.31380	0.71134
H	-3.58488	-3.90234	1.64786
H	-1.52138	-3.01467	0.59190
H	-3.93631	-0.95956	-2.39266
H	-6.00050	-1.82115	-1.30610
C	1.01124	2.49471	5.46495
C	2.32031	2.36896	4.97163
C	2.54119	2.10914	3.60796
C	0.13949	2.09662	3.22443
C	-0.07723	2.36068	4.58654
H	0.83846	2.69266	6.53601
H	3.18239	2.47370	5.65141
H	3.57354	2.01741	3.23678
H	-0.72723	1.97843	2.55962
H	-1.10934	2.44692	4.96365
C	1.36655	5.96815	-0.96174
C	1.40377	5.82397	0.43519
C	1.50484	4.54590	1.01257
C	1.51821	3.54621	-1.21037
C	1.42780	4.82668	-1.78079
H	1.28913	6.97154	-1.41327
H	1.35679	6.71303	1.08605
H	1.53678	4.44621	2.10911
H	1.56659	2.65334	-1.85495
H	1.40016	4.93177	-2.87842
C	6.24769	0.61089	0.71990
C	5.30990	-0.28363	1.26855
C	3.94797	0.05392	1.30317
C	4.45326	2.19391	0.25421
C	5.81621	1.84700	0.21056
H	7.31673	0.34161	0.68862
H	5.64005	-1.25807	1.66515
H	3.21675	-0.65714	1.71902
H	4.12583	3.16822	-0.14173
H	6.54459	2.55350	-0.22127
C	-1.11763	-0.85778	2.28665
C	-0.38951	-0.60045	1.26605
C	-1.48082	-1.55596	3.49093
H	-1.94059	0.21873	1.68857
C	-2.20592	-2.95064	5.86830
C	-0.98563	-3.22849	5.22332
C	-0.62487	-2.54441	4.05531
C	-2.70980	-1.28860	4.15534
C	-3.06269	-1.97623	5.32541
H	-2.48613	-3.49014	6.78837
H	-0.30353	-3.98997	5.63917
H	0.33384	-2.76219	3.55671
H	-3.38857	-0.52880	3.73400
H	-4.02224	-1.74848	5.82066

Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-778.00	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	10.51	0.02463	YES	YES
9	a	15.25	0.09851	YES	YES
10	a	19.33	0.06516	YES	YES
11	a	20.92	0.04905	YES	YES
12	a	23.43	0.08902	YES	YES
13	a	29.50	0.05955	YES	YES
14	a	33.85	0.01061	YES	YES
15	a	35.65	0.06263	YES	YES
16	a	39.24	0.42134	YES	YES

17	a	41.77	0.20435	YES	YES
18	a	43.63	0.01291	YES	YES
19	a	44.90	0.64543	YES	YES
20	a	49.39	0.37882	YES	YES
21	a	51.35	0.14830	YES	YES
22	a	56.61	0.21652	YES	YES
23	a	58.65	0.16078	YES	YES
24	a	62.26	0.17896	YES	YES
25	a	66.50	0.62370	YES	YES
26	a	68.15	0.15046	YES	YES
27	a	72.82	0.21832	YES	YES
28	a	74.97	0.68457	YES	YES
29	a	81.21	0.99097	YES	YES
30	a	82.63	0.60600	YES	YES
31	a	88.82	0.43871	YES	YES
32	a	90.19	0.28071	YES	YES
33	a	96.95	0.51471	YES	YES
34	a	101.53	2.57272	YES	YES
35	a	109.94	2.39295	YES	YES
36	a	116.36	1.78476	YES	YES
37	a	129.36	0.19600	YES	YES
38	a	141.97	0.30410	YES	YES
39	a	152.45	3.32617	YES	YES
40	a	155.91	3.94986	YES	YES
41	a	166.46	1.34100	YES	YES
42	a	183.08	1.34147	YES	YES
43	a	190.90	0.14761	YES	YES
44	a	194.88	0.82456	YES	YES
45	a	205.58	1.18547	YES	YES
46	a	214.22	4.97884	YES	YES
47	a	219.39	1.30774	YES	YES
48	a	221.59	2.77699	YES	YES
49	a	224.19	5.14402	YES	YES
50	a	235.85	10.68930	YES	YES
51	a	240.93	1.47353	YES	YES
52	a	246.17	1.00891	YES	YES
53	a	246.73	0.40275	YES	YES
54	a	251.47	0.24650	YES	YES
55	a	254.79	0.56394	YES	YES
56	a	260.10	1.24289	YES	YES
57	a	267.87	0.49790	YES	YES
58	a	271.68	2.77227	YES	YES
59	a	299.22	3.18888	YES	YES
60	a	303.40	2.18427	YES	YES
61	a	330.71	25.90791	YES	YES
62	a	396.70	0.19141	YES	YES
63	a	397.72	0.38038	YES	YES
64	a	398.63	0.24797	YES	YES
65	a	399.47	0.15840	YES	YES
66	a	403.93	10.14542	YES	YES
67	a	405.32	4.39664	YES	YES
68	a	405.52	27.20418	YES	YES
69	a	411.31	1.35428	YES	YES
70	a	420.42	12.31052	YES	YES
71	a	424.90	4.36286	YES	YES
72	a	434.60	3.50889	YES	YES
73	a	439.74	13.73642	YES	YES
74	a	446.68	0.47571	YES	YES
75	a	453.88	24.05133	YES	YES
76	a	471.82	5.75706	YES	YES
77	a	476.78	6.64851	YES	YES
78	a	487.16	30.15972	YES	YES
79	a	499.24	19.17151	YES	YES
80	a	504.35	38.04786	YES	YES
81	a	508.36	86.67216	YES	YES
82	a	512.53	170.90578	YES	YES
83	a	524.00	40.82391	YES	YES
84	a	526.43	0.67140	YES	YES
85	a	538.42	24.84926	YES	YES
86	a	590.18	2.78793	YES	YES
87	a	599.87	61.07726	YES	YES
88	a	601.62	5.56789	YES	YES
89	a	607.86	8.03687	YES	YES
90	a	608.73	1.33634	YES	YES
91	a	609.31	0.48075	YES	YES
92	a	609.54	3.38995	YES	YES
93	a	609.94	2.42392	YES	YES
94	a	610.36	1.11787	YES	YES
95	a	611.40	0.45383	YES	YES
96	a	647.30	22.73832	YES	YES
97	a	671.86	9.11428	YES	YES
98	a	672.66	35.15400	YES	YES
99	a	674.15	5.15369	YES	YES
100	a	684.64	2.00359	YES	YES
101	a	688.03	1.46528	YES	YES
102	a	689.27	1.73709	YES	YES
103	a	690.06	37.11090	YES	YES
104	a	690.96	50.05639	YES	YES
105	a	693.24	24.70324	YES	YES
106	a	696.10	42.03415	YES	YES
107	a	696.66	59.82749	YES	YES
108	a	698.29	34.52787	YES	YES
109	a	699.44	36.49870	YES	YES
110	a	701.02	31.94175	YES	YES
111	a	704.72	12.79247	YES	YES
112	a	736.44	7.25985	YES	YES
113	a	742.05	3.03353	YES	YES
114	a	743.29	2.29774	YES	YES
115	a	743.80	9.66829	YES	YES
116	a	746.54	2.86014	YES	YES
117	a	747.29	6.57907	YES	YES
118	a	753.62	24.83847	YES	YES
119	a	824.50	78.75772	YES	YES
120	a	825.61	0.01114	YES	YES
121	a	833.06	0.00959	YES	YES
122	a	834.66	1.10095	YES	YES
123	a	835.58	1.99464	YES	YES
124	a	836.50	0.28096	YES	YES
125	a	839.67	3.11047	YES	YES
126	a	844.78	0.90953	YES	YES
127	a	891.18	2.68311	YES	YES
128	a	904.49	0.46166	YES	YES
129	a	907.72	0.71675	YES	YES
130	a	909.12	0.74598	YES	YES
131	a	910.70	0.10477	YES	YES
132	a	912.02	1.21278	YES	YES
133	a	919.28	0.24136	YES	YES
134	a	926.66	17.72065	YES	YES
135	a	943.32	16.55777	YES	YES
136	a	949.94	0.01085	YES	YES
137	a	955.01	0.66027	YES	YES
138	a	958.16	0.23999	YES	YES
139	a	958.71	0.07038	YES	YES
140	a	959.79	0.48294	YES	YES
141	a	960.68	0.27556	YES	YES
142	a	969.36	0.34370	YES	YES
143	a	969.83	0.07323	YES	YES
144	a	978.57	2.35688	YES	YES
145	a	981.43	2.85280	YES	YES
146	a	982.22	0.27434	YES	YES
147	a	982.27	0.54035	YES	YES
148	a	982.43	0.31605	YES	YES
149	a	982.91	0.13583	YES	YES
150	a	983.03	1.51309	YES	YES
151	a	983.76	1.88437	YES	YES
152	a	984.58	1.80944	YES	YES
153	a	985.14	0.60643	YES	YES
154	a	985.36	0.26146	YES	YES
155	a	985.54	2.73748	YES	YES
156	a	985.75	0.52957	YES	YES
157	a	991.31	0.33056	YES	YES
158	a	1007.83	2.28818	YES	YES
159	a	1022.87	14.62959	YES	YES
160	a	1023.09	2.80670	YES	YES
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162	a	1024.16	12.90706	YES	YES
163	a	1024.60	3.64392	YES	YES
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165	a	1024.84	0.42576	YES	YES
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167	a	1025.73	4.46111	YES	YES
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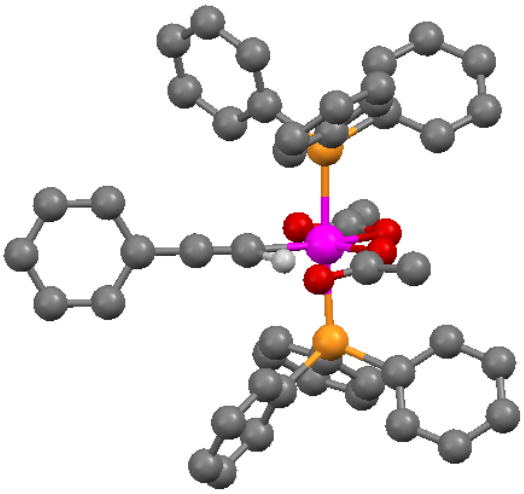
169	a	1072.14	7.95656	YES	YES
170	a	1072.46	7.19521	YES	YES
171	a	1072.78	0.09782	YES	YES
172	a	1074.70	2.79294	YES	YES
173	a	1074.98	11.57189	YES	YES
174	a	1075.18	16.76646	YES	YES
175	a	1075.67	0.92055	YES	YES
176	a	1077.31	31.89596	YES	YES
177	a	1077.39	15.85440	YES	YES
178	a	1080.36	2.30589	YES	YES
179	a	1082.38	26.73661	YES	YES
180	a	1082.58	4.73990	YES	YES
181	a	1084.03	32.13800	YES	YES
182	a	1135.62	0.01991	YES	YES
183	a	1141.85	0.28035	YES	YES
184	a	1142.06	0.47486	YES	YES
185	a	1142.08	0.47600	YES	YES
186	a	1142.39	0.36358	YES	YES
187	a	1142.52	0.14040	YES	YES
188	a	1143.42	0.45025	YES	YES
189	a	1157.21	1.05788	YES	YES
190	a	1167.28	3.65671	YES	YES
191	a	1167.71	4.51928	YES	YES
192	a	1168.69	4.19117	YES	YES
193	a	1169.89	2.70976	YES	YES
194	a	1171.91	11.01324	YES	YES
195	a	1174.62	1.20637	YES	YES
196	a	1227.86	20.30387	YES	YES
197	a	1279.03	16.24720	YES	YES
198	a	1290.25	10.10008	YES	YES

* zero point VIBRATIONAL energy : 0.7411365 Hartree *

Trans 3_ax



bp86-SVP SCF energy: -2931.4480524660
pbe-TZVPP SCF energy: -2930.992678771

XYZ Coordinates
97

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C	-3.12459	0.47866	1.61221
C	-2.89305	2.30182	-0.65190
C	3.31473	-1.17219	0.64924
C	3.20001	0.51034	-1.70326
C	3.19171	1.72146	0.94919
C	0.18208	1.51534	-2.37850
C	0.31502	2.16887	-3.72730
H	1.36219	2.05031	-4.08622
H	0.08015	3.25002	-3.65993
H	-0.35390	1.67432	-4.46183
C	0.06116	0.78630	2.88365
C	-0.03691	1.67435	4.11548
H	0.58849	1.25620	4.93065
H	0.26644	2.71689	3.89170
H	-1.09332	1.67888	4.46533
O	0.25168	2.20098	-1.29490
O	0.02693	0.24978	-2.26238
O	-0.01005	1.41646	1.74661
O	0.16495	-0.45356	2.99335
P	-2.34703	0.63056	-0.06832
P	2.44180	0.32630	-0.01794
Ru	0.03262	0.41805	-0.07469
C	-3.61253	4.90516	-1.47986
C	-4.23007	3.78503	-2.05983
C	-3.87545	2.48780	-1.64677
C	-2.25979	3.43336	-0.08572
C	-2.62807	4.72546	-0.49078
H	-3.89425	5.92156	-1.80228
H	-4.99827	3.91754	-2.83997
H	-4.36981	1.61617	-2.10465
H	-1.47151	3.29221	0.67175
H	-2.13240	5.60056	-0.03837
C	-4.27932	0.11969	4.16761
C	-3.52587	-0.91245	3.58086
C	-2.94873	-0.73600	2.31371
C	-3.88290	1.51061	2.20530
C	-4.45543	1.33052	3.47736
H	-4.72861	-0.02009	5.16507
H	-3.37453	-1.86356	4.11728
H	-2.35255	-1.55013	1.87047
H	-4.03376	2.46247	1.67252
H	-5.04633	2.14562	3.92780
C	-4.90017	-2.32634	-2.64286
C	-3.54933	-2.09660	-2.95383
C	-2.77876	-1.21757	-2.17235
C	-4.71942	-0.79365	-0.75819
C	-5.48394	-1.67303	-1.54281
H	-5.49962	-3.02097	-3.25493
H	-3.08233	-2.61354	-3.80835
H	-1.71917	-1.04158	-2.41365
H	-5.18364	-0.29391	0.10751
H	-6.54215	-1.85193	-1.28868
C	4.65001	-3.40491	1.76182
C	5.12013	-2.82225	0.57258
C	4.45920	-1.71154	0.01946
C	2.84563	-1.76341	1.84438
C	3.51501	-2.86976	2.39506
H	5.16848	-4.27672	2.19495
H	6.01172	-3.23128	0.06842
H	4.84464	-1.26383	-0.90956
H	1.95612	-1.36007	2.35663
H	3.13458	-3.31939	3.32706
C	4.28077	3.90705	2.37179
C	4.84266	2.62674	2.50810
C	4.30378	1.53859	1.79919
C	2.62256	3.01021	0.82439
C	3.17242	4.09521	1.52665
H	4.70473	4.76007	2.92779
H	5.70942	2.46900	3.17138
H	4.75263	0.53924	1.91269
H	1.74917	3.15929	0.17034
H	2.72371	5.09685	1.41819
C	4.26718	0.70382	-4.31487
C	3.42629	-0.37160	-3.97294
C	2.88761	-0.46474	-2.67993
C	4.04323	1.58585	-2.05309
C	4.57153	1.68214	-3.35352
H	4.68531	0.77796	-5.33274
H	3.18015	-1.14250	-4.72196
H	2.21808	-1.30146	-2.42447
H	4.29505	2.35377	-1.30496
H	5.23126	2.52719	-3.61204
C	-0.29503	-2.81281	0.12993
C	-0.15771	-1.57083	0.23358
C	-0.42758	-4.21954	-0.01553
H	-0.00637	-0.91899	1.26558
C	-0.68772	-7.03760	-0.30564
C	-1.83212	-6.21846	-0.27821
C	-1.71010	-4.83065	-0.13469
C	0.72085	-5.06425	-0.04661
C	0.58658	-6.45094	-0.18884
H	-0.78894	-8.12998	-0.41740
H	-2.83480	-6.66967	-0.36969
H	-2.60687	-4.19134	-0.11637
H	1.71783	-4.60566	0.04762
H	1.48897	-7.08520	-0.20891

Vibrational Frequencies

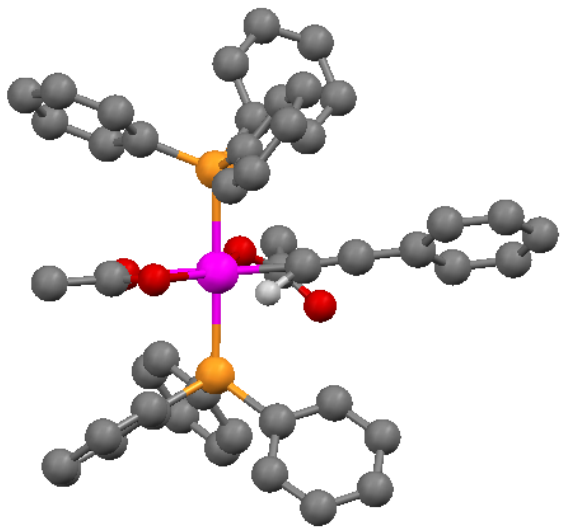
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.19	0.02947	YES	YES
8	a	16.50	0.04038	YES	YES
9	a	17.31	0.00272	YES	YES
10	a	22.07	0.04422	YES	YES
11	a	25.32	0.04053	YES	YES
12	a	27.61	0.09034	YES	YES
13	a	33.49	0.29918	YES	YES
14	a	34.78	0.10084	YES	YES
15	a	37.33	0.04720	YES	YES
16	a	40.92	0.16032	YES	YES
17	a	43.19	0.26303	YES	YES

18	a	50.61	0.03845	YES	YES
19	a	52.12	0.27126	YES	YES
20	a	54.41	0.12189	YES	YES
21	a	54.91	0.04072	YES	YES
22	a	57.93	0.19010	YES	YES
23	a	61.29	0.55638	YES	YES
24	a	64.44	0.28721	YES	YES
25	a	66.90	1.34457	YES	YES
26	a	70.52	0.49891	YES	YES
27	a	72.50	0.44045	YES	YES
28	a	76.38	0.15047	YES	YES
29	a	76.64	1.42249	YES	YES
30	a	79.15	0.36080	YES	YES
31	a	81.40	0.24580	YES	YES
32	a	84.08	0.64674	YES	YES
33	a	92.37	0.03426	YES	YES
34	a	99.41	0.29225	YES	YES
35	a	107.51	3.18419	YES	YES
36	a	118.95	4.02867	YES	YES
37	a	125.89	4.42900	YES	YES
38	a	140.96	0.59111	YES	YES
39	a	162.86	0.81257	YES	YES
40	a	180.88	0.01242	YES	YES
41	a	188.59	0.63854	YES	YES
42	a	192.23	1.71552	YES	YES
43	a	197.06	9.02331	YES	YES
44	a	198.60	2.31957	YES	YES
45	a	201.29	2.40163	YES	YES
46	a	210.29	0.05968	YES	YES
47	a	213.57	1.55597	YES	YES
48	a	219.45	0.59369	YES	YES
49	a	224.27	2.10073	YES	YES
50	a	240.51	5.01849	YES	YES
51	a	241.25	1.52962	YES	YES
52	a	243.15	11.57093	YES	YES
53	a	245.25	2.64731	YES	YES
54	a	251.30	1.93822	YES	YES
55	a	255.67	1.73961	YES	YES
56	a	262.57	0.94309	YES	YES
57	a	264.85	0.69879	YES	YES
58	a	278.10	7.74594	YES	YES
59	a	325.74	2.06588	YES	YES
60	a	337.32	21.68101	YES	YES
61	a	359.19	0.71488	YES	YES
62	a	395.09	9.03241	YES	YES
63	a	397.95	3.95280	YES	YES
64	a	398.20	1.07723	YES	YES
65	a	398.33	0.02912	YES	YES
66	a	400.55	18.69919	YES	YES
67	a	402.40	0.67229	YES	YES
68	a	403.54	0.35288	YES	YES
69	a	405.33	3.34135	YES	YES
70	a	409.04	38.43178	YES	YES
71	a	426.56	5.23476	YES	YES
72	a	429.12	1.71152	YES	YES
73	a	440.49	15.79259	YES	YES
74	a	442.05	5.35414	YES	YES
75	a	450.89	18.56311	YES	YES
76	a	474.23	2.45103	YES	YES
77	a	495.44	23.49916	YES	YES
78	a	497.85	1.85807	YES	YES
79	a	502.98	43.33957	YES	YES
80	a	506.73	48.42254	YES	YES
81	a	507.54	39.66283	YES	YES
82	a	509.85	9.48553	YES	YES
83	a	512.24	168.76001	YES	YES
84	a	521.30	45.76873	YES	YES
85	a	533.13	13.17023	YES	YES
86	a	543.81	48.40477	YES	YES
87	a	600.88	1.67607	YES	YES
88	a	605.82	2.99514	YES	YES
89	a	609.14	0.89269	YES	YES
90	a	609.70	0.47387	YES	YES
91	a	609.93	1.43034	YES	YES
92	a	609.93	0.89465	YES	YES
93	a	610.42	2.95375	YES	YES
94	a	610.64	1.00419	YES	YES
95	a	612.97	0.02689	YES	YES
96	a	668.83	63.88972	YES	YES
97	a	673.65	15.49924	YES	YES
98	a	674.35	19.58722	YES	YES
99	a	675.63	1.90617	YES	YES
100	a	687.93	0.74274	YES	YES
101	a	688.97	17.74016	YES	YES
102	a	689.53	23.64600	YES	YES
103	a	689.88	8.28112	YES	YES
104	a	692.42	13.05879	YES	YES
105	a	697.56	54.23641	YES	YES
106	a	697.85	21.26223	YES	YES
107	a	699.28	35.29117	YES	YES
108	a	700.91	30.44676	YES	YES
109	a	701.97	22.77359	YES	YES
110	a	703.20	24.35038	YES	YES
111	a	741.89	5.60512	YES	YES
112	a	743.23	6.77114	YES	YES
113	a	745.47	4.61313	YES	YES
114	a	746.07	0.65998	YES	YES
115	a	746.79	6.76072	YES	YES
116	a	747.40	9.94659	YES	YES
117	a	757.51	24.97595	YES	YES
118	a	768.97	41.24283	YES	YES
119	a	788.72	15.79050	YES	YES
120	a	826.36	0.18781	YES	YES
121	a	837.38	0.11515	YES	YES
122	a	837.67	0.21773	YES	YES
123	a	840.41	0.23006	YES	YES
124	a	843.23	0.47927	YES	YES
125	a	843.72	0.66455	YES	YES
126	a	847.53	0.26796	YES	YES
127	a	898.37	1.75065	YES	YES
128	a	909.79	0.74740	YES	YES
129	a	910.99	1.06148	YES	YES
130	a	915.51	0.11627	YES	YES
131	a	918.98	1.27008	YES	YES
132	a	919.72	0.21771	YES	YES
133	a	923.00	2.08531	YES	YES
134	a	935.76	10.64236	YES	YES
135	a	947.23	24.10002	YES	YES
136	a	954.24	0.01597	YES	YES
137	a	960.44	0.65649	YES	YES
138	a	960.62	0.96565	YES	YES
139	a	965.05	0.91988	YES	YES
140	a	966.71	5.81954	YES	YES
141	a	968.01	20.55945	YES	YES
142	a	968.39	13.82898	YES	YES
143	a	974.59	1.87234	YES	YES
144	a	975.72	15.70592	YES	YES
145	a	981.28	8.72742	YES	YES
146	a	982.57	3.49528	YES	YES
147	a	982.71	5.36185	YES	YES
148	a	983.61	0.12604	YES	YES
149	a	983.76	1.62977	YES	YES
150	a	984.43	1.16618	YES	YES
151	a	984.72	6.32434	YES	YES
152	a	984.80	1.50429	YES	YES
153	a	985.05	3.40362	YES	YES
154	a	986.26	38.56903	YES	YES
155	a	986.90	1.97804	YES	YES
156	a	988.54	0.04844	YES	YES
157	a	990.20	2.90697	YES	YES
158	a	994.71	8.53887	YES	YES
159	a	1007.02	28.74139	YES	YES
160	a	1023.37	2.82782	YES	YES
161	a	1023.54	0.95324	YES	YES
162	a	1023.59	2.91279	YES	YES
163	a	1023.88	0.86020	YES	YES
164	a	1024.32	2.20445	YES	YES
165	a	1024.58	6.51092	YES	YES

166	a	1024.92	1.46081	YES	YES
167	a	1025.28	6.79502	YES	YES
168	a	1027.62	17.91312	YES	YES
169	a	1068.69	3.25725	YES	YES
170	a	1072.11	1.82081	YES	YES
171	a	1073.04	3.44552	YES	YES
172	a	1073.97	11.36711	YES	YES
173	a	1074.36	5.63456	YES	YES
174	a	1075.18	5.58440	YES	YES
175	a	1075.78	0.25442	YES	YES
176	a	1076.21	18.55388	YES	YES
177	a	1078.60	19.51238	YES	YES
178	a	1079.00	24.24560	YES	YES
179	a	1080.72	9.31612	YES	YES
180	a	1083.45	15.18273	YES	YES
181	a	1085.22	6.17511	YES	YES
182	a	1137.72	0.03253	YES	YES
183	a	1141.59	0.23648	YES	YES
184	a	1141.80	0.33294	YES	YES
185	a	1141.91	0.48363	YES	YES
186	a	1142.30	0.36914	YES	YES
187	a	1142.43	0.18536	YES	YES
188	a	1142.50	0.61560	YES	YES
189	a	1156.39	1.65518	YES	YES
190	a	1166.63	6.12161	YES	YES
191	a	1168.18	5.82997	YES	YES
192	a	1170.28	3.73448	YES	YES
193	a	1171.28	5.51337	YES	YES
194	a	1172.83	8.20751	YES	YES
195	a	1177.96	5.06151	YES	YES
196	a	1215.98	6.12238	YES	YES
197	a	1284.79	0.00377	YES	YES
198	a	1291.36	6.94265	YES	YES

* zero point VIBRATIONAL energy : 0.7426180 Hartree *

Trans 3_ay



bp86-SVP SCF energy: -2931.4325244660
pbe-TZVPP SCF energy: -2930.979536879

XYZ Coordinates
97

C	-1.40676	-3.21582	-0.37816
C	-0.13170	-2.45387	-2.85632
C	1.50566	-3.11971	-0.53127
C	0.82849	3.09604	1.68149
C	1.12669	3.45953	-1.16979
C	-1.54495	3.34859	-0.03460
C	0.87156	0.67461	-2.80124
C	1.36739	1.00085	-4.18243
H	2.33019	0.48816	-4.37962
H	1.53087	2.09957	-4.25867
H	0.61296	0.70752	-4.94082
C	-2.61786	0.39488	1.11843
C	-4.11851	0.11983	0.97061
H	-4.65926	0.52017	1.85133
H	-4.50950	0.59115	0.04344
H	-4.29845	-0.97451	0.88692
O	-0.36357	0.79121	-2.48493
O	1.67849	0.29192	-1.87591
O	-1.94741	0.03016	0.05114
O	-2.15430	0.89603	2.14766
P	-0.01306	-2.17847	-1.02544
P	0.10646	2.52049	0.07271
Ru	0.05015	0.15689	-0.43138
C	3.86786	-4.48563	0.20465
C	2.61330	-5.08336	0.41094
C	1.43699	-4.40641	0.04385
C	2.77075	-2.51893	-0.73022
C	3.94264	-3.20361	-0.36862
H	4.78944	-5.01814	0.49353
H	2.54481	-6.08618	0.86449
H	0.45917	-4.88343	0.21507
H	2.83200	-1.51101	-1.17225
H	4.92363	-2.72642	-0.53019
C	-0.42426	-2.79321	-5.64776
C	-1.40040	-2.09299	-4.91522
C	-1.25323	-1.91622	-3.53057
C	0.84460	-3.15248	-3.59734
C	0.69798	-3.31870	-4.98658
H	-0.53967	-2.92851	-6.73618
H	-2.28335	-1.67495	-5.42674
H	-2.01560	-1.35590	-2.96550
H	1.72495	-3.57624	-3.08822
H	1.46731	-3.86965	-5.55299
C	-3.47414	-4.82922	0.67888
C	-2.90028	-3.81161	1.46056
C	-1.87543	-3.00594	0.93735
C	-1.98520	-4.24262	-1.15795
C	-3.01382	-5.04244	-0.63127
H	-4.28221	-5.45644	1.09122
H	-3.25322	-3.63662	2.49026
H	-1.43157	-2.21100	1.55460
H	-1.63285	-4.42400	-2.18558
H	-3.45648	-5.83945	-1.25223
C	1.87888	3.89634	4.17986
C	2.31375	4.52237	2.99929
C	1.79277	4.12750	1.75543
C	0.38619	2.47544	2.87251
C	0.91135	2.87961	4.11164
H	2.29314	4.20490	5.15452
H	3.06528	5.32856	3.04236
H	2.14112	4.63389	0.84222
H	-0.39423	1.69787	2.81112
H	0.56050	2.38525	5.03264
C	-4.06554	4.59123	-0.29576
C	-3.22490	4.92051	0.78086
C	-1.96938	4.30294	0.91274
C	-2.39701	3.01104	-1.11138
C	-3.64806	3.63709	-1.24064
H	-5.05111	5.07597	-0.39629
H	-3.54775	5.66265	1.52990
H	-1.31898	4.56129	1.76288
H	-2.07562	2.25807	-1.84864
H	-4.30510	3.37139	-2.08572
C	2.77136	4.83196	-3.02256
C	3.30551	3.79547	-2.23558
C	2.48900	3.10952	-1.32222
C	0.60074	4.50277	-1.96078
C	1.41786	5.18150	-2.88307
H	3.41162	5.36823	-3.74286
H	4.36692	3.51372	-2.33584
H	2.91775	2.29454	-0.71787
H	-0.45586	4.79340	-1.85490
H	0.98994	5.99566	-3.49164
C	0.64805	-1.05743	2.56910
C	0.48703	-0.54676	1.43896
C	0.65285	-1.56110	3.90016
H	1.30949	0.07514	0.76124
C	0.61798	-2.53810	6.56420
C	1.59624	-2.98786	5.65804
C	1.61562	-2.51149	4.34033
C	-0.33400	-1.11577	4.82746
C	-0.34687	-1.60472	6.14037
H	0.60607	-2.91667	7.59990
H	2.35285	-3.72180	5.98322
H	2.37865	-2.86448	3.62855
H	-1.09255	-0.39419	4.48309
H	-1.12002	-1.25311	6.84439

Vibrational Frequencies

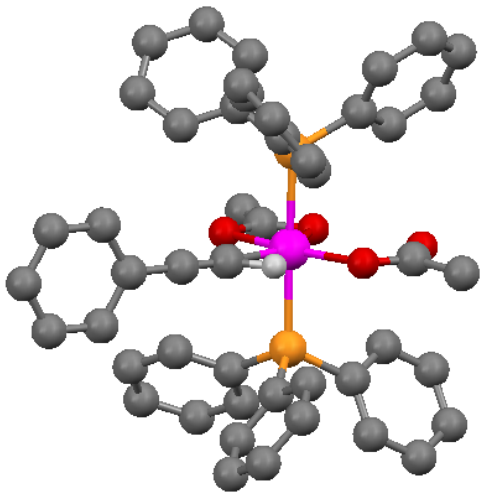
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.75	0.04485	YES	YES
8	a	14.53	0.51842	YES	YES
9	a	18.92	0.04030	YES	YES
10	a	20.02	0.23344	YES	YES
11	a	20.25	0.12112	YES	YES
12	a	24.71	0.08137	YES	YES
13	a	29.23	1.24984	YES	YES
14	a	30.40	0.73346	YES	YES
15	a	36.01	0.59724	YES	YES

16	a	38.69	0.62538	YES	YES
17	a	42.46	0.30909	YES	YES
18	a	43.01	0.14556	YES	YES
19	a	47.94	0.16373	YES	YES
20	a	49.90	0.70012	YES	YES
21	a	52.07	0.05119	YES	YES
22	a	52.58	0.15610	YES	YES
23	a	55.53	0.03728	YES	YES
24	a	56.76	1.15244	YES	YES
25	a	59.61	0.18658	YES	YES
26	a	68.03	1.56167	YES	YES
27	a	72.17	0.05851	YES	YES
28	a	75.95	0.35487	YES	YES
29	a	79.95	0.21204	YES	YES
30	a	81.81	0.62822	YES	YES
31	a	85.92	1.32105	YES	YES
32	a	93.96	0.93419	YES	YES
33	a	96.43	1.74864	YES	YES
34	a	105.80	0.21089	YES	YES
35	a	108.83	0.27758	YES	YES
36	a	111.71	0.63958	YES	YES
37	a	128.62	5.08191	YES	YES
38	a	140.53	1.08885	YES	YES
39	a	145.72	1.53747	YES	YES
40	a	171.81	0.81367	YES	YES
41	a	179.41	0.54164	YES	YES
42	a	190.83	0.59345	YES	YES
43	a	192.29	0.86693	YES	YES
44	a	195.63	0.14904	YES	YES
45	a	205.97	2.90335	YES	YES
46	a	213.20	3.16087	YES	YES
47	a	214.03	1.28350	YES	YES
48	a	221.93	1.95156	YES	YES
49	a	227.30	6.68656	YES	YES
50	a	238.44	4.38226	YES	YES
51	a	240.98	1.91080	YES	YES
52	a	241.99	0.07797	YES	YES
53	a	253.50	0.39103	YES	YES
54	a	255.97	0.59829	YES	YES
55	a	261.77	1.27205	YES	YES
56	a	262.25	0.53915	YES	YES
57	a	263.61	4.82235	YES	YES
58	a	277.05	5.39822	YES	YES
59	a	307.07	4.59569	YES	YES
60	a	332.45	4.08040	YES	YES
61	a	357.20	28.41948	YES	YES
62	a	397.03	0.74985	YES	YES
63	a	397.54	0.19869	YES	YES
64	a	398.20	1.74198	YES	YES
65	a	398.99	0.20551	YES	YES
66	a	402.48	6.96978	YES	YES
67	a	403.40	0.98219	YES	YES
68	a	404.86	26.16571	YES	YES
69	a	405.78	9.70247	YES	YES
70	a	416.01	13.61234	YES	YES
71	a	424.29	4.29998	YES	YES
72	a	432.33	3.50016	YES	YES
73	a	437.80	5.00237	YES	YES
74	a	441.35	14.07244	YES	YES
75	a	450.73	18.85772	YES	YES
76	a	471.35	32.88626	YES	YES
77	a	486.14	10.31101	YES	YES
78	a	496.98	8.67138	YES	YES
79	a	500.34	14.02446	YES	YES
80	a	503.08	56.26119	YES	YES
81	a	507.60	68.56359	YES	YES
82	a	508.71	105.06185	YES	YES
83	a	514.66	71.69972	YES	YES
84	a	518.48	7.18311	YES	YES
85	a	524.41	53.65940	YES	YES
86	a	537.71	14.53853	YES	YES
87	a	549.79	16.53489	YES	YES
88	a	586.99	3.89959	YES	YES
89	a	601.27	5.27987	YES	YES
90	a	609.17	0.65583	YES	YES
91	a	609.36	0.83076	YES	YES
92	a	609.45	0.83842	YES	YES
93	a	609.61	0.64045	YES	YES
94	a	610.42	1.22034	YES	YES
95	a	610.58	1.61873	YES	YES
96	a	612.50	0.16403	YES	YES
97	a	652.86	18.81438	YES	YES
98	a	671.64	50.67426	YES	YES
99	a	672.96	10.44000	YES	YES
100	a	674.82	2.23185	YES	YES
101	a	686.90	5.54846	YES	YES
102	a	689.85	12.12445	YES	YES
103	a	691.19	5.89592	YES	YES
104	a	693.24	8.17852	YES	YES
105	a	693.68	30.43488	YES	YES
106	a	695.88	39.74468	YES	YES
107	a	697.21	45.18059	YES	YES
108	a	697.91	19.78017	YES	YES
109	a	700.40	19.17744	YES	YES
110	a	702.15	41.55463	YES	YES
111	a	702.18	17.02066	YES	YES
112	a	743.35	2.23337	YES	YES
113	a	743.72	8.79151	YES	YES
114	a	744.48	10.64113	YES	YES
115	a	745.28	1.97616	YES	YES
116	a	745.56	4.70974	YES	YES
117	a	746.84	7.30268	YES	YES
118	a	760.81	23.31945	YES	YES
119	a	785.82	11.91776	YES	YES
120	a	834.04	0.31907	YES	YES
121	a	834.94	0.13707	YES	YES
122	a	835.77	0.23691	YES	YES
123	a	837.17	0.51442	YES	YES
124	a	842.67	0.01576	YES	YES
125	a	844.85	0.26814	YES	YES
126	a	845.78	0.77890	YES	YES
127	a	906.87	0.74451	YES	YES
128	a	908.07	0.44261	YES	YES
129	a	909.04	3.58662	YES	YES
130	a	910.69	0.43920	YES	YES
131	a	918.43	4.32150	YES	YES
132	a	918.70	0.31875	YES	YES
133	a	919.86	0.50817	YES	YES
134	a	923.93	0.58840	YES	YES
135	a	948.02	20.16778	YES	YES
136	a	957.62	0.05057	YES	YES
137	a	958.19	0.03066	YES	YES
138	a	960.55	0.17832	YES	YES
139	a	960.78	0.12852	YES	YES
140	a	967.06	0.11454	YES	YES
141	a	968.51	0.36295	YES	YES
142	a	971.52	0.26255	YES	YES
143	a	979.36	0.29160	YES	YES
144	a	981.23	0.28192	YES	YES
145	a	981.64	0.08972	YES	YES
146	a	981.86	1.01887	YES	YES
147	a	982.79	1.26872	YES	YES
148	a	982.96	1.02118	YES	YES
149	a	983.06	1.73950	YES	YES
150	a	983.54	1.04753	YES	YES
151	a	983.71	0.21171	YES	YES
152	a	984.03	0.33313	YES	YES
153	a	984.12	0.13062	YES	YES
154	a	986.59	4.29055	YES	YES
155	a	988.21	0.06432	YES	YES
156	a	989.68	6.39070	YES	YES
157	a	990.19	0.41959	YES	YES
158	a	1005.08	1.58202	YES	YES
159	a	1015.73	9.65252	YES	YES
160	a	1023.25	0.45066	YES	YES
161	a	1023.39	2.31208	YES	YES
162	a	1024.05	4.88144	YES	YES
163	a	1024.34	2.13502	YES	YES

164	a	1024.66	1.60329	YES	YES
165	a	1024.90	1.58767	YES	YES
166	a	1026.03	2.21247	YES	YES
167	a	1027.51	21.15816	YES	YES
168	a	1068.77	5.61578	YES	YES
169	a	1071.39	6.44623	YES	YES
170	a	1072.89	3.26342	YES	YES
171	a	1074.19	11.76503	YES	YES
172	a	1074.33	0.68979	YES	YES
173	a	1075.24	9.96258	YES	YES
174	a	1075.77	2.81127	YES	YES
175	a	1077.15	11.94660	YES	YES
176	a	1078.06	16.45840	YES	YES
177	a	1078.78	21.75646	YES	YES
178	a	1081.44	14.41758	YES	YES
179	a	1084.02	21.45013	YES	YES
180	a	1084.70	4.15315	YES	YES
181	a	1139.02	0.63198	YES	YES
182	a	1141.90	0.21500	YES	YES
183	a	1142.02	0.29520	YES	YES
184	a	1142.18	0.32545	YES	YES
185	a	1142.34	0.36354	YES	YES
186	a	1142.77	1.00775	YES	YES
187	a	1143.28	0.45972	YES	YES
188	a	1153.23	103.98482	YES	YES
189	a	1167.76	4.62125	YES	YES
190	a	1168.67	15.41292	YES	YES
191	a	1169.97	8.19541	YES	YES
192	a	1170.41	31.51975	YES	YES
193	a	1171.67	6.19666	YES	YES
194	a	1174.31	216.95333	YES	YES
195	a	1180.04	106.64478	YES	YES
196	a	1232.19	144.74474	YES	YES
197	a	1287.37	130.35740	YES	YES
198	a	1288.48	29.57946	YES	YES

* zero point VIBRATIONAL energy : 0.7426499 Hartree *

Trans 3_bx



bp86-SVP SCF energy: -2931.4347544050
pbe-TZVPP SCF energy: -2930.980793315

XYZ Coordinates
97

C	-1.29103	-3.12857	0.62933
C	-0.28509	-3.24749	-2.08545
C	1.58343	-3.20049	0.14585
C	-1.28282	3.12400	0.63817
C	1.59217	3.19012	0.15157
C	-0.27928	3.24485	-2.07701
C	2.52738	-0.00263	-1.14895
C	3.98314	0.02021	-1.52968
H	4.42937	0.99327	-1.22787
H	4.10121	-0.11384	-2.62333
H	4.52818	-0.78092	-0.98693
C	-1.99645	0.01951	-2.63716
C	-3.45545	0.09575	-3.09569
H	-3.52387	-0.18493	-4.16595
H	-4.11286	-0.56098	-2.48723
H	-3.82408	1.13998	-2.98093
O	1.59604	-0.00149	-2.03193
O	2.15859	-0.00882	0.07540
O	-1.87704	0.00539	-1.32128
O	-1.05910	0.00288	-3.43397
P	0.02254	-2.40611	-0.46254
P	0.02837	2.40017	-0.45547
Ru	0.06894	-0.00296	-0.45615
C	3.96375	-4.34170	1.15639
C	3.30020	-3.33404	1.88050
C	2.12341	-2.75849	1.37632
C	2.25469	-4.20976	-0.57702
C	3.44104	-4.77437	-0.07360
H	4.89229	-4.78703	1.55115
H	3.70721	-2.98308	2.84328
H	1.62100	-1.95269	1.93532
H	1.85051	-4.55972	-1.53990
H	3.95659	-5.56118	-0.64928
C	-0.64990	-4.53213	-4.57212
C	-1.21420	-5.08101	-3.40753
C	-1.03299	-4.44374	-2.16857
C	0.27378	-2.69554	-3.25926
C	0.09281	-3.34193	-4.49357
H	-0.79761	-5.02982	-5.54531
H	-1.80428	-6.01123	-3.46105
H	-1.48083	-4.88126	-1.26192
H	0.82765	-1.74612	-3.20830
H	0.52313	-2.89565	-5.40524
C	-3.38394	-4.18323	2.20680
C	-2.09022	-4.72264	2.29972
C	-1.04671	-4.20033	1.51381
C	-2.59406	-2.58685	0.54199
C	-3.63225	-3.11552	1.32560
H	-4.20046	-4.59300	2.82444
H	-1.88698	-5.55954	2.98866
H	-0.03646	-4.63266	1.59234
H	-2.78535	-1.74126	-0.14176
H	-4.64449	-2.68427	1.25135
C	-3.37217	4.17967	2.21935
C	-2.07590	4.71215	2.31689
C	-1.03408	4.18924	1.52907
C	-2.58843	2.58921	0.54590
C	-3.62482	3.11851	1.33145
H	-4.18736	4.58982	2.83851
H	-1.86937	5.54406	3.01087
H	-0.02180	4.61607	1.61130
H	-2.78270	1.74839	-0.14287
H	-4.63907	2.69261	1.25355
C	-0.64373	4.53429	-4.56145
C	-1.20957	5.08013	-3.39614
C	-1.02856	4.44045	-2.15834
C	0.28145	2.69619	-3.25155
C	0.10044	3.34486	-4.48473
H	-0.79120	5.03383	-5.53372
H	-1.80034	6.01000	-3.44817
H	-1.47703	4.87590	-1.25103
H	0.83781	1.74809	-3.20186
H	0.53218	2.90107	-5.39693
C	3.97823	4.32206	1.15891
C	3.31501	3.31275	1.88096
C	2.13536	2.74172	1.37831
C	2.26297	4.20124	-0.56922
C	3.45224	4.76119	-0.06746
H	4.90908	4.76371	1.55237
H	3.72458	2.95674	2.84078
H	1.63297	1.93485	1.93571
H	1.85611	4.55640	-1.52905
H	3.96725	5.54973	-0.64127
C	-0.38504	-0.00223	2.78806
C	-0.37944	-0.00275	1.53415
C	-0.34118	-0.00131	4.20699
H	-1.27956	-0.00578	0.77250
C	-0.24365	0.00055	7.04902
C	-0.27686	1.21610	6.33991
C	-0.32619	1.22144	4.94051
C	-0.31303	-1.22314	4.94169
C	-0.26373	-1.21596	6.34108
H	-0.20538	0.00125	8.15091
H	-0.26629	2.17363	6.88762
H	-0.35947	2.17292	4.38629
H	-0.33591	-2.17547	4.38838
H	-0.24284	-2.17281	6.88969

Vibrational Frequencies

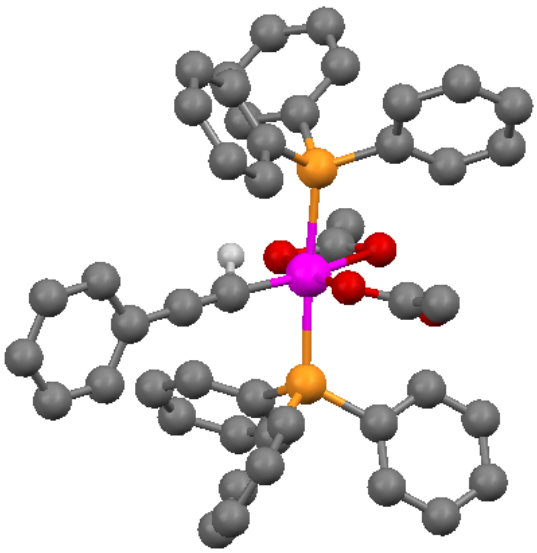
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.74	0.12044	YES	YES
8	a	13.68	0.05812	YES	YES
9	a	16.07	0.02338	YES	YES
10	a	20.52	0.14857	YES	YES
11	a	25.21	0.13038	YES	YES
12	a	27.33	0.24616	YES	YES
13	a	30.65	0.06258	YES	YES
14	a	33.72	0.27007	YES	YES
15	a	38.11	0.11737	YES	YES
16	a	40.60	0.75668	YES	YES
17	a	42.47	0.00159	YES	YES

18	a	47.76	0.32455	YES	YES
19	a	50.46	0.13250	YES	YES
20	a	50.96	0.15238	YES	YES
21	a	52.19	0.16434	YES	YES
22	a	53.50	0.03802	YES	YES
23	a	57.73	0.19528	YES	YES
24	a	58.44	0.26881	YES	YES
25	a	59.70	0.46233	YES	YES
26	a	65.38	0.65752	YES	YES
27	a	68.88	0.74945	YES	YES
28	a	74.27	0.07479	YES	YES
29	a	74.63	0.75458	YES	YES
30	a	77.25	0.64487	YES	YES
31	a	82.03	0.00375	YES	YES
32	a	89.06	1.51308	YES	YES
33	a	92.36	0.19619	YES	YES
34	a	97.56	2.04162	YES	YES
35	a	108.92	1.60735	YES	YES
36	a	112.18	6.77307	YES	YES
37	a	122.76	1.37855	YES	YES
38	a	128.80	4.31151	YES	YES
39	a	141.91	0.02145	YES	YES
40	a	153.83	2.38159	YES	YES
41	a	173.00	0.45410	YES	YES
42	a	186.95	0.00267	YES	YES
43	a	191.35	0.30047	YES	YES
44	a	192.59	0.11786	YES	YES
45	a	196.32	5.00235	YES	YES
46	a	210.83	0.78728	YES	YES
47	a	215.35	3.59830	YES	YES
48	a	217.23	0.04614	YES	YES
49	a	222.39	3.81689	YES	YES
50	a	241.15	0.22711	YES	YES
51	a	242.63	0.24823	YES	YES
52	a	244.69	8.41194	YES	YES
53	a	253.39	0.32525	YES	YES
54	a	253.77	0.26401	YES	YES
55	a	256.11	2.89981	YES	YES
56	a	262.70	0.26215	YES	YES
57	a	263.55	0.89833	YES	YES
58	a	269.48	11.18752	YES	YES
59	a	321.53	6.82643	YES	YES
60	a	334.92	13.40085	YES	YES
61	a	345.81	2.43121	YES	YES
62	a	396.64	2.88223	YES	YES
63	a	397.57	0.84471	YES	YES
64	a	397.68	1.00459	YES	YES
65	a	399.05	0.33491	YES	YES
66	a	400.89	1.13894	YES	YES
67	a	403.06	2.48045	YES	YES
68	a	403.59	0.11115	YES	YES
69	a	412.34	38.12059	YES	YES
70	a	418.81	30.84620	YES	YES
71	a	427.70	2.34162	YES	YES
72	a	428.93	0.34979	YES	YES
73	a	436.11	0.62411	YES	YES
74	a	442.46	20.84895	YES	YES
75	a	447.00	19.64950	YES	YES
76	a	479.52	69.87022	YES	YES
77	a	482.15	18.10412	YES	YES
78	a	499.07	0.51235	YES	YES
79	a	499.28	0.84115	YES	YES
80	a	504.11	7.43730	YES	YES
81	a	504.37	60.01172	YES	YES
82	a	508.16	114.06058	YES	YES
83	a	509.12	65.08826	YES	YES
84	a	512.20	60.70514	YES	YES
85	a	519.19	40.80183	YES	YES
86	a	536.29	13.87859	YES	YES
87	a	543.11	28.67585	YES	YES
88	a	587.29	3.58601	YES	YES
89	a	608.05	0.25394	YES	YES
90	a	608.91	0.52870	YES	YES
91	a	609.16	0.33983	YES	YES
92	a	609.64	0.03528	YES	YES
93	a	609.90	0.15296	YES	YES
94	a	610.01	5.19493	YES	YES
95	a	610.37	0.31260	YES	YES
96	a	612.72	0.01178	YES	YES
97	a	658.75	21.10336	YES	YES
98	a	672.19	45.58250	YES	YES
99	a	674.56	18.04274	YES	YES
100	a	676.22	0.45407	YES	YES
101	a	688.25	23.48098	YES	YES
102	a	689.69	0.77592	YES	YES
103	a	690.43	0.02679	YES	YES
104	a	691.11	18.55215	YES	YES
105	a	691.76	21.63867	YES	YES
106	a	695.56	20.89138	YES	YES
107	a	696.28	47.89171	YES	YES
108	a	699.62	31.00025	YES	YES
109	a	700.31	26.44028	YES	YES
110	a	706.26	27.15152	YES	YES
111	a	706.95	32.49233	YES	YES
112	a	742.58	3.54900	YES	YES
113	a	743.61	6.84302	YES	YES
114	a	744.87	1.36207	YES	YES
115	a	746.02	2.57345	YES	YES
116	a	746.14	8.93722	YES	YES
117	a	746.90	12.59709	YES	YES
118	a	757.33	22.24177	YES	YES
119	a	785.37	8.84738	YES	YES
120	a	825.70	0.02902	YES	YES
121	a	834.01	0.36368	YES	YES
122	a	834.75	0.47358	YES	YES
123	a	840.49	0.12034	YES	YES
124	a	840.81	0.09723	YES	YES
125	a	849.68	0.49832	YES	YES
126	a	850.62	0.34889	YES	YES
127	a	899.80	1.57932	YES	YES
128	a	911.26	1.58611	YES	YES
129	a	912.12	1.22511	YES	YES
130	a	913.88	1.14880	YES	YES
131	a	914.16	1.17024	YES	YES
132	a	914.22	1.47608	YES	YES
133	a	923.71	0.07132	YES	YES
134	a	924.58	0.12689	YES	YES
135	a	949.89	24.33804	YES	YES
136	a	954.44	0.00056	YES	YES
137	a	958.19	0.09421	YES	YES
138	a	958.88	0.07943	YES	YES
139	a	963.71	0.01079	YES	YES
140	a	963.90	0.01316	YES	YES
141	a	973.26	0.27041	YES	YES
142	a	974.03	0.31168	YES	YES
143	a	975.68	0.17910	YES	YES
144	a	978.85	1.09729	YES	YES
145	a	981.31	5.60542	YES	YES
146	a	982.04	0.10087	YES	YES
147	a	982.58	0.47463	YES	YES
148	a	982.61	0.23271	YES	YES
149	a	983.30	1.66724	YES	YES
150	a	984.30	0.22128	YES	YES
151	a	984.63	0.99353	YES	YES
152	a	984.90	1.60904	YES	YES
153	a	985.59	0.42397	YES	YES
154	a	985.82	0.93211	YES	YES
155	a	986.96	0.25585	YES	YES
156	a	987.23	0.10823	YES	YES
157	a	998.58	0.45444	YES	YES
158	a	1000.49	0.51253	YES	YES
159	a	1016.19	6.89958	YES	YES
160	a	1023.63	0.93732	YES	YES
161	a	1023.69	3.02418	YES	YES
162	a	1023.80	3.10642	YES	YES
163	a	1024.98	1.42627	YES	YES
164	a	1025.04	1.99315	YES	YES
165	a	1025.22	2.29485	YES	YES

166	a	1025.31	1.06006	YES	YES
167	a	1029.05	11.64714	YES	YES
168	a	1069.43	3.66632	YES	YES
169	a	1072.15	13.71409	YES	YES
170	a	1072.29	65.94867	YES	YES
171	a	1072.58	43.30550	YES	YES
172	a	1074.04	0.72361	YES	YES
173	a	1074.71	2.74870	YES	YES
174	a	1075.14	0.15129	YES	YES
175	a	1077.44	75.92413	YES	YES
176	a	1078.51	0.23743	YES	YES
177	a	1078.98	15.44056	YES	YES
178	a	1079.65	3.77621	YES	YES
179	a	1080.05	46.77880	YES	YES
180	a	1084.96	21.38799	YES	YES
181	a	1085.67	6.90255	YES	YES
182	a	1138.87	0.04333	YES	YES
183	a	1140.97	0.02421	YES	YES
184	a	1141.07	0.88431	YES	YES
185	a	1141.94	0.14118	YES	YES
186	a	1142.09	0.71932	YES	YES
187	a	1143.05	0.19352	YES	YES
188	a	1143.28	0.93855	YES	YES
189	a	1158.30	6.24445	YES	YES
190	a	1167.26	1.23929	YES	YES
191	a	1167.99	5.58429	YES	YES
192	a	1171.98	0.22443	YES	YES
193	a	1172.87	15.00070	YES	YES
194	a	1173.28	14.79095	YES	YES
195	a	1174.11	1.63197	YES	YES
196	a	1220.78	5.16667	YES	YES
197	a	1277.29	294.96578	YES	YES
198	a	1285.24	0.00552	YES	YES

* zero point VIBRATIONAL energy : 0.7429848 Hartree *

Trans 3_by



bp86-SVP SCF energy: -2931.4255705790
pbe-TZVPP SCF energy: -2930.971880729

XYZ Coordinates
97

C	-0.19086	-3.00794	1.83304
C	-1.26002	-3.49715	-0.82013
C	1.62645	-3.43170	-0.40659
C	-0.83768	3.28622	0.31564
C	1.69027	2.91760	-1.05860
C	-0.81107	2.71469	-2.52312
C	1.76471	-0.62256	-2.33178
C	2.83061	-0.88502	-3.36458
H	3.66989	-0.16913	-3.24742
H	2.40515	-0.81913	-4.38645
H	3.23106	-1.91334	-3.21895
C	-2.75010	-0.35134	-0.93157
C	-4.22324	-0.62457	-0.63784
H	-4.85251	-0.17529	-1.43303
H	-4.39123	-1.72487	-0.64224
H	-4.52722	-0.23899	0.35775
O	0.53213	-0.85515	-2.55283
O	2.08503	-0.17285	-1.17160
O	-1.97625	-0.35617	0.12717
O	-2.33165	-0.17068	-2.08228
P	0.06600	-2.54377	0.05881
P	-0.01250	2.18424	-0.92867
Ru	0.08628	-0.18866	-0.38709
C	4.06175	-4.70768	-1.07178
C	4.06505	-3.56137	-0.25669
C	2.85770	-2.92211	0.06718
C	1.63200	-4.58165	-1.22506
C	2.84386	-5.21364	-1.55610
H	5.01111	-5.20522	-1.33124
H	5.01626	-3.15433	0.12456
H	2.87592	-2.01557	0.69314
H	0.68270	-4.98898	-1.60737
H	2.83224	-6.11146	-2.19645
C	-3.21477	-4.97793	-2.22204
C	-2.93947	-5.27302	-0.87559
C	-1.96731	-4.53756	-0.17633
C	-1.54291	-3.19999	-2.17290
C	-2.51491	-3.94255	-2.86526
H	-3.98013	-5.55337	-2.76935
H	-3.48544	-6.08092	-0.36046
H	-1.76102	-4.77663	0.87864
H	-1.00889	-2.38099	-2.67667
H	-2.73277	-3.69628	-3.91758
C	-0.73240	-3.69074	4.51772
C	0.32547	-4.31224	3.83272
C	0.59420	-3.97722	2.49360
C	-1.24454	-2.37197	2.53024
C	-1.51569	-2.72258	3.86300
H	-0.94654	-3.96070	5.56554
H	0.94542	-5.07001	4.34029
H	1.41806	-4.47949	1.96232
H	-1.84473	-1.60323	2.01538
H	-2.34338	-2.22676	4.39662
C	-2.23362	4.96017	2.11304
C	-1.08128	5.43209	1.46198
C	-0.38423	4.59971	0.56770
C	-1.98675	2.81188	0.98503
C	-2.68053	3.64859	1.87472
H	-2.77907	5.61225	2.81561
H	-0.71848	6.45679	1.64905
H	0.51996	4.97961	0.06488
H	-2.31369	1.77104	0.82761
H	-3.57314	3.26534	2.39630
C	-1.90096	3.53439	-4.99937
C	-1.94220	4.39718	-3.89120
C	-1.39999	3.99162	-2.65993
C	-0.78800	1.84525	-3.63538
C	-1.32373	2.26034	-4.86585
H	-2.32943	3.85191	-5.96491
H	-2.40400	5.39489	-3.97972
H	-1.44546	4.67784	-1.80001
H	-0.37709	0.83045	-3.52713
H	-1.30534	1.56861	-5.72441
C	4.31911	3.95433	-1.17422
C	3.85280	3.33819	0.00193
C	2.55202	2.81598	0.05796
C	2.16371	3.53503	-2.23464
C	3.47333	4.04757	-2.29107
H	5.34367	4.36002	-1.21887
H	4.51113	3.25579	0.88271
H	2.19920	2.32162	0.97848
H	1.50730	3.62165	-3.11479
H	3.82971	4.52802	-3.21775
C	0.23751	0.88720	2.71541
C	0.20717	0.44553	1.54328
C	0.26497	1.40353	4.03987
H	1.09692	-0.21579	1.02049
C	0.33451	2.43598	6.68510
C	0.38785	3.30881	5.58230
C	0.35717	2.80576	4.27543
C	0.20730	0.53351	5.16664
C	0.24481	1.04812	6.46877
H	0.36245	2.83683	7.71199
H	0.45521	4.39784	5.74402
H	0.39334	3.48979	3.41285
H	0.13511	-0.55223	4.99511
H	0.20270	0.35804	7.32828

Vibrational Frequencies

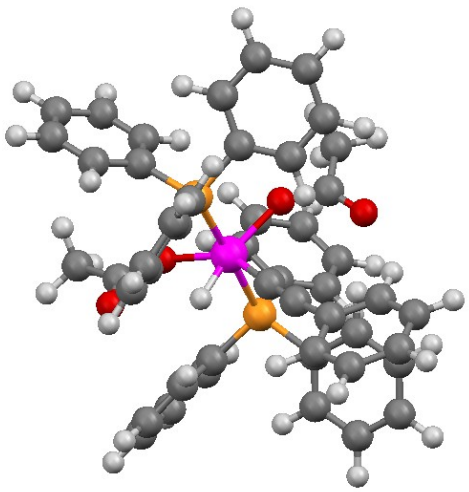
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.23	0.16546	YES	YES
8	a	16.08	0.22357	YES	YES
9	a	18.00	0.01538	YES	YES
10	a	20.31	0.00660	YES	YES
11	a	23.90	0.64834	YES	YES
12	a	28.35	0.10620	YES	YES
13	a	34.59	0.25536	YES	YES
14	a	35.89	0.89876	YES	YES

15	a	39.05	0.17637	YES	YES
16	a	41.29	0.26216	YES	YES
17	a	44.56	0.56983	YES	YES
18	a	47.31	1.33854	YES	YES
19	a	50.59	0.00365	YES	YES
20	a	51.35	0.35543	YES	YES
21	a	56.82	0.45938	YES	YES
22	a	57.48	0.37339	YES	YES
23	a	59.45	0.53592	YES	YES
24	a	61.07	0.75351	YES	YES
25	a	65.56	0.37472	YES	YES
26	a	66.93	1.34957	YES	YES
27	a	73.09	0.15757	YES	YES
28	a	73.83	2.74633	YES	YES
29	a	77.55	1.90042	YES	YES
30	a	79.52	0.94290	YES	YES
31	a	86.31	4.24484	YES	YES
32	a	86.91	0.91534	YES	YES
33	a	94.09	1.60438	YES	YES
34	a	99.69	1.56944	YES	YES
35	a	104.05	3.86134	YES	YES
36	a	110.35	2.22558	YES	YES
37	a	115.98	3.30860	YES	YES
38	a	122.22	2.75110	YES	YES
39	a	139.52	0.42875	YES	YES
40	a	161.22	1.33553	YES	YES
41	a	171.43	1.09356	YES	YES
42	a	183.52	2.10011	YES	YES
43	a	191.50	0.53495	YES	YES
44	a	193.39	1.82048	YES	YES
45	a	197.53	7.87804	YES	YES
46	a	208.48	1.06265	YES	YES
47	a	213.64	3.21241	YES	YES
48	a	217.99	2.29357	YES	YES
49	a	226.70	1.81210	YES	YES
50	a	240.72	1.35418	YES	YES
51	a	243.51	2.91371	YES	YES
52	a	245.71	3.26991	YES	YES
53	a	251.02	2.73853	YES	YES
54	a	256.76	0.69491	YES	YES
55	a	260.45	0.50512	YES	YES
56	a	263.77	1.12772	YES	YES
57	a	264.79	1.46798	YES	YES
58	a	274.38	5.05104	YES	YES
59	a	300.26	3.89063	YES	YES
60	a	324.27	17.07524	YES	YES
61	a	352.12	10.84954	YES	YES
62	a	394.73	5.92786	YES	YES
63	a	397.20	0.45936	YES	YES
64	a	398.93	0.41538	YES	YES
65	a	399.54	0.37343	YES	YES
66	a	400.80	2.62924	YES	YES
67	a	403.90	4.36707	YES	YES
68	a	404.43	1.15009	YES	YES
69	a	410.42	42.92029	YES	YES
70	a	416.27	19.17854	YES	YES
71	a	426.43	2.76782	YES	YES
72	a	428.60	11.29050	YES	YES
73	a	433.63	3.35412	YES	YES
74	a	442.79	19.30269	YES	YES
75	a	445.33	31.18478	YES	YES
76	a	463.13	36.56376	YES	YES
77	a	480.08	3.32491	YES	YES
78	a	487.47	5.15017	YES	YES
79	a	496.77	5.92861	YES	YES
80	a	502.49	11.25382	YES	YES
81	a	505.25	69.07950	YES	YES
82	a	507.16	69.36287	YES	YES
83	a	508.86	46.85750	YES	YES
84	a	512.20	88.74999	YES	YES
85	a	521.32	44.30447	YES	YES
86	a	534.77	13.85633	YES	YES
87	a	549.91	22.24606	YES	YES
88	a	588.86	3.79180	YES	YES
89	a	604.12	4.65403	YES	YES
90	a	608.96	0.60156	YES	YES
91	a	609.46	0.24243	YES	YES
92	a	609.72	0.15396	YES	YES
93	a	610.23	2.02249	YES	YES
94	a	610.32	2.53399	YES	YES
95	a	611.13	1.11569	YES	YES
96	a	612.68	0.26642	YES	YES
97	a	666.32	50.51070	YES	YES
98	a	673.48	12.73124	YES	YES
99	a	674.42	17.43758	YES	YES
100	a	675.89	1.50594	YES	YES
101	a	686.81	5.73225	YES	YES
102	a	689.04	3.75873	YES	YES
103	a	690.52	27.20942	YES	YES
104	a	691.17	15.28538	YES	YES
105	a	691.97	11.15039	YES	YES
106	a	695.26	33.79742	YES	YES
107	a	696.71	25.95367	YES	YES
108	a	698.70	25.95054	YES	YES
109	a	700.13	36.09102	YES	YES
110	a	703.47	24.89277	YES	YES
111	a	704.68	32.19162	YES	YES
112	a	742.09	3.53234	YES	YES
113	a	743.19	5.58652	YES	YES
114	a	744.66	9.34820	YES	YES
115	a	745.63	3.80424	YES	YES
116	a	747.20	1.66753	YES	YES
117	a	747.72	14.54134	YES	YES
118	a	760.14	21.36876	YES	YES
119	a	785.03	7.66890	YES	YES
120	a	829.11	0.22485	YES	YES
121	a	832.40	0.07956	YES	YES
122	a	837.05	0.47004	YES	YES
123	a	838.10	0.15407	YES	YES
124	a	841.39	0.55449	YES	YES
125	a	847.01	0.25072	YES	YES
126	a	847.86	1.34174	YES	YES
127	a	905.30	1.92870	YES	YES
128	a	905.37	0.74588	YES	YES
129	a	909.89	0.47754	YES	YES
130	a	914.46	0.93159	YES	YES
131	a	918.90	0.77000	YES	YES
132	a	920.73	4.48785	YES	YES
133	a	922.42	0.36880	YES	YES
134	a	922.91	1.32263	YES	YES
135	a	948.68	29.77693	YES	YES
136	a	957.22	0.45269	YES	YES
137	a	957.43	0.11236	YES	YES
138	a	961.15	0.00470	YES	YES
139	a	962.37	0.11898	YES	YES
140	a	965.96	0.01846	YES	YES
141	a	968.76	0.36222	YES	YES
142	a	971.93	0.12589	YES	YES
143	a	978.06	0.13555	YES	YES
144	a	979.78	0.15105	YES	YES
145	a	980.98	5.98895	YES	YES
146	a	981.75	0.31713	YES	YES
147	a	982.47	0.11945	YES	YES
148	a	983.52	2.48583	YES	YES
149	a	983.68	0.44164	YES	YES
150	a	984.00	1.69522	YES	YES
151	a	984.41	0.31198	YES	YES
152	a	984.61	0.25728	YES	YES
153	a	984.80	0.23900	YES	YES
154	a	985.51	1.78003	YES	YES
155	a	986.10	0.29800	YES	YES
156	a	988.30	0.12178	YES	YES
157	a	995.04	0.39047	YES	YES
158	a	998.03	0.05070	YES	YES
159	a	1017.39	10.39255	YES	YES
160	a	1023.90	0.90802	YES	YES
161	a	1024.02	2.42970	YES	YES
162	a	1024.25	1.35890	YES	YES

163	a	1024.36	2.50902	YES	YES
164	a	1024.51	2.34071	YES	YES
165	a	1024.72	1.44453	YES	YES
166	a	1026.31	6.83694	YES	YES
167	a	1027.89	11.82851	YES	YES
168	a	1069.78	3.00429	YES	YES
169	a	1072.63	2.83683	YES	YES
170	a	1072.98	8.84704	YES	YES
171	a	1074.64	2.28978	YES	YES
172	a	1075.13	10.47138	YES	YES
173	a	1075.31	5.76570	YES	YES
174	a	1076.65	11.85783	YES	YES
175	a	1078.20	31.87416	YES	YES
176	a	1078.57	14.84186	YES	YES
177	a	1079.94	20.40767	YES	YES
178	a	1081.58	4.05948	YES	YES
179	a	1084.60	19.14908	YES	YES
180	a	1084.99	0.96657	YES	YES
181	a	1139.45	0.72145	YES	YES
182	a	1141.52	7.34518	YES	YES
183	a	1141.54	0.30587	YES	YES
184	a	1141.98	34.38627	YES	YES
185	a	1142.23	7.06386	YES	YES
186	a	1142.30	8.35155	YES	YES
187	a	1142.87	38.00115	YES	YES
188	a	1143.69	312.91704	YES	YES
189	a	1165.21	203.25378	YES	YES
190	a	1168.49	9.53792	YES	YES
191	a	1169.71	9.86801	YES	YES
192	a	1170.77	6.85225	YES	YES
193	a	1171.67	13.95252	YES	YES
194	a	1173.31	41.01511	YES	YES
195	a	1180.06	6.42540	YES	YES
196	a	1222.10	62.72147	YES	YES
197	a	1287.13	0.02574	YES	YES
198	a	1291.71	6.35810	YES	YES

* zero point VIBRATIONAL energy : 0.7425341 Hartree *

Trans 4h



bp86-SVP SCF energy: -2931.4055150900
pbe-TZVPP SCF energy: -2930.946403926

XYZ Coordinates
97

C	-3.24786	1.42045	-0.11505
C	-3.22873	-1.11767	-1.52391
C	-3.21949	-1.09795	1.38669
C	3.26208	0.14971	-1.34351
C	3.16062	0.00675	1.56575
C	2.86719	-2.42694	0.00613
C	-0.39784	0.48734	3.10080
C	-0.46934	-0.32592	4.39111
H	0.49883	-0.83601	4.58475
H	-1.25126	-1.11221	4.30043
H	-0.71600	0.34602	5.23747
C	-0.01794	-2.76636	-1.99755
C	-0.21032	-4.27894	-2.04434
H	-0.34768	-4.59731	-3.09697
H	0.70251	-4.76927	-1.63861
H	-1.07530	-4.60246	-1.42930
O	-0.02495	-0.23549	2.06145
O	-0.64190	1.69310	3.05464
O	-0.29492	-2.26363	-0.80462
O	0.36525	-2.11284	-2.96531
P	-2.46126	-0.25110	-0.07703
P	2.33736	-0.65287	0.04389
Ru	-0.05837	-0.45197	0.03037
C	-4.25972	-2.46802	3.62787
C	-4.68171	-1.15925	3.34169
C	-4.16688	-0.47554	2.22523
C	-2.78882	-2.41216	1.68623
C	-3.31266	-3.09368	2.79576
H	-4.66609	-3.00162	4.50321
H	-5.41959	-0.66022	3.99152
H	-4.50289	0.55058	2.00798
H	-2.03848	-2.90199	1.04272
H	-2.97409	-4.11969	3.01697
C	-4.41018	-2.30700	-3.79846
C	-3.27071	-1.49560	-3.93737
C	-2.68022	-0.90620	-2.80787
C	-4.37420	-1.93254	-1.39073
C	-4.95913	-2.52510	-2.52334
H	-4.86932	-2.77349	-4.68606
H	-2.82554	-1.32719	-4.93152
H	-1.77532	-0.29029	-2.92747
H	-4.81605	-2.10568	-0.39662
H	-5.85223	-3.16119	-2.40528
C	-4.43659	3.97963	-0.10936
C	-3.37132	3.69214	0.76117
C	-2.76851	2.42285	0.75902
C	-4.32024	1.71123	-0.98773
C	-4.90927	2.98702	-0.98400
H	-4.89643	4.98211	-0.11036
H	-2.98984	4.46772	1.44511
H	-1.92722	2.21829	1.44518
H	-4.69914	0.94164	-1.67783
H	-5.74284	3.20311	-1.67285
C	4.64950	1.33603	-3.49710
C	5.11237	1.50612	-2.18174
C	4.42519	0.91438	-1.10796
C	2.79370	-0.01394	-2.66740
C	3.49266	0.57324	-3.73526
H	5.18932	1.80259	-4.33818
H	6.01496	2.10787	-1.98402
H	4.79632	1.05784	-0.08137
H	1.88641	-0.61099	-2.86578
H	3.12063	0.43651	-4.76430
C	3.57182	-5.16291	0.03367
C	4.12340	-4.30109	-0.92864
C	3.77487	-2.93817	-0.94364
C	2.30511	-3.30223	0.96434
C	2.66180	-4.65925	0.98179
H	3.84924	-6.23013	0.04534
H	4.83498	-4.68854	-1.67669
H	4.21285	-2.26992	-1.70180
H	1.58617	-2.91456	1.70609
H	2.22185	-5.33035	1.73823
C	4.41680	1.10830	3.84323
C	3.35736	1.79151	3.22033
C	2.72830	1.24593	2.08922
C	4.22563	-0.67575	2.19439
C	4.84907	-0.12579	3.32829
H	4.90479	1.53753	4.73422
H	3.00448	2.75574	3.62084
H	1.89013	1.78179	1.61620
H	4.57438	-1.64296	1.79902
H	5.67910	-0.66848	3.81074
C	0.38883	2.64709	-0.61639
C	0.19526	1.44206	-0.38067
C	0.58975	4.05633	-0.71990
H	0.03387	-0.15420	-1.53497
C	0.99131	6.86377	-0.89857
C	1.10586	6.05566	-2.04451
C	0.91213	4.66976	-1.96137
C	0.47468	4.88562	0.43127
C	0.67695	6.26944	0.33767
H	1.14726	7.95311	-0.96868
H	1.35305	6.51170	-3.01818
H	1.00857	4.03855	-2.85891
H	0.22613	4.41767	1.39738
H	0.58652	6.89394	1.24268

Vibrational Frequencies

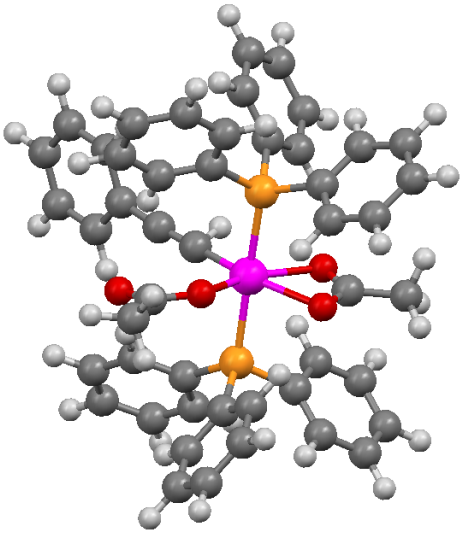
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.99	0.12761	YES	YES
8	a	12.73	0.41896	YES	YES
9	a	15.09	0.12064	YES	YES
10	a	17.31	0.66761	YES	YES
11	a	20.04	0.23544	YES	YES
12	a	23.53	0.01254	YES	YES

13	a	29.31	0.14932	YES	YES
14	a	30.71	0.09294	YES	YES
15	a	33.13	0.13568	YES	YES
16	a	38.13	0.01230	YES	YES
17	a	39.92	0.50882	YES	YES
18	a	42.72	0.20488	YES	YES
19	a	43.52	0.13984	YES	YES
20	a	47.97	0.32236	YES	YES
21	a	50.14	0.17253	YES	YES
22	a	52.55	0.23598	YES	YES
23	a	53.67	0.14408	YES	YES
24	a	57.82	0.09401	YES	YES
25	a	59.43	0.25575	YES	YES
26	a	63.23	0.17408	YES	YES
27	a	65.10	0.18592	YES	YES
28	a	70.02	0.73301	YES	YES
29	a	73.23	0.38722	YES	YES
30	a	74.43	0.21607	YES	YES
31	a	78.25	0.29192	YES	YES
32	a	79.46	3.60766	YES	YES
33	a	84.58	0.25879	YES	YES
34	a	98.27	0.20381	YES	YES
35	a	102.38	1.10861	YES	YES
36	a	104.63	4.51978	YES	YES
37	a	109.57	6.68839	YES	YES
38	a	113.04	7.97803	YES	YES
39	a	137.30	0.36693	YES	YES
40	a	141.01	1.20078	YES	YES
41	a	154.52	2.03111	YES	YES
42	a	165.37	0.53721	YES	YES
43	a	178.91	3.69999	YES	YES
44	a	191.60	0.91122	YES	YES
45	a	193.37	0.59506	YES	YES
46	a	204.52	1.58269	YES	YES
47	a	207.93	2.04050	YES	YES
48	a	210.19	8.16746	YES	YES
49	a	215.78	0.64571	YES	YES
50	a	220.52	2.39776	YES	YES
51	a	226.20	2.51159	YES	YES
52	a	240.16	1.54350	YES	YES
53	a	241.99	2.41551	YES	YES
54	a	247.84	5.54958	YES	YES
55	a	256.42	1.04182	YES	YES
56	a	256.59	0.47577	YES	YES
57	a	261.28	0.41434	YES	YES
58	a	262.52	0.61111	YES	YES
59	a	269.10	4.77332	YES	YES
60	a	303.97	6.95955	YES	YES
61	a	339.22	5.44193	YES	YES
62	a	387.50	1.06179	YES	YES
63	a	396.02	0.25812	YES	YES
64	a	396.64	0.19480	YES	YES
65	a	398.43	0.13870	YES	YES
66	a	399.06	0.28980	YES	YES
67	a	401.83	0.15199	YES	YES
68	a	402.89	0.06470	YES	YES
69	a	403.88	0.50603	YES	YES
70	a	411.42	25.33747	YES	YES
71	a	423.45	4.28185	YES	YES
72	a	433.32	0.34391	YES	YES
73	a	438.20	3.94814	YES	YES
74	a	445.46	16.24336	YES	YES
75	a	447.48	17.30255	YES	YES
76	a	495.96	3.34895	YES	YES
77	a	499.69	38.94956	YES	YES
78	a	500.48	6.49200	YES	YES
79	a	504.31	22.36064	YES	YES
80	a	507.86	66.54094	YES	YES
81	a	510.64	177.35038	YES	YES
82	a	513.63	12.93977	YES	YES
83	a	520.18	15.71972	YES	YES
84	a	529.83	3.44186	YES	YES
85	a	531.67	6.37600	YES	YES
86	a	562.36	2.23663	YES	YES
87	a	578.56	1.24685	YES	YES
88	a	581.02	21.75368	YES	YES
89	a	608.54	0.87924	YES	YES
90	a	608.99	5.32347	YES	YES
91	a	609.31	0.35434	YES	YES
92	a	609.73	0.19003	YES	YES
93	a	609.82	0.76163	YES	YES
94	a	610.41	0.98139	YES	YES
95	a	613.66	0.57205	YES	YES
96	a	620.32	39.90720	YES	YES
97	a	631.34	56.80629	YES	YES
98	a	665.11	44.39252	YES	YES
99	a	676.32	1.00674	YES	YES
100	a	676.53	3.36399	YES	YES
101	a	691.63	4.75732	YES	YES
102	a	691.94	10.95158	YES	YES
103	a	693.49	28.66588	YES	YES
104	a	693.83	11.00294	YES	YES
105	a	694.46	24.28432	YES	YES
106	a	696.49	23.18189	YES	YES
107	a	698.41	35.24099	YES	YES
108	a	699.08	22.19588	YES	YES
109	a	700.55	28.48335	YES	YES
110	a	702.06	28.90453	YES	YES
111	a	703.46	16.87811	YES	YES
112	a	742.92	5.57462	YES	YES
113	a	743.89	3.39443	YES	YES
114	a	744.19	10.79963	YES	YES
115	a	745.29	6.21397	YES	YES
116	a	746.94	4.94576	YES	YES
117	a	747.06	7.32079	YES	YES
118	a	754.95	23.52859	YES	YES
119	a	801.92	1.57987	YES	YES
120	a	829.04	0.52155	YES	YES
121	a	833.17	0.92712	YES	YES
122	a	838.84	0.13929	YES	YES
123	a	840.11	0.40206	YES	YES
124	a	842.36	0.35379	YES	YES
125	a	845.25	1.06384	YES	YES
126	a	847.00	0.57875	YES	YES
127	a	886.44	5.42299	YES	YES
128	a	898.89	3.58653	YES	YES
129	a	907.61	0.22184	YES	YES
130	a	911.32	0.47090	YES	YES
131	a	914.47	4.29096	YES	YES
132	a	915.42	0.13405	YES	YES
133	a	917.83	8.55707	YES	YES
134	a	924.24	0.93240	YES	YES
135	a	924.58	0.61046	YES	YES
136	a	936.07	11.34858	YES	YES
137	a	953.86	0.12433	YES	YES
138	a	957.69	0.11962	YES	YES
139	a	961.85	0.14798	YES	YES
140	a	964.00	0.00231	YES	YES
141	a	966.05	0.36925	YES	YES
142	a	972.13	0.28991	YES	YES
143	a	973.26	0.01848	YES	YES
144	a	974.48	0.33524	YES	YES
145	a	980.26	0.40409	YES	YES
146	a	981.75	3.87447	YES	YES
147	a	982.28	2.16345	YES	YES
148	a	982.84	0.72253	YES	YES
149	a	983.03	1.39392	YES	YES
150	a	983.71	1.14814	YES	YES
151	a	984.06	7.92767	YES	YES
152	a	984.86	0.67337	YES	YES
153	a	985.03	0.10318	YES	YES
154	a	985.21	0.10974	YES	YES
155	a	985.35	26.06848	YES	YES
156	a	987.27	2.34058	YES	YES
157	a	988.60	0.12046	YES	YES
158	a	999.60	1.25073	YES	YES
159	a	1001.08	0.34619	YES	YES
160	a	1018.64	13.38990	YES	YES

161	a	1021.32	10.35345	YES	YES
162	a	1023.64	1.27984	YES	YES
163	a	1023.95	2.16604	YES	YES
164	a	1024.05	2.54451	YES	YES
165	a	1024.51	1.17373	YES	YES
166	a	1024.73	7.55479	YES	YES
167	a	1025.46	0.88478	YES	YES
168	a	1026.06	0.58681	YES	YES
169	a	1068.19	5.66956	YES	YES
170	a	1073.21	2.99721	YES	YES
171	a	1074.14	0.16266	YES	YES
172	a	1074.72	3.37827	YES	YES
173	a	1075.69	14.11094	YES	YES
174	a	1077.21	0.72257	YES	YES
175	a	1077.81	8.07862	YES	YES
176	a	1079.82	11.40703	YES	YES
177	a	1080.01	30.27446	YES	YES
178	a	1082.09	16.43289	YES	YES
179	a	1083.11	10.59715	YES	YES
180	a	1085.79	10.79973	YES	YES
181	a	1087.66	6.02709	YES	YES
182	a	1138.25	0.00367	YES	YES
183	a	1141.81	0.66274	YES	YES
184	a	1142.51	0.28301	YES	YES
185	a	1142.63	0.29535	YES	YES
186	a	1143.21	0.44651	YES	YES
187	a	1143.27	0.38580	YES	YES
188	a	1143.75	0.65827	YES	YES
189	a	1157.97	0.25438	YES	YES
190	a	1168.43	1.39807	YES	YES
191	a	1169.36	4.61627	YES	YES
192	a	1170.05	4.74544	YES	YES
193	a	1171.03	2.66397	YES	YES
194	a	1177.29	5.67035	YES	YES
195	a	1181.27	3.98694	YES	YES
196	a	1227.33	43.44064	YES	YES
197	a	1250.64	502.55381	YES	YES
198	a	1275.67	254.28974	YES	YES

* zero point VIBRATIONAL energy : 0.7414234 Hartree *

Trans TS_{35}*_ay*



bp86-SVP SCF energy: -2931.4173649420
pbe-TZVPP SCF energy: -2930.964124190

XYZ Coordinates
97

C	-1.53920	-3.12294	-0.67758
C	-0.05834	-2.33884	-3.03888
C	1.36292	-3.11571	-0.61585
C	0.26298	2.99142	1.89595
C	1.31970	3.48514	-0.75496
C	-1.55598	3.39075	-0.33046
C	1.28927	0.79953	-2.65834
C	2.09259	1.08087	-3.90336
H	3.07843	1.51656	-3.64108
H	1.53586	1.76601	-4.57317
H	2.26879	0.12560	-4.44697
C	-2.84029	0.17455	0.73660
C	-4.32398	0.32174	0.38231
H	-4.94669	0.11415	1.27570
H	-4.52048	1.36134	0.03695
H	-4.60506	-0.36249	-0.44633
O	0.02184	0.93473	-2.63720
O	1.87420	0.37650	-1.59162
O	-2.07306	0.17098	-0.32188
O	-2.46533	0.08082	1.91519
P	-0.08344	-2.09887	-1.19920
P	0.00940	2.49836	0.12250
Ru	-0.01777	0.18183	-0.50993
C	3.61714	-4.58307	0.26520
C	2.33302	-5.14777	0.33904
C	1.21152	-4.42093	-0.09951
C	2.65915	-2.55080	-0.68419
C	3.77619	-3.28436	-0.24960
H	4.49467	-5.15428	0.61137
H	2.19848	-6.16577	0.74174
H	0.21042	-4.87647	-0.03741
H	2.78626	-1.53002	-1.08433
H	4.78056	-2.83256	-0.31047
C	-0.13949	-2.61379	-5.85024
C	-1.08948	-1.81208	-5.19121
C	-1.04551	-1.66612	-3.79606
C	0.89249	-3.14022	-3.70548
C	0.85228	-3.27363	-5.10563
H	-0.17190	-2.72203	-6.94735
H	-1.86703	-1.28614	-5.76964
H	-1.78007	-1.02254	-3.28564
H	1.66895	-3.66926	-3.13029
H	1.60051	-3.90394	-5.61490
C	-3.70046	-4.70992	0.21431
C	-3.15222	-3.72496	1.05378
C	-2.07868	-2.93271	0.61340
C	-2.09573	-4.11181	-1.51881
C	-3.17027	-4.90055	-1.07317
H	-4.54724	-5.32607	0.56081
H	-3.56938	-3.55463	2.05998
H	-1.67907	-2.14711	1.27417
H	-1.69013	-4.26996	-2.53090
H	-3.59644	-5.66845	-1.74060
C	0.48352	3.76858	4.60579
C	1.26705	4.40043	3.62550
C	1.15357	4.01973	2.27670
C	-0.51396	2.34738	2.88645
C	-0.40681	2.74690	4.23023
H	0.56497	4.07569	5.66226
H	1.96740	5.20507	3.90635
H	1.76077	4.53753	1.51807
H	-1.21076	1.53456	2.60645
H	-1.02848	2.24564	4.99080
C	-3.92489	4.72037	-1.10975
C	-3.32639	5.01292	0.12689
C	-2.14710	4.35348	0.51538
C	-2.16612	3.09408	-1.57118
C	-3.33976	3.76229	-1.95686
H	-4.85100	5.23703	-1.41327
H	-3.77902	5.76079	0.79939
H	-1.68846	4.59157	1.48807
H	-1.71329	2.34018	-2.23386
H	-3.80620	3.52390	-2.92750
C	3.39208	4.91147	-2.05334
C	3.69802	3.80834	-1.23583
C	2.67024	3.09500	-0.59824
C	1.02239	4.59253	-1.57731
C	2.05270	5.29854	-2.22423
H	4.19928	5.46817	-2.55817
H	4.74633	3.49484	-1.09777
H	2.91936	2.22458	0.02901
H	-0.02299	4.91119	-1.71305
H	1.80252	6.16202	-2.86315
C	0.62495	-0.86031	2.47962
C	0.40522	-0.43393	1.28637
C	0.94317	-1.40315	3.75129
H	1.55743	-0.67913	1.21566
C	1.52319	-2.49718	6.29995
C	1.60466	-1.10642	6.09420
C	1.32191	-0.55953	4.83734
C	0.86662	-2.81045	3.97652
C	1.15497	-3.34468	5.23686
H	1.74544	-2.92227	7.29276
H	1.89112	-0.44230	6.92651
H	1.37646	0.52752	4.66969
H	0.57440	-3.46606	3.14119
H	1.08896	-4.43369	5.39720

Vibrational Frequencies

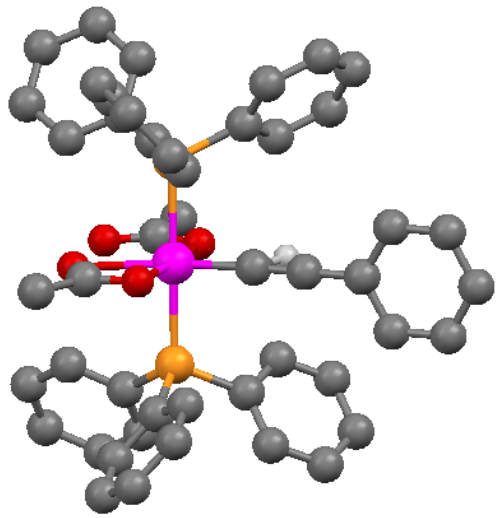
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-679.99	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	12.51	0.07662	YES	YES
9	a	15.75	0.16082	YES	YES
10	a	17.45	0.10505	YES	YES
11	a	17.87	0.11561	YES	YES
12	a	22.09	0.10402	YES	YES
13	a	29.17	0.03009	YES	YES
14	a	30.87	0.03935	YES	YES
15	a	32.02	0.13278	YES	YES

16	a	35.63	0.61331	YES	YES
17	a	41.94	0.11884	YES	YES
18	a	43.80	0.11455	YES	YES
19	a	49.48	0.06828	YES	YES
20	a	49.62	0.08138	YES	YES
21	a	51.29	1.44154	YES	YES
22	a	52.86	0.28727	YES	YES
23	a	54.17	0.53172	YES	YES
24	a	59.62	0.09631	YES	YES
25	a	62.36	0.02241	YES	YES
26	a	62.66	0.26174	YES	YES
27	a	68.53	0.63268	YES	YES
28	a	72.28	0.88320	YES	YES
29	a	75.12	0.03173	YES	YES
30	a	76.73	1.07326	YES	YES
31	a	80.06	0.75031	YES	YES
32	a	81.52	0.34254	YES	YES
33	a	90.15	0.46142	YES	YES
34	a	91.06	0.28778	YES	YES
35	a	102.20	2.92010	YES	YES
36	a	107.90	0.52098	YES	YES
37	a	115.55	5.49378	YES	YES
38	a	125.20	6.82467	YES	YES
39	a	141.60	1.06507	YES	YES
40	a	153.87	1.88081	YES	YES
41	a	168.13	2.87776	YES	YES
42	a	177.92	0.02759	YES	YES
43	a	183.60	2.62912	YES	YES
44	a	190.21	0.53982	YES	YES
45	a	194.02	0.24587	YES	YES
46	a	209.31	1.07729	YES	YES
47	a	214.60	0.44805	YES	YES
48	a	215.61	4.51884	YES	YES
49	a	220.75	2.57685	YES	YES
50	a	225.36	10.52157	YES	YES
51	a	237.31	8.10770	YES	YES
52	a	240.52	3.85666	YES	YES
53	a	242.61	0.59911	YES	YES
54	a	245.65	6.50787	YES	YES
55	a	253.81	0.39859	YES	YES
56	a	256.83	1.00093	YES	YES
57	a	258.32	7.05080	YES	YES
58	a	261.23	7.03863	YES	YES
59	a	261.83	2.36611	YES	YES
60	a	266.61	18.18008	YES	YES
61	a	313.28	2.86343	YES	YES
62	a	329.45	18.46675	YES	YES
63	a	394.99	3.35449	YES	YES
64	a	397.55	0.37547	YES	YES
65	a	398.60	0.33660	YES	YES
66	a	399.59	0.69512	YES	YES
67	a	400.53	0.29248	YES	YES
68	a	404.46	1.94868	YES	YES
69	a	406.37	29.96194	YES	YES
70	a	408.05	12.02893	YES	YES
71	a	411.27	1.16195	YES	YES
72	a	411.84	67.53720	YES	YES
73	a	424.01	3.11764	YES	YES
74	a	435.45	3.59007	YES	YES
75	a	437.97	0.53849	YES	YES
76	a	443.58	16.05563	YES	YES
77	a	447.35	22.39273	YES	YES
78	a	472.63	7.80433	YES	YES
79	a	481.34	5.73116	YES	YES
80	a	499.29	16.68997	YES	YES
81	a	501.51	3.48769	YES	YES
82	a	505.15	64.98002	YES	YES
83	a	507.58	66.25566	YES	YES
84	a	511.54	163.79438	YES	YES
85	a	511.89	16.88951	YES	YES
86	a	522.45	37.69903	YES	YES
87	a	540.27	21.71275	YES	YES
88	a	559.68	48.76111	YES	YES
89	a	588.91	7.23844	YES	YES
90	a	606.78	2.74700	YES	YES
91	a	608.54	0.69100	YES	YES
92	a	609.22	0.99180	YES	YES
93	a	609.32	1.72336	YES	YES
94	a	609.68	2.26740	YES	YES
95	a	610.17	0.39895	YES	YES
96	a	610.23	0.05142	YES	YES
97	a	610.53	0.87213	YES	YES
98	a	653.16	19.81331	YES	YES
99	a	665.28	57.43556	YES	YES
100	a	672.78	16.63157	YES	YES
101	a	674.58	1.89713	YES	YES
102	a	684.06	27.97241	YES	YES
103	a	687.12	1.14249	YES	YES
104	a	687.66	10.33726	YES	YES
105	a	689.01	13.95043	YES	YES
106	a	690.26	13.39550	YES	YES
107	a	695.84	34.91923	YES	YES
108	a	697.93	30.70502	YES	YES
109	a	699.59	31.25038	YES	YES
110	a	701.59	21.42758	YES	YES
111	a	704.27	31.73476	YES	YES
112	a	706.36	27.39771	YES	YES
113	a	743.08	1.88507	YES	YES
114	a	743.81	11.78549	YES	YES
115	a	745.25	4.60781	YES	YES
116	a	745.82	6.29953	YES	YES
117	a	746.55	2.78397	YES	YES
118	a	748.10	8.23302	YES	YES
119	a	761.55	20.32108	YES	YES
120	a	796.73	12.76467	YES	YES
121	a	827.12	0.33828	YES	YES
122	a	831.37	0.09847	YES	YES
123	a	835.93	0.35850	YES	YES
124	a	842.17	0.53460	YES	YES
125	a	843.62	0.61321	YES	YES
126	a	847.57	1.09331	YES	YES
127	a	853.87	1.69642	YES	YES
128	a	902.63	0.94417	YES	YES
129	a	908.06	0.39527	YES	YES
130	a	911.02	2.61749	YES	YES
131	a	913.55	4.44426	YES	YES
132	a	917.39	0.82235	YES	YES
133	a	919.84	1.97472	YES	YES
134	a	920.75	0.71143	YES	YES
135	a	928.32	0.16568	YES	YES
136	a	942.89	18.98493	YES	YES
137	a	953.99	0.06089	YES	YES
138	a	958.13	0.06435	YES	YES
139	a	960.25	0.33366	YES	YES
140	a	965.09	0.59431	YES	YES
141	a	967.10	0.08979	YES	YES
142	a	971.11	0.60791	YES	YES
143	a	974.80	0.18471	YES	YES
144	a	980.44	1.27365	YES	YES
145	a	980.58	0.49779	YES	YES
146	a	981.11	1.16434	YES	YES
147	a	981.31	0.34288	YES	YES
148	a	981.60	0.60100	YES	YES
149	a	982.03	0.16212	YES	YES
150	a	982.87	0.10282	YES	YES
151	a	983.08	0.16021	YES	YES
152	a	984.23	0.88813	YES	YES
153	a	984.65	1.92360	YES	YES
154	a	986.32	4.79855	YES	YES
155	a	987.89	0.18744	YES	YES
156	a	989.83	1.04998	YES	YES
157	a	991.85	5.29353	YES	YES
158	a	993.53	0.25776	YES	YES
159	a	1014.70	1.45706	YES	YES
160	a	1018.26	9.69318	YES	YES
161	a	1021.38	3.59447	YES	YES
162	a	1023.09	1.06520	YES	YES
163	a	1023.27	1.81888	YES	YES

164	a	1023.38	1.66714	YES	YES
165	a	1024.31	2.20854	YES	YES
166	a	1024.80	1.36557	YES	YES
167	a	1025.52	1.22360	YES	YES
168	a	1028.54	16.14042	YES	YES
169	a	1069.29	2.66305	YES	YES
170	a	1072.64	3.90879	YES	YES
171	a	1072.77	3.09329	YES	YES
172	a	1073.84	5.89355	YES	YES
173	a	1074.16	7.38834	YES	YES
174	a	1074.31	5.16286	YES	YES
175	a	1074.89	7.02054	YES	YES
176	a	1076.22	16.68150	YES	YES
177	a	1076.30	15.84299	YES	YES
178	a	1077.51	22.51885	YES	YES
179	a	1080.36	9.85985	YES	YES
180	a	1083.04	12.58288	YES	YES
181	a	1085.22	5.79189	YES	YES
182	a	1140.99	0.27723	YES	YES
183	a	1141.08	0.49673	YES	YES
184	a	1141.12	0.28128	YES	YES
185	a	1141.54	0.30512	YES	YES
186	a	1142.07	0.49775	YES	YES
187	a	1142.10	0.50937	YES	YES
188	a	1142.50	0.45569	YES	YES
189	a	1153.24	0.11378	YES	YES
190	a	1167.05	3.91104	YES	YES
191	a	1167.22	1.61086	YES	YES
192	a	1168.08	4.79112	YES	YES
193	a	1171.58	14.70109	YES	YES
194	a	1172.04	3.16779	YES	YES
195	a	1181.14	4.38632	YES	YES
196	a	1208.51	5.48702	YES	YES
197	a	1284.58	0.04908	YES	YES
198	a	1289.60	10.47902	YES	YES

* zero point VIBRATIONAL energy : 0.7400469 Hartree *

Trans TS_{35}_bx



bp86-SVP SCF energy: -2931.4174273710
pbe-TZVPP SCF energy: -2930.963852812

XYZ Coordinates
97

C	-1.00210	-3.15248	0.70925
C	-0.52446	-3.20373	-2.14846
C	1.72033	-3.21542	-0.29717
C	-0.97715	3.15097	0.72613
C	1.74863	3.19183	-0.27050
C	-0.48656	3.22079	-2.13013
C	2.47326	0.00350	-1.72825
C	3.87548	0.06215	-2.28433
H	4.23916	1.11327	-2.25025
H	3.88879	-0.28163	-3.33803
H	4.56230	-0.55457	-1.66901
C	-2.35845	0.00106	-2.17345
C	-3.87931	-0.08783	-2.33410
H	-4.16688	0.23778	-3.35438
H	-4.20049	-1.14603	-2.20102
H	-4.41308	0.52330	-1.57494
O	1.44768	0.00117	-2.48547
O	2.28454	-0.01110	-0.45878
O	-1.96434	-0.00146	-0.91612
O	-1.60243	0.03676	-3.14668
P	0.08315	-2.39322	-0.59535
P	0.10275	2.38978	-0.58106
Ru	0.14218	-0.00245	-0.57394
C	4.22275	-4.40805	0.25650
C	3.73191	-3.37985	1.08175
C	2.49446	-2.77951	0.80262
C	2.22043	-4.24390	-1.12329
C	3.46701	-4.83428	-0.84772
H	5.19878	-4.87375	0.47334
H	4.32359	-3.03311	1.94557
H	2.12629	-1.95865	1.43874
H	1.63336	-4.58856	-1.98945
H	3.84632	-5.63645	-1.50288
C	-1.34089	-4.42745	-4.55709
C	-1.71025	-4.98908	-3.32265
C	-1.30329	-4.38210	-2.12228
C	-0.16458	-2.63633	-3.39114
C	-0.56830	-3.25407	-4.58653
H	-1.66398	-4.90227	-5.49890
H	-2.32208	-5.90633	-3.29033
H	-1.59836	-4.83090	-1.16018
H	0.41629	-1.70146	-3.41661
H	-0.28893	-2.79876	-5.55096
C	-2.75459	-4.24453	2.64130
C	-1.46900	-4.78398	2.46852
C	-0.59597	-4.24329	1.50622
C	-2.29636	-2.61110	0.88956
C	-3.16493	-3.15782	1.84811
H	-3.43770	-4.67082	3.39502
H	-1.13949	-5.63822	3.08399
H	0.40769	-4.67909	1.37708
H	-2.60742	-1.74748	0.27424
H	-4.17212	-2.72765	1.97903
C	-2.72218	4.24979	2.66062
C	-1.43577	4.78622	2.48405
C	-0.56652	4.24215	1.52035
C	-2.27183	2.61248	0.91050
C	-3.13690	3.16273	1.87019
H	-3.40247	4.67870	3.41541
H	-1.10278	5.64054	3.09753
H	0.43787	4.67534	1.38798
H	-2.58584	1.74820	0.29776
H	-4.14467	2.73505	2.00459
C	-1.26994	4.47767	-4.53240
C	-1.66291	5.01753	-3.29580
C	-1.27206	4.39416	-2.09835
C	-0.10387	2.67425	-3.37538
C	-0.49057	3.30876	-4.56734
H	-1.57991	4.96560	-5.47191
H	-2.28069	5.93060	-3.25916
H	-1.58548	4.82636	-1.13452
H	0.48155	1.74223	-3.40562
H	-0.19286	2.87026	-5.53411
C	4.26380	4.35093	0.29893
C	3.75844	3.32256	1.11507
C	2.51482	2.73902	0.82805
C	2.26303	4.22111	-1.08714
C	3.51587	4.79473	-0.80383
H	5.24473	4.80325	0.52189
H	4.34365	2.96191	1.97755
H	2.13532	1.91805	1.45723
H	1.68201	4.58001	-1.95161
H	3.90594	5.59808	-1.45123
C	-0.15593	-0.00343	2.61548
C	-0.13695	-0.00497	1.32771
C	-0.24648	0.00648	4.03420
H	-1.28967	-0.03981	1.61481
C	-0.38714	0.02917	6.86318
C	-0.36803	1.24269	6.14874
C	-0.30042	1.23882	4.75086
C	-0.27037	-1.21414	4.77209
C	-0.33966	-1.19575	6.16976
H	-0.44041	0.03807	7.96446
H	-0.40769	2.20203	6.69109
H	-0.29045	2.18363	4.18446
H	-0.23628	-2.16794	4.22205
H	-0.35687	-2.14625	6.72855

Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-751.20	0.00000	YES	YES
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		0.00	0.00000	-	-
8	a	9.36	0.15411	YES	YES
9	a	10.27	0.00677	YES	YES
10	a	15.76	0.03128	YES	YES
11	a	19.11	0.18863	YES	YES
12	a	26.90	0.06412	YES	YES
13	a	29.13	0.09507	YES	YES
14	a	31.13	0.36167	YES	YES
15	a	37.03	0.12001	YES	YES
16	a	39.41	0.30041	YES	YES

17	a	42.71	0.05410	YES	YES
18	a	48.97	0.26799	YES	YES
19	a	50.51	0.49009	YES	YES
20	a	51.44	0.08288	YES	YES
21	a	52.47	0.46724	YES	YES
22	a	52.70	0.09763	YES	YES
23	a	54.49	0.39625	YES	YES
24	a	56.86	0.02818	YES	YES
25	a	59.58	0.54051	YES	YES
26	a	59.75	0.56698	YES	YES
27	a	70.10	0.66343	YES	YES
28	a	70.68	1.30233	YES	YES
29	a	73.55	0.08825	YES	YES
30	a	74.55	0.24005	YES	YES
31	a	77.46	1.02604	YES	YES
32	a	79.30	1.55149	YES	YES
33	a	85.63	1.16002	YES	YES
34	a	92.95	0.79034	YES	YES
35	a	95.63	3.60088	YES	YES
36	a	103.69	4.61445	YES	YES
37	a	107.44	2.67769	YES	YES
38	a	120.38	1.15237	YES	YES
39	a	123.80	4.66298	YES	YES
40	a	143.61	0.11239	YES	YES
41	a	157.68	7.98087	YES	YES
42	a	173.54	1.37883	YES	YES
43	a	176.81	3.72948	YES	YES
44	a	188.08	3.99216	YES	YES
45	a	192.02	0.15546	YES	YES
46	a	198.80	27.39551	YES	YES
47	a	201.05	18.37372	YES	YES
48	a	211.80	0.51752	YES	YES
49	a	217.06	3.33879	YES	YES
50	a	219.31	2.88285	YES	YES
51	a	221.07	4.04514	YES	YES
52	a	241.16	1.17322	YES	YES
53	a	242.91	0.09431	YES	YES
54	a	245.40	6.19472	YES	YES
55	a	254.18	0.23784	YES	YES
56	a	254.49	0.72471	YES	YES
57	a	260.20	0.84743	YES	YES
58	a	261.38	1.22045	YES	YES
59	a	263.41	1.90567	YES	YES
60	a	274.14	10.26400	YES	YES
61	a	306.25	13.39169	YES	YES
62	a	324.89	10.60158	YES	YES
63	a	395.70	0.11197	YES	YES
64	a	397.00	0.21769	YES	YES
65	a	397.65	0.18612	YES	YES
66	a	399.09	0.29747	YES	YES
67	a	399.30	0.73274	YES	YES
68	a	404.87	0.71612	YES	YES
69	a	406.06	0.76907	YES	YES
70	a	408.77	0.21164	YES	YES
71	a	413.03	45.83151	YES	YES
72	a	427.71	11.94024	YES	YES
73	a	432.63	0.11100	YES	YES
74	a	436.65	0.04865	YES	YES
75	a	439.93	18.33335	YES	YES
76	a	445.37	35.39282	YES	YES
77	a	447.01	10.93445	YES	YES
78	a	473.20	6.64447	YES	YES
79	a	477.69	15.56502	YES	YES
80	a	492.72	0.21119	YES	YES
81	a	499.36	0.70247	YES	YES
82	a	503.94	10.80217	YES	YES
83	a	504.84	58.66559	YES	YES
84	a	509.74	89.16417	YES	YES
85	a	510.31	183.58781	YES	YES
86	a	521.59	29.05954	YES	YES
87	a	555.27	12.04011	YES	YES
88	a	567.00	67.79458	YES	YES
89	a	593.56	3.55363	YES	YES
90	a	602.65	2.63116	YES	YES
91	a	608.97	0.38590	YES	YES
92	a	609.28	0.38431	YES	YES
93	a	609.54	0.79602	YES	YES
94	a	609.85	1.03772	YES	YES
95	a	609.90	4.70022	YES	YES
96	a	610.28	0.44919	YES	YES
97	a	610.59	0.02863	YES	YES
98	a	661.09	31.19286	YES	YES
99	a	670.54	37.61000	YES	YES
100	a	673.79	19.85461	YES	YES
101	a	675.62	0.27089	YES	YES
102	a	686.08	22.14740	YES	YES
103	a	687.45	0.15158	YES	YES
104	a	688.94	26.52012	YES	YES
105	a	689.42	2.43787	YES	YES
106	a	690.79	18.36951	YES	YES
107	a	696.81	20.32555	YES	YES
108	a	697.32	27.13661	YES	YES
109	a	698.09	24.38261	YES	YES
110	a	698.92	47.32189	YES	YES
111	a	708.29	29.41770	YES	YES
112	a	708.81	30.20502	YES	YES
113	a	742.93	2.67752	YES	YES
114	a	743.54	0.11192	YES	YES
115	a	744.03	7.49230	YES	YES
116	a	744.78	12.55441	YES	YES
117	a	746.68	1.62914	YES	YES
118	a	747.53	10.94889	YES	YES
119	a	761.72	18.84006	YES	YES
120	a	798.01	11.65765	YES	YES
121	a	829.32	0.02174	YES	YES
122	a	835.12	0.03014	YES	YES
123	a	835.19	0.05970	YES	YES
124	a	838.84	0.32748	YES	YES
125	a	839.52	0.92278	YES	YES
126	a	851.43	0.86380	YES	YES
127	a	851.90	0.51814	YES	YES
128	a	908.45	0.46405	YES	YES
129	a	908.69	1.67247	YES	YES
130	a	912.71	0.30894	YES	YES
131	a	913.58	5.53110	YES	YES
132	a	915.85	0.88413	YES	YES
133	a	916.64	0.03715	YES	YES
134	a	924.52	0.09128	YES	YES
135	a	924.89	0.21406	YES	YES
136	a	945.42	27.73541	YES	YES
137	a	957.79	0.09018	YES	YES
138	a	958.24	0.05294	YES	YES
139	a	961.66	0.00651	YES	YES
140	a	963.43	0.09493	YES	YES
141	a	964.02	0.11777	YES	YES
142	a	972.38	0.36943	YES	YES
143	a	972.88	0.51311	YES	YES
144	a	980.31	1.28517	YES	YES
145	a	980.72	0.26642	YES	YES
146	a	981.29	2.03915	YES	YES
147	a	981.65	0.28201	YES	YES
148	a	982.01	1.95203	YES	YES
149	a	982.30	0.55017	YES	YES
150	a	982.44	2.65257	YES	YES
151	a	982.51	3.53691	YES	YES
152	a	982.68	0.05217	YES	YES
153	a	983.10	0.48967	YES	YES
154	a	983.86	0.07438	YES	YES
155	a	984.46	2.86674	YES	YES
156	a	987.87	0.08352	YES	YES
157	a	988.14	0.03291	YES	YES
158	a	1002.22	1.00197	YES	YES
159	a	1003.92	0.99518	YES	YES
160	a	1019.17	7.96877	YES	YES
161	a	1021.24	3.23960	YES	YES
162	a	1023.65	0.28965	YES	YES
163	a	1023.70	2.53420	YES	YES
164	a	1024.24	0.43421	YES	YES

165	a	1024.35	2.29245	YES	YES
166	a	1025.05	2.74652	YES	YES
167	a	1025.21	2.06928	YES	YES
168	a	1026.77	12.11574	YES	YES
169	a	1068.92	3.37247	YES	YES
170	a	1072.33	0.68912	YES	YES
171	a	1072.84	4.39988	YES	YES
172	a	1072.92	2.49075	YES	YES
173	a	1073.55	6.37630	YES	YES
174	a	1075.89	0.43064	YES	YES
175	a	1076.28	8.09255	YES	YES
176	a	1078.78	6.43758	YES	YES
177	a	1079.16	28.14471	YES	YES
178	a	1079.75	2.15401	YES	YES
179	a	1080.30	41.34136	YES	YES
180	a	1085.10	20.60456	YES	YES
181	a	1085.67	2.96510	YES	YES
182	a	1140.76	0.41571	YES	YES
183	a	1140.83	0.19581	YES	YES
184	a	1141.03	0.83210	YES	YES
185	a	1141.12	0.08825	YES	YES
186	a	1141.21	0.62718	YES	YES
187	a	1142.00	0.11300	YES	YES
188	a	1142.17	0.76437	YES	YES
189	a	1152.81	0.03911	YES	YES
190	a	1168.32	0.83151	YES	YES
191	a	1169.03	7.06743	YES	YES
192	a	1170.46	4.55290	YES	YES
193	a	1171.58	6.11678	YES	YES
194	a	1173.97	12.01664	YES	YES
195	a	1175.41	11.08081	YES	YES
196	a	1206.42	4.15357	YES	YES
197	a	1283.94	0.02108	YES	YES
198	a	1287.12	194.64564	YES	YES

* zero point VIBRATIONAL energy : 0.7397156 Hartree *

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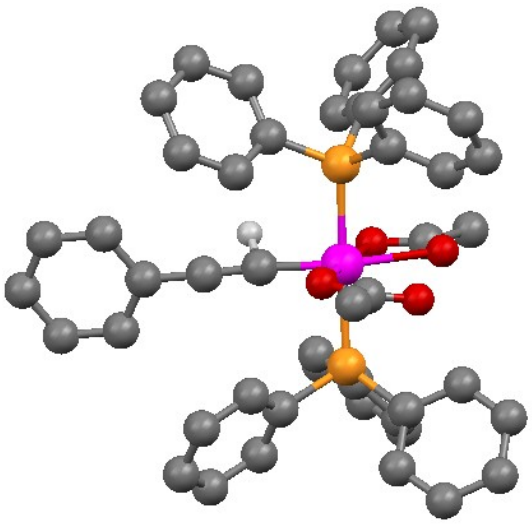

bp86-SVP SCF energy: -2931.4124726440
pbe-TZVPP SCF energy: -2930.958027080

XYZ Coordinates
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C	1.98560	-3.25590	0.15767
C	-1.12796	3.14974	-0.11962
C	1.47038	2.99804	-1.38780
C	-0.91954	2.33000	-2.89616
C	2.23925	-0.52563	-2.03789
C	3.52569	-0.59730	-2.82672
H	3.67027	0.36010	-3.37573
H	3.47422	-1.41803	-3.57109
H	4.39370	-0.74231	-2.15222
C	-2.55728	-0.75456	-1.46911
C	-4.04817	-1.06844	-1.33210
H	-4.54832	-0.95066	-2.31437
H	-4.16851	-2.12497	-1.00336
H	-4.53865	-0.42249	-0.57347
O	1.12426	-0.86901	-2.54031
O	2.25456	-0.06809	-0.83470
O	-1.96481	-0.47178	-0.33138
O	-1.97740	-0.80119	-2.55974
P	0.28860	-2.49861	0.17472
P	-0.12711	2.05593	-1.24020
Ru	0.14739	-0.20248	-0.48905
C	4.59892	-4.34127	0.20940
C	4.33575	-3.10412	0.82437
C	3.04142	-2.56139	0.79097
C	2.25997	-4.49495	-0.46029
C	3.55938	-5.03181	-0.43524
H	5.61714	-4.76459	0.22950
H	5.14686	-2.55082	1.32645
H	2.85329	-1.58045	1.25551
H	1.45196	-5.04733	-0.96532
H	3.75721	-6.00092	-0.92315
C	-2.12948	-5.46880	-2.50730
C	-2.16027	-5.62120	-1.11034
C	-1.44994	-4.72985	-0.28792
C	-0.68272	-3.51932	-2.26371
C	-1.38933	-4.41951	-3.07864
H	-2.69004	-6.16685	-3.15175
H	-2.74198	-6.43925	-0.65317
H	-1.47943	-4.85904	0.80559
H	-0.12226	-2.68476	-2.71226
H	-1.37173	-4.28513	-4.17272
C	-1.35638	-3.37645	4.46667
C	-0.13408	-3.94855	4.07525
C	0.38756	-3.69484	2.79351
C	-1.53100	-2.27177	2.29824
C	-2.05247	-2.53971	3.57465
H	-1.76804	-3.58385	5.46886
H	0.41795	-4.60593	4.76787
H	1.34068	-4.15782	2.49227
H	-2.06269	-1.60402	1.59768
H	-3.01031	-2.08450	3.87747
C	-2.76302	4.75800	1.53208
C	-1.62978	5.30982	0.91012
C	-0.81476	4.51088	0.08783
C	-2.26319	2.59725	0.51558
C	-3.07528	3.40147	1.33298
H	-3.40180	5.38551	2.17608
H	-1.37645	6.37272	1.06165
H	0.07001	4.95412	-0.39666
H	-2.49149	1.52647	0.37236
H	-3.95775	2.95979	1.82516
C	-2.01084	2.73644	-5.46785
C	-2.34647	3.60497	-4.41592
C	-1.80189	3.40597	-3.13521
C	-0.59763	1.44912	-3.95274
C	-1.13607	1.66152	-5.23189
H	-2.44015	2.89195	-6.47202
H	-3.03981	4.44518	-4.58887
H	-2.07273	4.09416	-2.31908
H	0.05508	0.58289	-3.76168
H	-0.88315	0.96429	-6.04781
C	3.92123	4.40764	-1.49730
C	3.55893	3.70831	-0.33128
C	2.34838	3.00131	-0.28023
C	1.84166	3.69866	-2.55449
C	3.06246	4.39693	-2.60825
H	4.87632	4.95761	-1.53937
H	4.23106	3.70376	0.54303
H	2.07898	2.44049	0.62916
H	1.17287	3.70388	-3.42990
H	3.33884	4.93991	-3.52765
C	-0.05828	0.96807	2.49120
C	0.08341	0.45075	1.31811
C	-0.09846	1.51503	3.79914
H	1.09839	0.13914	1.83439
C	-0.20239	2.63015	6.40081
C	-0.07502	3.47101	5.27824
C	-0.01094	2.92692	3.99067
C	-0.24495	0.67709	4.94539
C	-0.28261	1.23435	6.22803
H	-0.24194	3.06411	7.41370
H	-0.01669	4.56403	5.41199
H	0.09153	3.57835	3.10854
H	-0.32680	-0.41204	4.80147
H	-0.38645	0.57566	7.10620

Vibrational Frequencies

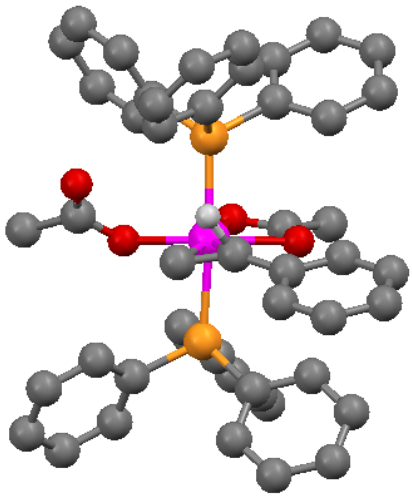
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-690.15	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	14.04	0.06078	YES	YES
9	a	18.91	0.02591	YES	YES
10	a	20.82	0.07891	YES	YES
11	a	24.63	0.13883	YES	YES
12	a	27.59	0.09234	YES	YES
13	a	33.03	0.47121	YES	YES
14	a	37.05	0.06763	YES	YES
15	a	39.66	0.23287	YES	YES
16	a	45.46	0.04954	YES	YES

17	a	48.08	0.46166	YES	YES
18	a	49.17	0.32659	YES	YES
19	a	50.62	0.49904	YES	YES
20	a	52.37	0.52384	YES	YES
21	a	54.71	0.22361	YES	YES
22	a	56.50	0.58839	YES	YES
23	a	58.77	0.95884	YES	YES
24	a	59.76	0.53929	YES	YES
25	a	63.66	1.13443	YES	YES
26	a	65.14	0.32240	YES	YES
27	a	69.51	0.38786	YES	YES
28	a	71.68	0.28400	YES	YES
29	a	74.64	0.24544	YES	YES
30	a	76.19	1.06513	YES	YES
31	a	78.75	0.56711	YES	YES
32	a	81.18	0.86060	YES	YES
33	a	84.27	4.61597	YES	YES
34	a	88.64	1.09859	YES	YES
35	a	94.49	0.33384	YES	YES
36	a	107.77	5.33393	YES	YES
37	a	110.07	1.20585	YES	YES
38	a	114.53	6.07982	YES	YES
39	a	121.91	1.58861	YES	YES
40	a	142.59	0.23820	YES	YES
41	a	155.95	5.27294	YES	YES
42	a	171.32	0.45304	YES	YES
43	a	181.66	1.26065	YES	YES
44	a	190.50	0.52898	YES	YES
45	a	193.43	1.73956	YES	YES
46	a	202.20	17.60505	YES	YES
47	a	211.15	1.32897	YES	YES
48	a	215.22	2.11990	YES	YES
49	a	218.19	5.80891	YES	YES
50	a	221.98	5.08185	YES	YES
51	a	234.58	38.78740	YES	YES
52	a	242.74	1.44885	YES	YES
53	a	244.64	2.24640	YES	YES
54	a	247.65	5.30744	YES	YES
55	a	253.29	1.89086	YES	YES
56	a	256.41	0.40632	YES	YES
57	a	260.30	0.74265	YES	YES
58	a	261.27	0.32319	YES	YES
59	a	264.94	0.56987	YES	YES
60	a	268.60	4.55700	YES	YES
61	a	301.94	6.13228	YES	YES
62	a	321.72	14.82157	YES	YES
63	a	389.31	11.65337	YES	YES
64	a	397.39	0.24542	YES	YES
65	a	397.72	0.42349	YES	YES
66	a	399.74	1.16004	YES	YES
67	a	400.06	0.29814	YES	YES
68	a	404.64	1.59108	YES	YES
69	a	404.81	3.82757	YES	YES
70	a	405.77	6.66127	YES	YES
71	a	412.96	41.88423	YES	YES
72	a	427.09	17.38184	YES	YES
73	a	428.74	2.51811	YES	YES
74	a	432.56	6.52446	YES	YES
75	a	437.92	4.45815	YES	YES
76	a	442.90	20.90179	YES	YES
77	a	445.32	21.10132	YES	YES
78	a	471.55	6.69873	YES	YES
79	a	481.33	1.40524	YES	YES
80	a	491.17	4.82652	YES	YES
81	a	499.52	2.64318	YES	YES
82	a	503.62	10.51456	YES	YES
83	a	506.48	44.22896	YES	YES
84	a	508.59	182.91614	YES	YES
85	a	510.39	78.06270	YES	YES
86	a	519.55	38.95553	YES	YES
87	a	541.90	11.88651	YES	YES
88	a	565.31	54.83902	YES	YES
89	a	595.20	3.19388	YES	YES
90	a	607.03	1.95710	YES	YES
91	a	608.95	0.07441	YES	YES
92	a	609.46	1.99018	YES	YES
93	a	609.49	0.52276	YES	YES
94	a	609.76	2.53116	YES	YES
95	a	610.23	0.05204	YES	YES
96	a	610.50	2.01398	YES	YES
97	a	610.85	0.86589	YES	YES
98	a	663.69	45.42577	YES	YES
99	a	671.58	22.47346	YES	YES
100	a	673.97	20.39938	YES	YES
101	a	675.72	0.60910	YES	YES
102	a	685.92	23.37482	YES	YES
103	a	686.97	8.01246	YES	YES
104	a	688.82	1.41422	YES	YES
105	a	689.67	16.35338	YES	YES
106	a	690.52	15.06514	YES	YES
107	a	694.59	30.83153	YES	YES
108	a	698.19	22.09862	YES	YES
109	a	699.27	31.34181	YES	YES
110	a	701.22	34.48876	YES	YES
111	a	706.26	25.54479	YES	YES
112	a	707.11	35.92518	YES	YES
113	a	742.87	3.70783	YES	YES
114	a	743.39	1.77800	YES	YES
115	a	744.49	10.10120	YES	YES
116	a	744.81	6.93671	YES	YES
117	a	747.29	4.26631	YES	YES
118	a	748.33	9.54527	YES	YES
119	a	759.73	19.85368	YES	YES
120	a	797.92	15.35819	YES	YES
121	a	829.27	0.68698	YES	YES
122	a	829.52	0.26049	YES	YES
123	a	836.82	0.03462	YES	YES
124	a	839.17	0.54644	YES	YES
125	a	842.77	0.84143	YES	YES
126	a	850.17	0.94607	YES	YES
127	a	852.06	1.18079	YES	YES
128	a	902.18	0.72113	YES	YES
129	a	909.22	1.18588	YES	YES
130	a	911.84	1.08457	YES	YES
131	a	916.83	6.30404	YES	YES
132	a	917.36	1.61486	YES	YES
133	a	920.45	0.18419	YES	YES
134	a	924.03	0.33792	YES	YES
135	a	925.06	0.21736	YES	YES
136	a	943.98	23.48480	YES	YES
137	a	954.81	0.14382	YES	YES
138	a	959.47	0.02704	YES	YES
139	a	961.83	0.37255	YES	YES
140	a	963.66	0.13416	YES	YES
141	a	967.40	0.11811	YES	YES
142	a	972.56	0.24187	YES	YES
143	a	973.72	0.17084	YES	YES
144	a	978.78	1.73419	YES	YES
145	a	982.04	0.48524	YES	YES
146	a	982.34	0.20460	YES	YES
147	a	982.81	0.03893	YES	YES
148	a	982.93	2.83876	YES	YES
149	a	983.12	0.26629	YES	YES
150	a	983.32	2.98859	YES	YES
151	a	983.82	0.76898	YES	YES
152	a	983.97	2.57245	YES	YES
153	a	984.14	0.97091	YES	YES
154	a	984.59	1.15372	YES	YES
155	a	986.82	0.07407	YES	YES
156	a	988.11	3.22976	YES	YES
157	a	991.48	0.00610	YES	YES
158	a	1004.07	0.01268	YES	YES
159	a	1007.08	1.03657	YES	YES
160	a	1019.77	8.07471	YES	YES
161	a	1021.99	2.92197	YES	YES
162	a	1023.61	1.57028	YES	YES
163	a	1023.98	1.83851	YES	YES
164	a	1024.31	0.69802	YES	YES

165	a	1024.50	2.47703	YES	YES
166	a	1024.71	2.05769	YES	YES
167	a	1025.88	2.69359	YES	YES
168	a	1029.55	11.65092	YES	YES
169	a	1071.56	0.99023	YES	YES
170	a	1071.82	3.40177	YES	YES
171	a	1072.50	2.06711	YES	YES
172	a	1073.89	6.74960	YES	YES
173	a	1074.76	1.52355	YES	YES
174	a	1075.13	19.67739	YES	YES
175	a	1075.61	7.80416	YES	YES
176	a	1078.12	14.40374	YES	YES
177	a	1078.70	14.01681	YES	YES
178	a	1079.56	17.05687	YES	YES
179	a	1080.84	12.32561	YES	YES
180	a	1084.55	23.13037	YES	YES
181	a	1085.12	1.76702	YES	YES
182	a	1140.09	0.35122	YES	YES
183	a	1141.01	0.45457	YES	YES
184	a	1141.24	0.40397	YES	YES
185	a	1141.44	0.34075	YES	YES
186	a	1141.68	0.16626	YES	YES
187	a	1142.29	0.53968	YES	YES
188	a	1142.57	0.65190	YES	YES
189	a	1157.03	0.01599	YES	YES
190	a	1164.79	3.13164	YES	YES
191	a	1167.31	5.06899	YES	YES
192	a	1169.89	5.15378	YES	YES
193	a	1173.45	10.11818	YES	YES
194	a	1175.72	7.11642	YES	YES
195	a	1179.02	11.73451	YES	YES
196	a	1208.12	7.46437	YES	YES
197	a	1286.90	0.03895	YES	YES
198	a	1289.10	5.42504	YES	YES

* zero point VIBRATIONAL energy : 0.7400659 Hartree *

Trans TS_{25}*_ax*



bp86-SVP SCF energy: -2931.3690851740
pbe-TZVPP SCF energy: -2930.918195741

XYZ Coordinates
97

C	-0.42972	-3.56485	0.94704
C	-0.09285	-3.03833	-1.89072
C	2.22927	-3.01630	-0.17871
C	-1.46449	3.21554	0.37115
C	1.11357	3.11657	1.70838
C	1.01372	3.19460	-1.16907
C	2.61998	-0.54632	1.94416
C	4.01245	-0.00155	2.27960
H	4.50782	-0.66783	3.01384
H	3.92554	1.02250	2.70429
H	4.63330	0.07097	1.36111
C	0.12050	0.19262	-2.51221
C	0.04162	0.39905	-4.00074
H	0.85835	-0.15544	-4.50600
H	-0.94243	0.07034	-4.39059
H	0.17245	1.48148	-4.22395
O	2.04087	0.14470	0.98840
O	2.15174	-1.52019	2.53733
O	-0.94427	0.16696	-1.78960
O	1.23899	0.07867	-1.90929
P	0.47155	-2.42998	-0.22044
P	0.18580	2.37581	0.27854
Ru	0.19965	-0.04138	0.05683
C	4.91808	-3.88053	-0.22006
C	3.94587	-4.62859	0.46498
C	2.60788	-4.20065	0.48623
C	3.20963	-2.26311	-0.86392
C	4.54524	-2.69922	-0.88472
H	5.96840	-4.21686	-0.23339
H	4.22953	-5.55359	0.99430
H	1.85696	-4.79182	1.03319
H	2.92213	-1.33579	-1.38318
H	5.30225	-2.10539	-1.42409
C	-1.04106	-3.92627	-4.41177
C	-1.91008	-3.27461	-3.51869
C	-1.43720	-2.82711	-2.27449
C	0.77005	-3.69572	-2.79410
C	0.29920	-4.13231	-4.04559
H	-1.40963	-4.27446	-5.39109
H	-2.96548	-3.10918	-3.79222
H	-2.12770	-2.31952	-1.58413
H	1.82045	-3.87511	-2.51943
H	0.98960	-4.64505	-4.73609
C	-1.79241	-5.20297	2.80977
C	-0.92148	-4.19569	3.25786
C	-0.24229	-3.37620	2.33894
C	-1.29874	-4.58672	0.50303
C	-1.97418	-5.39886	1.43035
H	-2.32614	-5.84047	3.53460
H	-0.76153	-4.04011	4.33781
H	0.47472	-2.60853	2.68305
H	-1.44788	-4.76411	-0.57281
H	-2.64576	-6.19465	1.06663
C	-4.00590	4.45293	0.42868
C	-3.04634	4.76536	1.40570
C	-1.78046	4.15454	1.37688
C	-2.44218	2.89134	-0.59838
C	-3.69960	3.51568	-0.57359
H	-4.99773	4.93449	0.45212
H	-3.28061	5.49359	2.20003
H	-1.03448	4.41211	2.14443
H	-2.21498	2.13773	-1.36952
H	-4.45176	3.25500	-1.33608
C	2.41516	4.37321	-3.32193
C	1.09120	4.75449	-3.04927
C	0.39280	4.17117	-1.97521
C	2.34403	2.80729	-1.45497
C	3.03965	3.40024	-2.51942
H	2.96278	4.83471	-4.16067
H	0.59443	5.51909	-3.66976
H	-0.63995	4.48882	-1.76168
H	2.82876	2.03460	-0.83714
H	4.07768	3.09320	-2.72963
C	2.41686	4.28851	3.92528
C	1.77765	3.04344	4.05591
C	1.13122	2.45539	2.95506
C	1.75823	4.36778	1.58110
C	2.40567	4.94892	2.68460
H	2.92766	4.74416	4.79032
H	1.78609	2.51435	5.02348
H	0.63574	1.47186	3.05470
H	1.75749	4.89697	0.61483
H	2.90563	5.92541	2.57095
C	-0.58673	-0.06254	2.06349
C	-1.58269	-0.26635	1.17722
H	-1.33012	-1.27348	1.85156
C	-3.04112	-0.08996	0.99195
C	-5.84423	0.18522	0.74266
C	-5.06493	-0.15506	-0.37601
C	-3.67258	-0.29309	-0.25434
C	-3.83246	0.26390	2.11261
C	-5.22207	0.39702	1.98698
H	-6.93773	0.29143	0.64553
H	-5.54578	-0.31405	-1.35590
H	-3.05210	-0.52235	-1.13211
H	-3.33866	0.43456	3.08263
H	-5.82579	0.67409	2.86728

Vibrational Frequencies

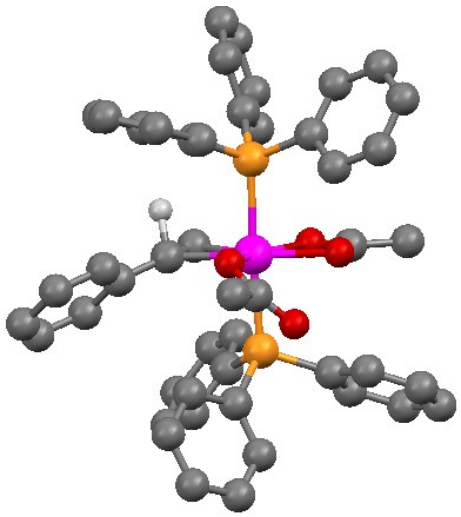
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-741.78	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	3.00	0.05016	YES	YES
9	a	16.95	0.18351	YES	YES
10	a	20.46	0.01757	YES	YES
11	a	22.41	0.07204	YES	YES
12	a	25.48	0.22690	YES	YES
13	a	30.63	0.14174	YES	YES
14	a	36.14	0.07358	YES	YES
15	a	39.05	0.27537	YES	YES
16	a	41.74	0.02421	YES	YES
17	a	46.52	0.08298	YES	YES

18	a	47.99	0.51525	YES	YES
19	a	49.72	0.11456	YES	YES
20	a	54.88	0.18029	YES	YES
21	a	56.32	0.34352	YES	YES
22	a	58.34	1.10297	YES	YES
23	a	60.85	0.98841	YES	YES
24	a	63.22	1.10803	YES	YES
25	a	66.64	0.20565	YES	YES
26	a	70.19	0.99552	YES	YES
27	a	76.03	0.00441	YES	YES
28	a	76.88	1.36159	YES	YES
29	a	77.35	0.99033	YES	YES
30	a	78.56	0.49224	YES	YES
31	a	83.84	0.67378	YES	YES
32	a	84.50	0.08315	YES	YES
33	a	90.79	1.56415	YES	YES
34	a	105.06	0.06196	YES	YES
35	a	108.40	3.23977	YES	YES
36	a	112.42	1.33752	YES	YES
37	a	134.28	3.52492	YES	YES
38	a	138.31	0.52687	YES	YES
39	a	146.26	0.21604	YES	YES
40	a	157.50	1.89739	YES	YES
41	a	172.24	0.43664	YES	YES
42	a	180.23	0.70844	YES	YES
43	a	192.64	0.87880	YES	YES
44	a	196.54	3.95093	YES	YES
45	a	198.68	0.30855	YES	YES
46	a	209.04	0.13140	YES	YES
47	a	212.53	2.11974	YES	YES
48	a	219.14	1.39116	YES	YES
49	a	222.15	4.79072	YES	YES
50	a	224.78	2.90498	YES	YES
51	a	229.36	1.89797	YES	YES
52	a	241.68	1.36464	YES	YES
53	a	244.24	1.59959	YES	YES
54	a	249.93	0.55156	YES	YES
55	a	255.94	0.43592	YES	YES
56	a	258.47	0.75129	YES	YES
57	a	260.35	0.96720	YES	YES
58	a	262.58	2.67786	YES	YES
59	a	265.97	1.74911	YES	YES
60	a	306.52	1.46931	YES	YES
61	a	317.32	13.41150	YES	YES
62	a	396.91	1.66378	YES	YES
63	a	397.93	0.05275	YES	YES
64	a	398.23	1.15516	YES	YES
65	a	399.37	0.33093	YES	YES
66	a	400.45	5.48396	YES	YES
67	a	402.94	30.73728	YES	YES
68	a	404.69	0.98951	YES	YES
69	a	407.55	0.97548	YES	YES
70	a	408.78	0.65814	YES	YES
71	a	419.53	1.98344	YES	YES
72	a	431.77	4.37769	YES	YES
73	a	437.54	5.45377	YES	YES
74	a	440.97	0.84593	YES	YES
75	a	444.36	14.45588	YES	YES
76	a	451.61	21.24011	YES	YES
77	a	456.86	0.37485	YES	YES
78	a	490.40	4.34422	YES	YES
79	a	494.37	14.08442	YES	YES
80	a	499.06	10.05185	YES	YES
81	a	502.76	55.41390	YES	YES
82	a	508.11	38.19702	YES	YES
83	a	511.80	104.37471	YES	YES
84	a	513.60	93.53811	YES	YES
85	a	525.52	3.66805	YES	YES
86	a	581.92	21.47198	YES	YES
87	a	589.06	3.21974	YES	YES
88	a	597.05	9.87046	YES	YES
89	a	606.16	14.13039	YES	YES
90	a	609.30	1.33546	YES	YES
91	a	609.87	0.65862	YES	YES
92	a	610.05	0.23587	YES	YES
93	a	610.24	3.50021	YES	YES
94	a	610.54	0.31473	YES	YES
95	a	611.80	1.77752	YES	YES
96	a	617.34	20.94052	YES	YES
97	a	646.27	19.43409	YES	YES
98	a	669.61	37.28018	YES	YES
99	a	671.42	9.50126	YES	YES
100	a	674.23	5.26953	YES	YES
101	a	684.25	6.64980	YES	YES
102	a	688.33	8.91525	YES	YES
103	a	689.44	2.98089	YES	YES
104	a	690.81	16.25283	YES	YES
105	a	695.71	72.94937	YES	YES
106	a	697.23	26.42059	YES	YES
107	a	700.04	33.38862	YES	YES
108	a	700.20	8.26785	YES	YES
109	a	702.09	15.86870	YES	YES
110	a	702.32	25.48945	YES	YES
111	a	707.68	24.26102	YES	YES
112	a	742.69	1.03449	YES	YES
113	a	742.90	14.19613	YES	YES
114	a	744.30	5.75988	YES	YES
115	a	744.91	5.71755	YES	YES
116	a	746.08	1.26128	YES	YES
117	a	748.07	8.45619	YES	YES
118	a	760.58	17.14091	YES	YES
119	a	789.62	11.81984	YES	YES
120	a	835.88	1.03914	YES	YES
121	a	837.66	0.47026	YES	YES
122	a	839.19	0.49421	YES	YES
123	a	839.94	0.18409	YES	YES
124	a	844.00	1.36389	YES	YES
125	a	848.43	0.47631	YES	YES
126	a	853.43	0.76753	YES	YES
127	a	908.21	11.38491	YES	YES
128	a	911.34	1.17898	YES	YES
129	a	912.33	0.20178	YES	YES
130	a	912.77	7.37104	YES	YES
131	a	917.32	2.68109	YES	YES
132	a	918.27	3.48632	YES	YES
133	a	925.17	0.23720	YES	YES
134	a	929.60	1.51928	YES	YES
135	a	944.51	36.41961	YES	YES
136	a	950.08	19.21574	YES	YES
137	a	960.25	0.57716	YES	YES
138	a	961.90	0.37511	YES	YES
139	a	962.41	0.10643	YES	YES
140	a	963.84	0.29885	YES	YES
141	a	967.03	0.30298	YES	YES
142	a	973.94	0.13250	YES	YES
143	a	977.25	1.88854	YES	YES
144	a	980.96	0.31373	YES	YES
145	a	981.22	0.16859	YES	YES
146	a	982.51	0.64231	YES	YES
147	a	983.00	0.35211	YES	YES
148	a	983.27	0.45638	YES	YES
149	a	983.43	0.69398	YES	YES
150	a	983.89	0.16587	YES	YES
151	a	983.94	0.51774	YES	YES
152	a	984.78	0.73532	YES	YES
153	a	985.71	6.36143	YES	YES
154	a	986.22	1.03494	YES	YES
155	a	988.36	0.56784	YES	YES
156	a	988.87	9.14944	YES	YES
157	a	991.16	0.80878	YES	YES
158	a	1005.57	0.13671	YES	YES
159	a	1016.79	7.91213	YES	YES
160	a	1022.97	7.27733	YES	YES
161	a	1023.76	0.25635	YES	YES
162	a	1023.86	2.35320	YES	YES
163	a	1024.29	1.56114	YES	YES
164	a	1024.98	3.44728	YES	YES
165	a	1025.52	0.43258	YES	YES

166	a	1025.88	4.82731	YES	YES
167	a	1026.14	13.64847	YES	YES
168	a	1026.72	8.20206	YES	YES
169	a	1068.96	1.26295	YES	YES
170	a	1071.89	17.38525	YES	YES
171	a	1072.92	8.31595	YES	YES
172	a	1073.35	10.35171	YES	YES
173	a	1074.90	1.19857	YES	YES
174	a	1074.99	1.09372	YES	YES
175	a	1075.68	20.29741	YES	YES
176	a	1076.09	0.91503	YES	YES
177	a	1077.40	19.59277	YES	YES
178	a	1078.14	12.35152	YES	YES
179	a	1079.82	9.16366	YES	YES
180	a	1083.16	16.88094	YES	YES
181	a	1084.39	7.48911	YES	YES
182	a	1139.87	0.41425	YES	YES
183	a	1141.15	0.46719	YES	YES
184	a	1141.53	0.46150	YES	YES
185	a	1141.99	0.42813	YES	YES
186	a	1142.23	0.51091	YES	YES
187	a	1142.72	0.61465	YES	YES
188	a	1143.54	0.46082	YES	YES
189	a	1151.74	10.19514	YES	YES
190	a	1167.05	6.78392	YES	YES
191	a	1169.83	2.45277	YES	YES
192	a	1170.27	1.44769	YES	YES
193	a	1171.63	9.58080	YES	YES
194	a	1172.05	8.79190	YES	YES
195	a	1174.49	6.28924	YES	YES
196	a	1178.60	12.77597	YES	YES
197	a	1282.01	244.13149	YES	YES
198	a	1290.65	5.14992	YES	YES

* zero point VIBRATIONAL energy : 0.7409657 Hartree *

Trans TS_{25}*_ay*



bp86-SVP SCF energy: -2931.3691795850
pbe-TZVPP SCF energy: -2930.919420420

XYZ Coordinates
97

C	2.09502	-2.88325	-0.49392
C	-0.75621	-3.35440	-0.52446
C	0.57391	-2.27632	-2.87849
C	-2.55398	2.82042	0.43611
C	-0.04285	3.01342	1.85852
C	-0.15360	3.71269	-0.97531
C	2.85369	0.52129	-0.17283
C	4.09050	1.01495	0.58562
H	4.87137	1.32626	-0.13845
H	4.50054	0.16740	1.17963
H	3.85418	1.84334	1.28473
C	-0.89610	0.55320	-2.75752
C	-1.30305	0.76267	-4.19123
H	-0.99328	-0.12527	-4.78718
H	-2.40369	0.87381	-4.27174
H	-0.79161	1.65340	-4.60959
O	1.73754	0.70645	0.49634
O	2.96361	-0.01546	-1.27886
O	-1.69575	0.02688	-1.90307
O	0.27197	0.86428	-2.34386
P	0.50702	-2.08033	-1.02673
P	-0.74961	2.43547	0.23936
Ru	-0.11995	0.16530	-0.32554
C	0.76534	-2.50775	-5.69056
C	1.66921	-1.69476	-4.98235
C	1.57541	-1.56954	-3.58665
C	-0.33040	-3.09144	-3.59267
C	-0.23512	-3.20377	-4.99190
H	0.84239	-2.60054	-6.78715
H	2.45817	-1.14472	-5.52217
H	2.27426	-0.92730	-3.02752
H	-1.11290	-3.65281	-3.05954
H	-0.94689	-3.84778	-5.53518
C	-2.75121	-5.22463	0.20531
C	-1.39698	-5.50411	0.45163
C	-0.40382	-4.57748	0.08570
C	-2.12398	-3.07345	-0.75701
C	-3.11008	-4.00873	-0.40283
H	-3.52869	-5.95327	0.49025
H	-1.10421	-6.45369	0.93031
H	0.65385	-4.81329	0.27973
H	-2.41362	-2.11657	-1.21881
H	-4.17106	-3.77680	-0.59420
C	4.44210	-4.18184	0.40480
C	3.91217	-4.47746	-0.86260
C	2.74517	-3.83501	-1.30994
C	2.63556	-2.58844	0.77440
C	3.79899	-3.23653	1.22178
H	5.35834	-4.68640	0.75460
H	4.41038	-5.21573	-1.51323
H	2.34106	-4.07863	-2.30519
H	2.15043	-1.83714	1.41449
H	4.20499	-2.99362	2.21763
C	-5.31131	3.40830	0.63877
C	-4.36516	4.25195	1.24835
C	-2.99482	3.96177	1.14823
C	-3.50938	1.97719	-0.17133
C	-4.88005	2.27526	-0.06993
H	-6.38759	3.63470	0.72207
H	-4.69522	5.14235	1.80928
H	-2.26437	4.62792	1.63550
H	-3.17199	1.08446	-0.72037
H	-5.61611	1.60582	-0.54490
C	0.84901	5.62318	-2.80699
C	-0.44290	5.76478	-2.27438
C	-0.94222	4.81732	-1.36397
C	1.13635	3.56392	-1.53505
C	1.63537	4.51948	-2.43513
H	1.23889	6.36723	-3.52164
H	-1.07453	6.61959	-2.56900
H	-1.95941	4.94193	-0.96197
H	1.74401	2.68100	-1.29018
H	2.64306	4.38594	-2.86206
C	1.09770	3.71400	4.35729
C	-0.15797	3.08613	4.30555
C	-0.72407	2.73822	3.06747
C	1.21924	3.64211	1.92256
C	1.78213	3.99196	3.16156
H	1.54008	3.99124	5.32850
H	-0.70764	2.86556	5.23544
H	-1.72216	2.27003	3.05006
H	1.76661	3.87446	0.99631
H	2.76486	4.49158	3.18907
C	-1.62525	-0.62147	0.92580
C	-0.51384	-0.52195	1.67996
H	-1.45856	0.24074	1.99923
C	0.20536	-1.05077	2.84561
C	1.54174	-2.10262	5.10059
C	1.92127	-0.85491	4.57281
C	1.26326	-0.32903	3.44988
C	-0.17392	-2.30655	3.38378
C	0.49477	-2.82704	4.50153
H	2.06423	-2.51365	5.98073
H	2.74159	-0.28531	5.04024
H	1.56489	0.63474	3.01731
H	-0.99222	-2.86766	2.90616
H	0.19525	-3.80750	4.90887

Vibrational Frequencies

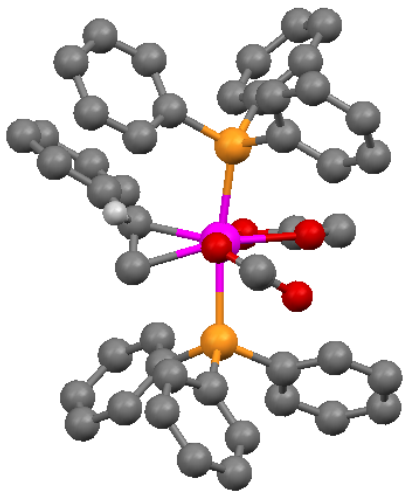
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-820.66	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	11.10	0.35137	YES	YES
9	a	14.42	0.44270	YES	YES
10	a	24.55	0.21685	YES	YES
11	a	25.49	0.35943	YES	YES
12	a	29.59	0.07086	YES	YES
13	a	35.52	0.14967	YES	YES
14	a	41.32	0.17283	YES	YES
15	a	44.60	0.35153	YES	YES
16	a	46.08	0.12662	YES	YES

17	a	48.07	0.08620	YES	YES
18	a	50.00	0.20936	YES	YES
19	a	54.73	0.38827	YES	YES
20	a	55.10	0.38027	YES	YES
21	a	58.36	0.20632	YES	YES
22	a	59.33	0.07946	YES	YES
23	a	61.44	0.07013	YES	YES
24	a	64.49	0.17003	YES	YES
25	a	65.37	1.97077	YES	YES
26	a	71.63	1.56296	YES	YES
27	a	72.59	0.41769	YES	YES
28	a	74.35	0.31314	YES	YES
29	a	78.11	1.08534	YES	YES
30	a	81.41	0.49607	YES	YES
31	a	84.66	1.07817	YES	YES
32	a	90.40	0.95895	YES	YES
33	a	92.93	0.11012	YES	YES
34	a	100.63	0.81969	YES	YES
35	a	105.36	1.38696	YES	YES
36	a	109.58	4.64327	YES	YES
37	a	135.08	2.44623	YES	YES
38	a	139.99	0.20424	YES	YES
39	a	144.63	3.31767	YES	YES
40	a	151.86	1.37039	YES	YES
41	a	165.60	0.74010	YES	YES
42	a	177.26	2.38792	YES	YES
43	a	192.92	0.30765	YES	YES
44	a	193.68	0.90073	YES	YES
45	a	198.90	0.38135	YES	YES
46	a	201.07	2.54434	YES	YES
47	a	206.57	0.54564	YES	YES
48	a	211.18	1.93079	YES	YES
49	a	223.23	1.32140	YES	YES
50	a	224.51	1.69260	YES	YES
51	a	229.32	1.87551	YES	YES
52	a	242.79	3.02734	YES	YES
53	a	244.98	1.52808	YES	YES
54	a	248.39	0.03009	YES	YES
55	a	253.03	0.40567	YES	YES
56	a	256.02	0.84167	YES	YES
57	a	259.75	3.05625	YES	YES
58	a	263.84	1.53727	YES	YES
59	a	266.26	0.31537	YES	YES
60	a	299.50	3.88522	YES	YES
61	a	323.06	11.03359	YES	YES
62	a	394.76	0.59330	YES	YES
63	a	395.92	1.73567	YES	YES
64	a	398.24	0.26445	YES	YES
65	a	399.79	0.36573	YES	YES
66	a	400.66	0.05852	YES	YES
67	a	404.99	0.32491	YES	YES
68	a	406.21	12.71320	YES	YES
69	a	406.74	26.06672	YES	YES
70	a	407.27	0.28962	YES	YES
71	a	416.43	1.51081	YES	YES
72	a	424.61	4.22212	YES	YES
73	a	434.36	11.08334	YES	YES
74	a	441.89	0.84136	YES	YES
75	a	447.25	8.50307	YES	YES
76	a	454.86	16.85586	YES	YES
77	a	465.22	0.85075	YES	YES
78	a	485.95	25.81911	YES	YES
79	a	496.12	1.77899	YES	YES
80	a	498.64	20.36913	YES	YES
81	a	501.12	5.52464	YES	YES
82	a	505.64	77.61471	YES	YES
83	a	508.30	63.34165	YES	YES
84	a	516.24	136.34790	YES	YES
85	a	525.65	1.60744	YES	YES
86	a	564.66	9.81488	YES	YES
87	a	583.44	21.27560	YES	YES
88	a	591.90	4.81210	YES	YES
89	a	597.48	0.91030	YES	YES
90	a	609.19	1.62718	YES	YES
91	a	609.57	0.73503	YES	YES
92	a	609.90	0.33306	YES	YES
93	a	610.33	0.21463	YES	YES
94	a	610.50	2.01271	YES	YES
95	a	611.57	1.22307	YES	YES
96	a	612.77	2.08319	YES	YES
97	a	666.51	22.56895	YES	YES
98	a	671.35	34.07436	YES	YES
99	a	672.06	9.50407	YES	YES
100	a	673.56	2.84678	YES	YES
101	a	684.67	3.79653	YES	YES
102	a	685.70	17.47813	YES	YES
103	a	689.05	11.33948	YES	YES
104	a	691.59	16.04724	YES	YES
105	a	693.03	28.33223	YES	YES
106	a	695.33	39.00695	YES	YES
107	a	696.99	32.94903	YES	YES
108	a	697.79	26.34036	YES	YES
109	a	700.94	41.93737	YES	YES
110	a	702.66	16.86242	YES	YES
111	a	704.35	24.90697	YES	YES
112	a	735.67	5.96006	YES	YES
113	a	743.20	8.82261	YES	YES
114	a	743.72	5.68197	YES	YES
115	a	744.42	0.75820	YES	YES
116	a	747.95	11.66266	YES	YES
117	a	749.18	6.25689	YES	YES
118	a	758.37	11.80811	YES	YES
119	a	775.58	1.99867	YES	YES
120	a	831.74	0.25067	YES	YES
121	a	833.59	0.55380	YES	YES
122	a	834.61	0.49094	YES	YES
123	a	838.17	0.24169	YES	YES
124	a	841.86	0.59096	YES	YES
125	a	844.11	0.14366	YES	YES
126	a	848.99	0.74370	YES	YES
127	a	901.12	7.49821	YES	YES
128	a	903.59	1.46232	YES	YES
129	a	908.95	0.84206	YES	YES
130	a	910.03	0.88721	YES	YES
131	a	916.90	0.85892	YES	YES
132	a	918.02	0.24215	YES	YES
133	a	922.60	0.70160	YES	YES
134	a	924.69	0.04228	YES	YES
135	a	941.92	23.48614	YES	YES
136	a	949.44	10.41999	YES	YES
137	a	955.92	0.35430	YES	YES
138	a	958.40	0.15902	YES	YES
139	a	958.65	0.17925	YES	YES
140	a	961.41	0.48199	YES	YES
141	a	966.04	0.28580	YES	YES
142	a	968.15	0.40753	YES	YES
143	a	972.22	0.20926	YES	YES
144	a	979.90	0.24144	YES	YES
145	a	981.88	1.20924	YES	YES
146	a	981.98	1.01660	YES	YES
147	a	982.32	0.75378	YES	YES
148	a	982.55	0.80122	YES	YES
149	a	983.11	0.45464	YES	YES
150	a	983.27	0.82696	YES	YES
151	a	983.50	4.57170	YES	YES
152	a	984.12	1.89606	YES	YES
153	a	984.15	0.69478	YES	YES
154	a	984.43	2.77126	YES	YES
155	a	986.46	0.37530	YES	YES
156	a	986.50	0.17966	YES	YES
157	a	986.94	0.12975	YES	YES
158	a	991.37	0.48957	YES	YES
159	a	1002.98	0.13438	YES	YES
160	a	1016.39	8.53266	YES	YES
161	a	1024.18	1.67256	YES	YES
162	a	1024.32	1.42331	YES	YES
163	a	1024.44	2.78788	YES	YES
164	a	1024.56	0.86594	YES	YES

165	a	1024.81	5.26866	YES	YES
166	a	1025.07	0.61206	YES	YES
167	a	1025.22	15.81465	YES	YES
168	a	1025.65	2.31127	YES	YES
169	a	1070.84	1.41861	YES	YES
170	a	1072.46	12.16079	YES	YES
171	a	1073.02	11.66433	YES	YES
172	a	1074.39	10.61469	YES	YES
173	a	1074.95	11.50985	YES	YES
174	a	1075.23	0.96967	YES	YES
175	a	1076.06	6.74429	YES	YES
176	a	1076.40	13.68961	YES	YES
177	a	1076.89	4.38361	YES	YES
178	a	1078.70	10.64766	YES	YES
179	a	1080.27	6.67147	YES	YES
180	a	1083.31	25.61393	YES	YES
181	a	1084.41	5.72007	YES	YES
182	a	1140.42	0.54485	YES	YES
183	a	1141.36	0.44573	YES	YES
184	a	1141.43	0.38782	YES	YES
185	a	1141.77	0.81901	YES	YES
186	a	1142.50	0.39641	YES	YES
187	a	1142.76	0.20714	YES	YES
188	a	1142.91	0.45034	YES	YES
189	a	1154.62	1.14329	YES	YES
190	a	1167.63	1.08138	YES	YES
191	a	1170.15	3.34328	YES	YES
192	a	1171.60	3.83906	YES	YES
193	a	1172.34	1.90680	YES	YES
194	a	1173.44	8.05016	YES	YES
195	a	1174.26	14.77764	YES	YES
196	a	1176.18	9.58901	YES	YES
197	a	1285.77	134.68411	YES	YES
198	a	1293.26	3.29420	YES	YES

* zero point VIBRATIONAL energy : 0.7401734 Hartree *

Trans TS_{25}_bx



bp86-SVP SCF energy: -2931.3685945370
pbe-TZVPP SCF energy: -2930.921062173

XYZ Coordinates
97

C	3.33205	1.37715	0.91787
C	3.31246	-1.52304	1.22460
C	3.33195	-0.34279	-1.43222
C	-2.80051	-0.01614	2.20619
C	-3.12644	1.66878	-0.12671
C	-3.22719	-1.24267	-0.38425
C	0.27996	2.55466	0.21839
C	0.46113	4.04869	0.24127
H	1.49550	4.28265	0.57984
H	-0.24442	4.50717	0.96464
H	0.30748	4.47988	-0.76829
C	0.28345	-1.42621	2.71020
C	-0.08383	-2.54196	3.68650
H	0.07139	-3.54071	3.22610
H	0.52604	-2.45067	4.60718
H	-1.16042	-2.45809	3.95528
O	0.37105	1.88808	-0.87736
O	0.06963	1.89052	1.28735
O	-0.19277	-1.60758	1.50335
O	0.95117	-0.44424	3.06347
P	2.53218	-0.15840	0.23628
P	-2.26588	0.11965	0.42998
Ru	0.11566	-0.01760	0.13655
C	4.46044	-0.56654	-4.01702
C	3.54457	0.46200	-3.73321
C	2.97854	0.57058	-2.45286
C	4.25458	-1.36947	-1.72413
C	4.81199	-1.48031	-3.00995
H	4.89688	-0.65745	-5.02575
H	3.25961	1.18173	-4.51853
H	2.25968	1.37571	-2.23163
H	4.53701	-2.09318	-0.94432
H	5.52713	-2.29207	-3.22402
C	4.52785	-3.63180	2.66563
C	5.03396	-2.32525	2.76496
C	4.43159	-1.27639	2.04962
C	2.80787	-2.83983	1.12518
C	3.41594	-3.88336	1.84331
H	5.00032	-4.45423	3.22867
H	5.90627	-2.11474	3.40610
H	4.83940	-0.25791	2.14041
H	1.94096	-3.03384	0.47541
H	3.01219	-4.90632	1.75771
C	4.47653	3.70672	2.04237
C	3.52253	2.96602	2.76365
C	2.94520	1.81155	2.20888
C	4.29666	2.11936	0.20122
C	4.86218	3.27960	0.76053
H	4.92355	4.61456	2.48146
H	3.21824	3.29030	3.77290
H	2.19814	1.22729	2.76907
H	4.61931	1.79123	-0.79879
H	5.61548	3.84710	0.18864
C	-3.63913	-0.10768	4.90579
C	-2.51946	0.65738	4.53677
C	-2.09782	0.70651	3.19718
C	-3.92635	-0.78216	2.58201
C	-4.34137	-0.82756	3.92429
H	-3.96345	-0.14584	5.95930
H	-1.95558	1.21872	5.30001
H	-1.21338	1.29838	2.91945
H	-4.48942	-1.34954	1.82439
H	-5.22117	-1.43228	4.20156
C	-4.57406	-3.41672	-1.59270
C	-3.49852	-3.65196	-0.71667
C	-2.82416	-2.57505	-0.11614
C	-4.30429	-1.01478	-1.26585
C	-4.97344	-2.09754	-1.86485
H	-5.10237	-4.26372	-2.06149
H	-3.17957	-4.68423	-0.49533
H	-1.98521	-2.75497	0.57940
H	-4.62983	0.01419	-1.48570
H	-5.81657	-1.90399	-2.54874
C	-4.38978	4.02620	-1.05460
C	-4.65353	3.54467	0.23883
C	-4.02898	2.37324	0.70093
C	-2.85814	2.16684	-1.42163
C	-3.49232	3.33174	-1.88412
H	-4.88243	4.94435	-1.41601
H	-5.35505	4.08305	0.89791
H	-4.24760	2.00672	1.71592
H	-2.15008	1.63744	-2.07750
H	-3.27689	3.69966	-2.90102
C	-0.24254	-1.03169	-1.72368
C	0.65126	-1.79411	-1.07547
C	-0.75301	-0.66606	-3.06071
H	-0.70337	-2.12453	-1.34927
C	-1.60279	-0.04258	-5.68793
C	-1.91370	-1.29146	-5.12177
C	-1.49640	-1.60198	-3.81917
C	-0.45872	0.59531	-3.62852
C	-0.87756	0.89606	-4.93447
H	-1.92967	0.19984	-6.71266
H	-2.48762	-2.03484	-5.69955
H	-1.74792	-2.58195	-3.38177
H	0.09168	1.33591	-3.03123
H	-0.63284	1.88079	-5.36694

Vibrational Frequencies

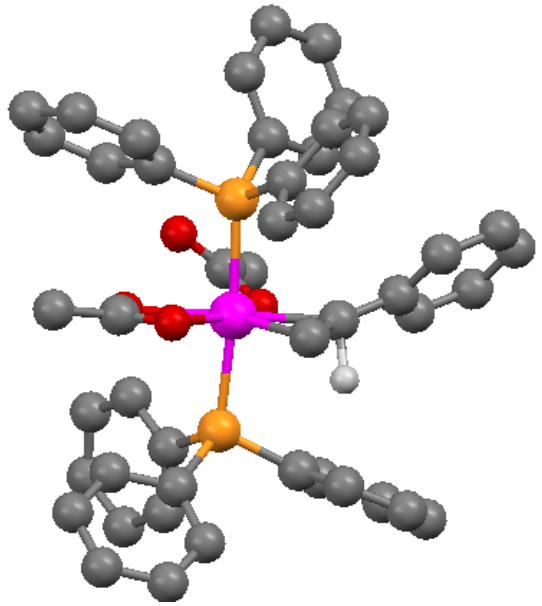
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-684.90	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	14.95	0.10606	YES	YES
9	a	17.76	0.01505	YES	YES
10	a	18.19	0.05409	YES	YES
11	a	28.42	0.01643	YES	YES
12	a	31.53	0.02775	YES	YES
13	a	33.78	0.07860	YES	YES
14	a	36.88	0.09885	YES	YES
15	a	43.81	0.17960	YES	YES
16	a	47.09	0.02005	YES	YES
17	a	49.98	0.01345	YES	YES

18	a	53.30	0.15239	YES	YES
19	a	56.23	0.11245	YES	YES
20	a	56.49	0.08508	YES	YES
21	a	58.49	0.27673	YES	YES
22	a	63.08	0.41468	YES	YES
23	a	64.51	0.12244	YES	YES
24	a	69.13	0.52810	YES	YES
25	a	70.18	0.16170	YES	YES
26	a	71.14	0.81375	YES	YES
27	a	74.36	0.49521	YES	YES
28	a	77.16	1.16761	YES	YES
29	a	78.90	0.76399	YES	YES
30	a	81.89	0.07441	YES	YES
31	a	83.86	0.58527	YES	YES
32	a	89.76	0.09392	YES	YES
33	a	95.46	3.34286	YES	YES
34	a	103.68	5.73480	YES	YES
35	a	105.25	5.11599	YES	YES
36	a	118.08	4.76216	YES	YES
37	a	121.04	7.42165	YES	YES
38	a	135.25	1.74372	YES	YES
39	a	143.28	0.00897	YES	YES
40	a	149.91	1.48349	YES	YES
41	a	161.75	0.78462	YES	YES
42	a	172.41	0.51713	YES	YES
43	a	182.72	1.12746	YES	YES
44	a	192.42	0.26870	YES	YES
45	a	196.70	0.32302	YES	YES
46	a	211.27	0.58869	YES	YES
47	a	214.27	3.05422	YES	YES
48	a	214.44	1.65828	YES	YES
49	a	219.02	2.87495	YES	YES
50	a	223.76	2.15762	YES	YES
51	a	226.06	4.32793	YES	YES
52	a	240.24	2.24672	YES	YES
53	a	242.19	1.56929	YES	YES
54	a	253.08	1.57093	YES	YES
55	a	255.65	1.37921	YES	YES
56	a	256.40	0.83722	YES	YES
57	a	261.13	0.29454	YES	YES
58	a	261.40	0.86124	YES	YES
59	a	270.39	2.89243	YES	YES
60	a	312.21	4.34851	YES	YES
61	a	322.31	10.99012	YES	YES
62	a	359.97	9.12960	YES	YES
63	a	396.60	1.26279	YES	YES
64	a	397.84	1.49999	YES	YES
65	a	398.51	0.28557	YES	YES
66	a	398.95	0.89375	YES	YES
67	a	401.13	25.86977	YES	YES
68	a	403.32	0.24481	YES	YES
69	a	405.20	0.80503	YES	YES
70	a	408.89	4.63016	YES	YES
71	a	411.23	8.28633	YES	YES
72	a	425.94	1.71235	YES	YES
73	a	434.98	1.99991	YES	YES
74	a	440.21	1.70522	YES	YES
75	a	443.41	19.98738	YES	YES
76	a	449.13	20.84439	YES	YES
77	a	474.50	0.84283	YES	YES
78	a	494.92	16.87168	YES	YES
79	a	496.44	6.26067	YES	YES
80	a	498.97	8.27998	YES	YES
81	a	502.94	49.73175	YES	YES
82	a	506.95	33.72140	YES	YES
83	a	508.85	15.53877	YES	YES
84	a	512.98	196.37748	YES	YES
85	a	523.39	13.99251	YES	YES
86	a	552.27	52.05227	YES	YES
87	a	593.85	5.55968	YES	YES
88	a	600.28	3.41389	YES	YES
89	a	605.01	0.79860	YES	YES
90	a	609.33	0.97722	YES	YES
91	a	609.74	2.41170	YES	YES
92	a	610.21	0.88723	YES	YES
93	a	610.66	0.43800	YES	YES
94	a	610.83	0.54009	YES	YES
95	a	611.12	1.08041	YES	YES
96	a	631.99	3.66804	YES	YES
97	a	663.66	37.66561	YES	YES
98	a	671.47	14.45709	YES	YES
99	a	672.13	13.71688	YES	YES
100	a	673.68	0.16696	YES	YES
101	a	686.56	1.89672	YES	YES
102	a	687.92	10.81209	YES	YES
103	a	689.00	4.86171	YES	YES
104	a	690.05	21.08383	YES	YES
105	a	695.46	55.42201	YES	YES
106	a	697.76	25.16913	YES	YES
107	a	697.98	32.03828	YES	YES
108	a	698.39	6.50592	YES	YES
109	a	701.87	31.21308	YES	YES
110	a	704.02	26.72919	YES	YES
111	a	705.46	31.68897	YES	YES
112	a	741.98	4.48547	YES	YES
113	a	743.23	11.84105	YES	YES
114	a	744.73	4.71857	YES	YES
115	a	745.72	4.03530	YES	YES
116	a	746.54	5.18171	YES	YES
117	a	747.76	6.53344	YES	YES
118	a	754.45	14.88580	YES	YES
119	a	767.30	9.33202	YES	YES
120	a	834.26	1.09378	YES	YES
121	a	837.68	0.80749	YES	YES
122	a	838.88	0.31402	YES	YES
123	a	840.49	0.30973	YES	YES
124	a	842.78	0.39660	YES	YES
125	a	847.15	0.41486	YES	YES
126	a	847.66	3.35675	YES	YES
127	a	908.16	4.59402	YES	YES
128	a	911.34	19.17939	YES	YES
129	a	912.36	2.81109	YES	YES
130	a	913.21	1.60495	YES	YES
131	a	916.82	0.99363	YES	YES
132	a	917.24	0.38870	YES	YES
133	a	921.67	1.72857	YES	YES
134	a	923.71	1.47109	YES	YES
135	a	931.46	27.13226	YES	YES
136	a	951.71	7.82104	YES	YES
137	a	959.21	0.79521	YES	YES
138	a	962.53	0.19133	YES	YES
139	a	962.75	0.79196	YES	YES
140	a	966.96	0.95355	YES	YES
141	a	967.51	0.84377	YES	YES
142	a	971.19	0.34405	YES	YES
143	a	972.91	0.52299	YES	YES
144	a	981.09	0.53611	YES	YES
145	a	982.32	0.71388	YES	YES
146	a	982.88	0.31184	YES	YES
147	a	983.08	1.18760	YES	YES
148	a	983.72	0.44637	YES	YES
149	a	983.91	0.81663	YES	YES
150	a	984.40	0.77670	YES	YES
151	a	985.26	0.95722	YES	YES
152	a	985.57	0.60167	YES	YES
153	a	985.98	6.52123	YES	YES
154	a	986.30	1.25910	YES	YES
155	a	986.47	1.99446	YES	YES
156	a	987.92	0.79449	YES	YES
157	a	991.02	0.99148	YES	YES
158	a	996.43	0.15222	YES	YES
159	a	997.33	1.92417	YES	YES
160	a	1021.72	8.82916	YES	YES
161	a	1023.61	2.89561	YES	YES
162	a	1023.72	1.76389	YES	YES
163	a	1024.43	1.27261	YES	YES
164	a	1024.75	2.48177	YES	YES
165	a	1025.86	3.18717	YES	YES

166	a	1026.10	1.99820	YES	YES
167	a	1027.27	18.24494	YES	YES
168	a	1028.91	5.15494	YES	YES
169	a	1071.77	3.79094	YES	YES
170	a	1072.21	8.33177	YES	YES
171	a	1073.34	3.97639	YES	YES
172	a	1074.51	8.86059	YES	YES
173	a	1075.27	4.89181	YES	YES
174	a	1075.34	5.14392	YES	YES
175	a	1076.14	12.14983	YES	YES
176	a	1076.93	22.52230	YES	YES
177	a	1077.72	14.56884	YES	YES
178	a	1078.03	21.53603	YES	YES
179	a	1079.23	2.12196	YES	YES
180	a	1082.86	16.98187	YES	YES
181	a	1083.50	4.74571	YES	YES
182	a	1140.12	0.49540	YES	YES
183	a	1141.63	0.47158	YES	YES
184	a	1141.75	0.99231	YES	YES
185	a	1141.84	0.35440	YES	YES
186	a	1142.05	0.41549	YES	YES
187	a	1142.36	0.24117	YES	YES
188	a	1142.69	0.59578	YES	YES
189	a	1159.11	6.15119	YES	YES
190	a	1167.65	1.90381	YES	YES
191	a	1170.32	3.72041	YES	YES
192	a	1170.54	1.34971	YES	YES
193	a	1171.17	12.78263	YES	YES
194	a	1172.56	11.30071	YES	YES
195	a	1173.05	9.89980	YES	YES
196	a	1174.48	4.85321	YES	YES
197	a	1292.91	11.48533	YES	YES
198	a	1294.89	3.80412	YES	YES

* zero point VIBRATIONAL energy : 0.7410996 Hartree *

Trans TS_{25}*_by*



bp86-SVP SCF energy: -2931.3644455140
pbe-TZVPP SCF energy: -2930.915253984

XYZ Coordinates
97

C	3.38829	0.93070	1.28550
C	3.27462	-1.39001	-0.47850
C	3.47493	1.38377	-1.49733
C	-2.87327	2.20833	0.03602
C	-3.12335	-0.13021	-1.68038
C	-3.24556	-0.39752	1.20343
C	0.10135	2.81474	-0.82537
C	-0.02184	4.28229	-1.13945
H	0.51315	4.88958	-0.38124
H	-1.09800	4.56531	-1.11011
H	0.36601	4.49549	-2.15683
C	-0.05972	-0.20186	2.67526
C	0.32486	-0.99534	3.92621
H	-0.38230	-0.76005	4.74739
H	0.33887	-2.08823	3.73199
H	1.34805	-0.69397	4.24603
O	-0.02771	1.92673	-1.73645
O	0.30620	2.40038	0.36960
O	0.41422	-0.72478	1.56937
O	-0.71901	0.84157	2.75621
P	2.57172	0.30945	-0.26747
P	-2.27250	0.45480	-0.13097
Ru	0.14483	0.29625	-0.26064
C	4.78172	3.20137	-3.23910
C	3.92297	3.67787	-2.23345
C	3.27878	2.77891	-1.37053
C	4.35610	0.91751	-2.49496
C	5.00070	1.82048	-3.35978
H	5.28825	3.90642	-3.91890
H	3.75662	4.76130	-2.11329
H	2.63839	3.16777	-0.56316
H	4.57120	-0.15586	-2.59728
H	5.68778	1.43357	-4.13091
C	4.09101	-4.09566	-0.75414
C	4.11654	-3.47021	0.50414
C	3.70535	-2.13441	0.64374
C	3.22816	-2.03919	-1.73958
C	3.64219	-3.37740	-1.87370
H	4.41351	-5.14455	-0.86041
H	4.45924	-4.02751	1.39192
H	3.72066	-1.66386	1.63866
H	2.87498	-1.50002	-2.63358
H	3.60573	-3.85931	-2.86482
C	4.69214	1.96522	3.56946
C	5.44036	1.34410	2.55256
C	4.79413	0.83629	1.41566
C	2.64447	1.56543	2.30079
C	3.29933	2.07833	3.43685
H	5.19962	2.36800	4.46211
H	6.53648	1.26028	2.64108
H	5.39278	0.36464	0.61857
H	1.55564	1.68523	2.20349
H	2.70464	2.57387	4.22211
C	-3.76318	4.86384	0.40952
C	-4.08609	4.17169	-0.76962
C	-3.64512	2.84878	-0.95657
C	-2.53942	2.91177	1.21777
C	-2.99153	4.22876	1.39976
H	-4.11422	5.89906	0.55812
H	-4.69293	4.65833	-1.55159
H	-3.91413	2.31463	-1.88118
H	-1.92478	2.41335	1.98507
H	-2.73205	4.76608	2.32743
C	-4.76978	-1.77190	3.15152
C	-5.22774	-0.55013	2.62909
C	-4.47246	0.13359	1.66143
C	-2.79135	-1.62169	1.73596
C	-3.55006	-2.30459	2.70168
H	-5.36258	-2.30657	3.91254
H	-6.18216	-0.12111	2.97753
H	-4.84440	1.09013	1.26203
H	-1.82974	-2.03841	1.40528
H	-3.17649	-3.25913	3.10715
C	-4.35154	-0.95970	-4.09022
C	-3.21587	-0.13176	-4.12383
C	-2.59729	0.27559	-2.93007
C	-4.26427	-0.96099	-1.65387
C	-4.87155	-1.37522	-2.85303
H	-4.82989	-1.28417	-5.02965
H	-2.79558	0.19451	-5.08966
H	-1.69875	0.91194	-2.96498
H	-4.68468	-1.29245	-0.69175
H	-5.76070	-2.02699	-2.81545
C	-0.05357	-1.73860	-0.97230
C	0.05670	-0.90011	-2.01295
C	-0.51658	-3.04822	-0.50239
H	1.00924	-1.83098	-1.64151
C	-1.41666	-5.58924	0.34335
C	-2.04852	-4.93997	-0.73298
C	-1.60101	-3.68106	-1.16069
C	0.11220	-3.70508	0.58315
C	-0.33436	-4.97005	0.99538
H	-1.76756	-6.58126	0.67362
H	-2.89608	-5.42118	-1.24870
H	-2.08884	-3.16792	-2.00347
H	0.94782	-3.20504	1.09329
H	0.16656	-5.47829	1.83613

Vibrational Frequencies

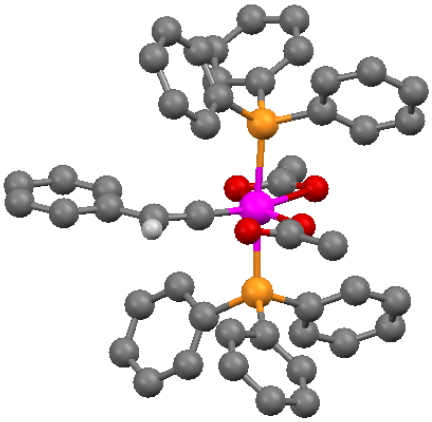
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-758.97	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	1.81	0.02248	YES	YES
9	a	18.60	0.14335	YES	YES
10	a	23.44	0.13519	YES	YES
11	a	28.65	0.39645	YES	YES
12	a	32.01	0.16036	YES	YES
13	a	40.06	0.04786	YES	YES

14	a	46.50	0.03036	YES	YES
15	a	46.67	0.06589	YES	YES
16	a	49.97	0.01819	YES	YES
17	a	50.97	0.13745	YES	YES
18	a	54.24	0.23756	YES	YES
19	a	56.57	0.16107	YES	YES
20	a	58.19	0.03442	YES	YES
21	a	63.22	0.85348	YES	YES
22	a	65.02	0.10105	YES	YES
23	a	65.81	0.25510	YES	YES
24	a	67.77	0.33286	YES	YES
25	a	74.26	2.85652	YES	YES
26	a	76.52	0.80221	YES	YES
27	a	78.98	0.05724	YES	YES
28	a	85.43	0.11230	YES	YES
29	a	89.64	1.01470	YES	YES
30	a	92.99	4.20160	YES	YES
31	a	97.27	0.56180	YES	YES
32	a	103.75	1.91090	YES	YES
33	a	107.43	1.57799	YES	YES
34	a	109.55	1.50203	YES	YES
35	a	111.38	2.10048	YES	YES
36	a	119.03	2.12356	YES	YES
37	a	135.93	0.70908	YES	YES
38	a	139.72	0.20417	YES	YES
39	a	144.82	3.09140	YES	YES
40	a	149.25	0.91324	YES	YES
41	a	163.26	1.18002	YES	YES
42	a	175.60	3.20921	YES	YES
43	a	185.80	0.63846	YES	YES
44	a	190.25	1.64673	YES	YES
45	a	196.11	0.06300	YES	YES
46	a	200.51	0.10530	YES	YES
47	a	207.70	1.85570	YES	YES
48	a	210.81	0.76392	YES	YES
49	a	221.67	2.38314	YES	YES
50	a	222.79	3.59626	YES	YES
51	a	226.10	1.31436	YES	YES
52	a	243.59	1.78316	YES	YES
53	a	245.00	1.90836	YES	YES
54	a	248.20	0.78054	YES	YES
55	a	252.58	0.94521	YES	YES
56	a	255.25	0.48043	YES	YES
57	a	261.96	1.05902	YES	YES
58	a	263.36	1.15981	YES	YES
59	a	268.69	0.32245	YES	YES
60	a	298.97	4.69062	YES	YES
61	a	320.98	11.53272	YES	YES
62	a	390.53	3.16860	YES	YES
63	a	398.03	0.42520	YES	YES
64	a	398.47	0.27543	YES	YES
65	a	398.94	0.10906	YES	YES
66	a	401.42	31.48237	YES	YES
67	a	403.16	1.82256	YES	YES
68	a	403.55	3.63240	YES	YES
69	a	405.08	1.11577	YES	YES
70	a	414.15	2.89215	YES	YES
71	a	417.84	3.13611	YES	YES
72	a	426.04	4.75076	YES	YES
73	a	432.32	7.67072	YES	YES
74	a	439.41	1.93463	YES	YES
75	a	445.49	12.03138	YES	YES
76	a	458.26	20.53380	YES	YES
77	a	468.14	0.95479	YES	YES
78	a	486.53	18.96652	YES	YES
79	a	498.43	6.84548	YES	YES
80	a	499.23	20.15116	YES	YES
81	a	501.33	26.18838	YES	YES
82	a	509.10	32.02284	YES	YES
83	a	510.61	60.34852	YES	YES
84	a	513.41	163.58165	YES	YES
85	a	524.13	10.94856	YES	YES
86	a	556.67	12.50270	YES	YES
87	a	588.08	17.39461	YES	YES
88	a	595.16	5.79514	YES	YES
89	a	605.43	3.22349	YES	YES
90	a	608.17	0.14447	YES	YES
91	a	609.00	2.37750	YES	YES
92	a	609.54	0.32309	YES	YES
93	a	609.76	0.29023	YES	YES
94	a	611.17	1.05889	YES	YES
95	a	611.96	0.03143	YES	YES
96	a	614.86	2.29576	YES	YES
97	a	665.20	32.29604	YES	YES
98	a	670.09	11.09013	YES	YES
99	a	671.11	22.11401	YES	YES
100	a	673.86	6.22544	YES	YES
101	a	683.21	5.51853	YES	YES
102	a	685.47	7.65519	YES	YES
103	a	688.86	8.60033	YES	YES
104	a	690.35	21.80331	YES	YES
105	a	691.20	31.70410	YES	YES
106	a	697.75	44.16549	YES	YES
107	a	698.57	36.82030	YES	YES
108	a	698.83	34.63423	YES	YES
109	a	701.17	6.65358	YES	YES
110	a	702.12	50.59680	YES	YES
111	a	711.69	13.06953	YES	YES
112	a	735.72	8.85693	YES	YES
113	a	739.67	6.66333	YES	YES
114	a	743.33	8.54988	YES	YES
115	a	744.46	3.77700	YES	YES
116	a	747.13	4.52764	YES	YES
117	a	748.80	6.62279	YES	YES
118	a	755.81	12.99482	YES	YES
119	a	771.96	1.21673	YES	YES
120	a	828.99	0.09742	YES	YES
121	a	833.88	1.36814	YES	YES
122	a	835.43	0.83600	YES	YES
123	a	838.08	0.35959	YES	YES
124	a	844.06	1.40616	YES	YES
125	a	847.71	2.05344	YES	YES
126	a	848.15	0.30583	YES	YES
127	a	898.02	8.02850	YES	YES
128	a	904.54	0.39940	YES	YES
129	a	910.35	0.72275	YES	YES
130	a	911.65	0.92013	YES	YES
131	a	914.49	0.09640	YES	YES
132	a	918.20	1.23325	YES	YES
133	a	922.13	1.00104	YES	YES
134	a	922.90	0.25459	YES	YES
135	a	944.11	31.82851	YES	YES
136	a	949.21	4.61388	YES	YES
137	a	956.03	0.05163	YES	YES
138	a	957.59	2.20934	YES	YES
139	a	960.55	0.50614	YES	YES
140	a	961.23	0.53512	YES	YES
141	a	967.08	1.68691	YES	YES
142	a	968.34	0.31279	YES	YES
143	a	970.65	0.21727	YES	YES
144	a	979.73	2.24291	YES	YES
145	a	980.39	0.25348	YES	YES
146	a	981.23	0.15836	YES	YES
147	a	981.33	1.59009	YES	YES
148	a	982.31	0.69026	YES	YES
149	a	982.82	0.64114	YES	YES
150	a	983.97	0.48257	YES	YES
151	a	984.40	0.33096	YES	YES
152	a	985.06	0.12563	YES	YES
153	a	985.41	1.99560	YES	YES
154	a	986.15	6.41445	YES	YES
155	a	986.26	1.35953	YES	YES
156	a	986.82	0.34879	YES	YES
157	a	988.24	2.82022	YES	YES
158	a	991.63	0.40744	YES	YES
159	a	998.54	0.12230	YES	YES
160	a	1021.14	11.37153	YES	YES
161	a	1023.50	0.37835	YES	YES

162	a	1023.78	1.48788	YES	YES
163	a	1024.21	2.76058	YES	YES
164	a	1024.46	1.45144	YES	YES
165	a	1024.79	1.93809	YES	YES
166	a	1024.94	3.74272	YES	YES
167	a	1026.07	0.87959	YES	YES
168	a	1027.47	22.19088	YES	YES
169	a	1069.97	2.31411	YES	YES
170	a	1070.39	0.69978	YES	YES
171	a	1072.75	13.30712	YES	YES
172	a	1072.83	14.60349	YES	YES
173	a	1074.57	7.58912	YES	YES
174	a	1074.78	1.06625	YES	YES
175	a	1075.94	2.84124	YES	YES
176	a	1076.42	28.09953	YES	YES
177	a	1076.65	7.33940	YES	YES
178	a	1078.23	11.95818	YES	YES
179	a	1078.90	2.63659	YES	YES
180	a	1081.93	7.94623	YES	YES
181	a	1083.15	10.49920	YES	YES
182	a	1139.34	0.32738	YES	YES
183	a	1140.49	0.38853	YES	YES
184	a	1141.02	0.38268	YES	YES
185	a	1141.98	0.42333	YES	YES
186	a	1142.18	0.35839	YES	YES
187	a	1142.68	0.33979	YES	YES
188	a	1143.30	0.13910	YES	YES
189	a	1153.60	0.59127	YES	YES
190	a	1166.36	0.51060	YES	YES
191	a	1168.32	5.50886	YES	YES
192	a	1169.25	0.61628	YES	YES
193	a	1170.19	4.28142	YES	YES
194	a	1173.00	8.25232	YES	YES
195	a	1174.78	5.36682	YES	YES
196	a	1175.49	9.14867	YES	YES
197	a	1287.20	0.87931	YES	YES
198	a	1291.27	31.17853	YES	YES

* zero point VIBRATIONAL energy : 0.7412549 Hartree *

Trans 5_ax



bp86-SVP SCF energy: -2931.4845362850
pbe-TZVPP SCF energy: -2931.028268646

XYZ Coordinates
97

C	1.25205	0.03235	0.84455
C	2.46681	0.00045	1.41826
H	2.46833	0.01750	2.52503
C	3.76077	-0.10737	0.73265
C	3.87228	-0.21793	-0.67946
H	2.95440	-0.21320	-1.29053
C	5.12501	-0.33218	-1.29625
H	5.18318	-0.41865	-2.39490
C	6.30618	-0.33941	-0.52858
H	7.29022	-0.42969	-1.01791
C	6.21227	-0.23145	0.86979
H	7.12671	-0.23620	1.48719
C	4.95936	-0.11726	1.49138
H	4.89801	-0.03531	2.59024
C	-1.72153	3.10222	-1.09599
C	-3.01151	2.55606	-0.90060
H	-3.15866	1.75511	-0.15797
C	-4.09897	3.02822	-1.65157
H	-5.10127	2.59870	-1.48813
C	-3.91049	4.03302	-2.61826
H	-4.76545	4.39591	-3.21291
C	-2.62860	4.56807	-2.82713
H	-2.47225	5.35453	-3.58422
C	-1.53730	4.10861	-2.06731
H	-0.53693	4.53961	-2.23157
C	-0.62459	3.22867	1.59563
C	-1.67284	4.14466	1.82923
H	-2.37476	4.40239	1.02040
C	-1.82836	4.73738	3.09483
H	-2.65304	5.44978	3.26411
C	-0.93783	4.42668	4.13594
H	-1.06191	4.89178	5.12819
C	0.11004	3.51772	3.90774
H	0.80953	3.26073	4.71996
C	0.26680	2.91886	2.64795
H	1.08385	2.20022	2.48197
C	1.15954	3.33920	-0.68607
C	1.55835	4.58330	-0.14824
H	0.99684	5.03096	0.68684
C	2.67801	5.25343	-0.66937
H	2.98383	6.22098	-0.23749
C	3.40804	4.69143	-1.73066
H	4.29096	5.21516	-2.13360
C	3.01405	3.45518	-2.26994
H	3.58863	3.00264	-3.09474
C	1.89788	2.77772	-1.75127
H	1.59242	1.80568	-2.17079
C	-2.10917	-2.97223	0.54892
C	-3.26640	-2.30600	0.08296
H	-3.16453	-1.45904	-0.61342
C	-4.53877	-2.72775	0.50163
H	-5.43463	-2.20302	0.12953
C	-4.67295	-3.80391	1.39698
H	-5.67379	-4.12703	1.72927
C	-3.52584	-4.46320	1.86891
H	-3.62088	-5.30735	2.57222
C	-2.24929	-4.05281	1.44602
H	-1.35739	-4.57830	1.82174
C	-0.27928	-3.14742	-1.72177
C	-1.30678	-3.89792	-2.33114
H	-2.25652	-4.06398	-1.79901
C	-1.12411	-4.44305	-3.61466
H	-1.93506	-5.03063	-4.07646
C	0.08675	-4.24975	-4.29969
H	0.23064	-4.68214	-5.30398
C	1.11519	-3.50127	-3.69900
H	2.06915	-3.34476	-4.22963
C	0.93243	-2.94562	-2.42297
H	1.74377	-2.35922	-1.96254
C	0.73946	-3.38867	0.98108
C	1.02952	-2.96526	2.29809
H	0.59101	-2.03289	2.69388
C	1.88052	-3.73386	3.11043
H	2.09857	-3.39348	4.13628
C	2.45961	-4.91697	2.62098
H	3.13413	-5.51108	3.26021
C	2.17671	-5.33899	1.31100
H	2.62438	-6.26626	0.91633
C	1.31985	-4.58145	0.49451
H	1.10196	-4.92871	-0.52718
C	-0.85793	-0.04216	-2.61135
C	-1.06958	-0.00917	-4.10466
H	-1.92588	-0.65795	-4.38075
H	-0.15575	-0.33246	-4.64193
H	-1.31729	1.03108	-4.41357
C	-1.35017	0.00566	2.75931
C	-2.59051	0.07965	3.64746
H	-2.28879	0.19915	4.70688
H	-3.17579	-0.86035	3.54020
H	-3.24848	0.91940	3.34062
O	0.33685	0.03026	-2.13073
O	-1.83076	-0.10126	-1.79675
O	-1.63284	0.12890	1.48161
O	-0.22000	-0.17708	3.22921
P	-0.33491	2.44348	-0.05902
P	-0.44723	-2.39335	-0.03565
Ru	-0.29697	0.03436	-0.06226

Vibrational Frequencies

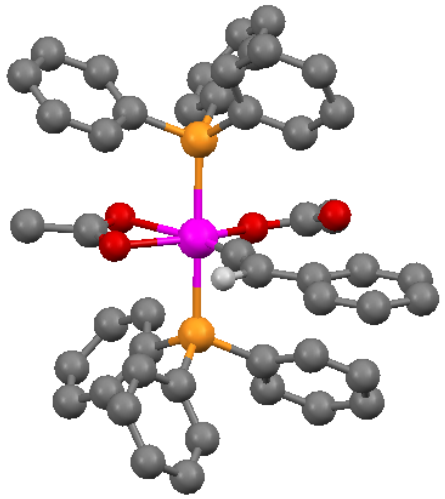
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	4.94	0.03969	YES	YES
8	a	16.00	0.10831	YES	YES
9	a	20.09	0.05515	YES	YES
10	a	22.27	0.06367	YES	YES
11	a	23.46	0.08992	YES	YES
12	a	26.79	0.10866	YES	YES
13	a	32.46	0.23903	YES	YES
14	a	37.34	0.18582	YES	YES
15	a	39.56	0.06621	YES	YES
16	a	42.42	0.38067	YES	YES
17	a	43.64	0.15643	YES	YES
18	a	45.16	0.27170	YES	YES
19	a	49.09	0.15131	YES	YES

20	a	51.36	0.20808	YES	YES
21	a	54.64	0.23014	YES	YES
22	a	57.12	0.05767	YES	YES
23	a	59.14	0.07919	YES	YES
24	a	61.26	0.10621	YES	YES
25	a	64.74	0.41853	YES	YES
26	a	66.30	0.27819	YES	YES
27	a	69.30	0.22070	YES	YES
28	a	75.38	0.12311	YES	YES
29	a	76.15	0.42715	YES	YES
30	a	77.11	2.15631	YES	YES
31	a	80.16	0.12715	YES	YES
32	a	82.20	0.14647	YES	YES
33	a	89.21	0.05315	YES	YES
34	a	106.29	4.53753	YES	YES
35	a	115.48	0.14735	YES	YES
36	a	121.45	5.59713	YES	YES
37	a	130.59	6.93113	YES	YES
38	a	139.04	0.44539	YES	YES
39	a	158.15	1.21181	YES	YES
40	a	165.56	3.12951	YES	YES
41	a	181.52	1.03592	YES	YES
42	a	190.09	0.71944	YES	YES
43	a	191.46	0.23894	YES	YES
44	a	194.83	0.25976	YES	YES
45	a	211.57	0.21545	YES	YES
46	a	213.77	3.30304	YES	YES
47	a	218.33	1.13087	YES	YES
48	a	221.67	2.97664	YES	YES
49	a	231.95	3.16694	YES	YES
50	a	241.32	1.93337	YES	YES
51	a	241.89	1.11952	YES	YES
52	a	247.10	5.09431	YES	YES
53	a	254.18	0.89279	YES	YES
54	a	256.87	0.16693	YES	YES
55	a	260.27	1.63081	YES	YES
56	a	263.27	0.75938	YES	YES
57	a	263.51	1.11982	YES	YES
58	a	268.24	0.30569	YES	YES
59	a	302.89	3.68546	YES	YES
60	a	314.40	14.82771	YES	YES
61	a	396.47	0.40114	YES	YES
62	a	398.23	0.20924	YES	YES
63	a	398.66	0.16370	YES	YES
64	a	400.50	0.31983	YES	YES
65	a	402.85	0.36981	YES	YES
66	a	406.58	2.45434	YES	YES
67	a	407.69	22.88031	YES	YES
68	a	409.08	0.48547	YES	YES
69	a	415.04	6.08889	YES	YES
70	a	422.99	7.16606	YES	YES
71	a	433.36	1.06150	YES	YES
72	a	437.41	0.42675	YES	YES
73	a	443.86	17.15543	YES	YES
74	a	448.43	20.01401	YES	YES
75	a	472.23	0.26456	YES	YES
76	a	486.03	10.38525	YES	YES
77	a	493.58	15.02390	YES	YES
78	a	498.51	17.08513	YES	YES
79	a	502.76	19.31595	YES	YES
80	a	505.36	62.14186	YES	YES
81	a	506.98	34.72402	YES	YES
82	a	512.19	179.44213	YES	YES
83	a	518.78	9.10873	YES	YES
84	a	524.38	4.84716	YES	YES
85	a	583.11	25.56203	YES	YES
86	a	593.93	4.03341	YES	YES
87	a	602.72	3.96747	YES	YES
88	a	609.35	1.26893	YES	YES
89	a	609.50	1.32314	YES	YES
90	a	609.76	0.43109	YES	YES
91	a	609.93	0.81857	YES	YES
92	a	610.16	2.87954	YES	YES
93	a	610.39	0.43834	YES	YES
94	a	613.67	3.21100	YES	YES
95	a	656.66	24.00687	YES	YES
96	a	671.07	35.30908	YES	YES
97	a	673.90	15.00119	YES	YES
98	a	675.80	4.92376	YES	YES
99	a	684.75	18.52626	YES	YES
100	a	689.68	3.74447	YES	YES
101	a	690.92	2.95053	YES	YES
102	a	691.52	17.97097	YES	YES
103	a	692.73	12.89054	YES	YES
104	a	695.91	38.23418	YES	YES
105	a	696.63	26.64370	YES	YES
106	a	697.48	21.63256	YES	YES
107	a	700.88	25.85156	YES	YES
108	a	701.52	27.85818	YES	YES
109	a	703.03	24.53607	YES	YES
110	a	704.36	27.53063	YES	YES
111	a	714.67	9.38364	YES	YES
112	a	742.73	5.98779	YES	YES
113	a	743.24	5.00866	YES	YES
114	a	745.30	1.74643	YES	YES
115	a	745.67	6.70512	YES	YES
116	a	746.04	9.89697	YES	YES
117	a	746.66	3.96684	YES	YES
118	a	762.03	34.21330	YES	YES
119	a	818.43	1.68660	YES	YES
120	a	829.90	0.05183	YES	YES
121	a	835.06	0.30385	YES	YES
122	a	835.72	0.11626	YES	YES
123	a	840.89	0.33951	YES	YES
124	a	844.05	0.32132	YES	YES
125	a	845.91	1.16338	YES	YES
126	a	846.97	0.49405	YES	YES
127	a	891.98	6.23448	YES	YES
128	a	908.20	0.83958	YES	YES
129	a	910.61	0.22168	YES	YES
130	a	914.75	0.32446	YES	YES
131	a	920.68	0.33731	YES	YES
132	a	923.18	2.26345	YES	YES
133	a	923.45	0.50482	YES	YES
134	a	924.52	1.30385	YES	YES
135	a	945.13	10.66592	YES	YES
136	a	951.00	0.24372	YES	YES
137	a	958.55	0.04649	YES	YES
138	a	959.27	0.09170	YES	YES
139	a	963.78	0.11922	YES	YES
140	a	970.13	0.82822	YES	YES
141	a	970.25	0.17250	YES	YES
142	a	971.88	0.04257	YES	YES
143	a	973.24	0.34928	YES	YES
144	a	979.72	1.57349	YES	YES
145	a	982.56	1.08549	YES	YES
146	a	982.94	1.22101	YES	YES
147	a	983.38	0.76880	YES	YES
148	a	983.45	0.07518	YES	YES
149	a	983.59	0.70251	YES	YES
150	a	983.72	0.25586	YES	YES
151	a	984.26	1.00158	YES	YES
152	a	985.00	0.31154	YES	YES
153	a	986.51	0.10541	YES	YES
154	a	987.37	3.06618	YES	YES
155	a	990.76	0.04528	YES	YES
156	a	993.95	11.48401	YES	YES
157	a	996.25	0.36215	YES	YES
158	a	1002.28	0.20046	YES	YES
159	a	1021.46	9.20414	YES	YES
160	a	1023.59	1.41751	YES	YES
161	a	1024.14	1.47702	YES	YES
162	a	1025.10	2.51329	YES	YES
163	a	1025.39	1.37946	YES	YES
164	a	1026.10	0.98491	YES	YES
165	a	1026.29	0.81203	YES	YES
166	a	1026.65	4.81980	YES	YES
167	a	1027.18	15.42385	YES	YES

168	a	1069.51	6.21427	YES	YES
169	a	1073.30	2.32072	YES	YES
170	a	1074.00	3.99134	YES	YES
171	a	1075.00	9.54509	YES	YES
172	a	1075.97	2.37308	YES	YES
173	a	1077.35	18.01900	YES	YES
174	a	1078.14	3.36439	YES	YES
175	a	1078.39	12.28010	YES	YES
176	a	1079.88	20.98548	YES	YES
177	a	1081.46	20.83208	YES	YES
178	a	1082.23	3.90356	YES	YES
179	a	1084.78	11.18317	YES	YES
180	a	1085.83	9.95487	YES	YES
181	a	1130.97	19.99487	YES	YES
182	a	1136.85	4.35356	YES	YES
183	a	1141.30	0.19215	YES	YES
184	a	1142.20	0.35762	YES	YES
185	a	1142.48	0.48816	YES	YES
186	a	1142.78	0.41447	YES	YES
187	a	1143.40	0.75747	YES	YES
188	a	1144.71	0.42342	YES	YES
189	a	1161.62	3.52298	YES	YES
190	a	1167.33	1.84940	YES	YES
191	a	1169.52	4.12014	YES	YES
192	a	1173.76	12.27056	YES	YES
193	a	1173.93	2.39800	YES	YES
194	a	1175.18	6.70850	YES	YES
195	a	1181.62	4.98151	YES	YES
196	a	1243.31	1.19554	YES	YES
197	a	1291.19	5.79991	YES	YES
198	a	1291.93	169.58038	YES	YES

* zero point VIBRATIONAL energy : 0.7456610 Hartree *

Trans 5_ay



bp86-SVP SCF energy: -2931.4836757520
pbe-TZVPP SCF energy: -2931.027752225

XYZ Coordinates
97

C	1.26701	0.15448	-0.69069
C	2.39365	0.31939	-1.40557
H	2.21076	0.33243	-2.50104
C	3.79349	0.50564	-0.99769
C	4.22291	0.49302	0.35686
H	3.48585	0.31732	1.15768
C	5.57426	0.69142	0.67805
H	5.88095	0.67589	1.73804
C	6.53527	0.90252	-0.32851
H	7.59557	1.05685	-0.06763
C	6.12378	0.91149	-1.67307
H	6.86223	1.07289	-2.47705
C	4.77463	0.71596	-2.00219
H	4.46467	0.72626	-3.06144
C	-2.41409	2.87844	0.20562
C	-3.14563	2.27131	1.25298
H	-2.66535	1.50122	1.87847
C	-4.47726	2.64416	1.49200
H	-5.03665	2.16809	2.31423
C	-5.10001	3.60835	0.67837
H	-6.14902	3.89407	0.86359
C	-4.38307	4.20216	-0.37363
H	-4.86645	4.95582	-1.01750
C	-3.04376	3.84279	-0.60910
H	-2.48692	4.31944	-1.43154
C	0.24772	3.18827	1.34437
C	-0.39024	4.04991	2.26216
H	-1.47196	4.24024	2.18359
C	0.35057	4.67297	3.28246
H	-0.16120	5.34174	3.99454
C	1.73292	4.44697	3.39268
H	2.31202	4.93640	4.19352
C	2.37390	3.59302	2.47749
H	3.45701	3.40358	2.55393
C	1.63755	2.96443	1.46137
H	2.15338	2.29440	0.75618
C	-0.10242	3.29163	-1.53517
C	0.45864	4.58357	-1.43020
H	0.60033	5.04616	-0.44044
C	0.84683	5.28373	-2.58501
H	1.28844	6.28968	-2.48978
C	0.67844	4.70339	-3.85368
H	0.98779	5.25283	-4.75852
C	0.12047	3.41789	-3.96382
H	-0.00928	2.95469	-4.95622
C	-0.26579	2.71023	-2.81297
H	-0.69609	1.69899	-2.89924
C	-0.90572	-3.17117	1.55559
C	-2.11686	-2.66612	2.08467
H	-2.65475	-1.86718	1.55030
C	-2.63347	-3.18633	3.28277
H	-3.58107	-2.78929	3.68352
C	-1.94395	-4.19867	3.97423
H	-2.34786	-4.59848	4.91941
C	-0.73480	-4.69422	3.45859
H	-0.18445	-5.48403	3.99646
C	-0.21735	-4.18605	2.25389
H	0.73174	-4.58073	1.85921
C	-1.30598	-3.27505	-1.33749
C	-2.37677	-4.14340	-1.03884
H	-2.62187	-4.37521	0.00960
C	-3.13231	-4.72386	-2.07396
H	-3.96387	-5.40410	-1.82501
C	-2.82478	-4.44601	-3.41636
H	-3.41483	-4.90527	-4.22699
C	-1.75845	-3.58028	-3.72182
H	-1.51007	-3.35617	-4.77254
C	-1.00901	-2.99156	-2.69114
H	-0.18069	-2.30897	-2.93928
C	1.37820	-3.28788	-0.25974
C	2.50129	-2.74714	0.40429
H	2.38796	-1.84673	1.03272
C	3.75611	-3.36700	0.27970
H	4.62616	-2.92872	0.79507
C	3.90490	-4.52242	-0.50631
H	4.89405	-4.99953	-0.60885
C	2.78844	-5.06706	-1.16356
H	2.89416	-5.97652	-1.77842
C	1.52909	-4.45568	-1.04141
H	0.66210	-4.89541	-1.55851
C	-2.63905	-0.31262	-1.43547
C	-3.85167	-0.48948	-2.31402
H	-4.77311	-0.23284	-1.75378
H	-3.91426	-1.55471	-2.63156
H	-3.76900	0.13452	-3.22734
C	0.70653	-0.08543	2.74448
C	0.34878	0.12885	4.21438
H	0.51302	1.20031	4.46674
H	1.02065	-0.48108	4.85209
H	-0.71134	-0.12081	4.42262
O	-1.48392	-0.10426	-1.97215
O	-2.70340	-0.39152	-0.16936
O	-0.32427	0.05299	1.94315
O	1.86746	-0.32534	2.39563
P	-0.65689	2.35162	-0.03876
P	-0.26412	-2.46480	-0.03267
Ru	-0.41972	-0.04237	-0.09141

Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	10.31	0.02648	YES	YES
8	a	17.30	0.04932	YES	YES
9	a	18.76	0.00749	YES	YES
10	a	23.83	0.03494	YES	YES
11	a	24.85	0.13025	YES	YES
12	a	29.77	0.08610	YES	YES
13	a	35.99	0.23851	YES	YES
14	a	36.49	0.20771	YES	YES
15	a	41.40	0.27189	YES	YES
16	a	43.60	0.35068	YES	YES
17	a	45.51	0.10283	YES	YES

18	a	47.57	0.28296	YES	YES
19	a	50.95	0.19739	YES	YES
20	a	54.08	0.25332	YES	YES
21	a	54.78	0.29559	YES	YES
22	a	55.89	0.27779	YES	YES
23	a	59.36	0.35297	YES	YES
24	a	64.27	0.14671	YES	YES
25	a	67.42	0.41583	YES	YES
26	a	69.82	0.01768	YES	YES
27	a	70.85	0.91331	YES	YES
28	a	74.72	1.19026	YES	YES
29	a	75.81	0.88949	YES	YES
30	a	78.98	0.07796	YES	YES
31	a	83.11	0.12457	YES	YES
32	a	91.51	0.05580	YES	YES
33	a	96.16	0.88113	YES	YES
34	a	106.08	4.50336	YES	YES
35	a	108.97	6.13922	YES	YES
36	a	116.62	1.43352	YES	YES
37	a	120.67	2.07796	YES	YES
38	a	139.02	0.53927	YES	YES
39	a	157.04	0.43484	YES	YES
40	a	167.16	2.89974	YES	YES
41	a	172.58	0.70404	YES	YES
42	a	188.21	1.07243	YES	YES
43	a	190.46	0.49741	YES	YES
44	a	193.46	0.20251	YES	YES
45	a	209.99	0.79580	YES	YES
46	a	213.27	3.70345	YES	YES
47	a	218.38	1.15975	YES	YES
48	a	221.30	2.76286	YES	YES
49	a	228.40	6.77215	YES	YES
50	a	236.11	4.01192	YES	YES
51	a	240.99	2.92246	YES	YES
52	a	241.89	0.27780	YES	YES
53	a	253.51	0.37283	YES	YES
54	a	254.74	0.26977	YES	YES
55	a	256.05	2.15270	YES	YES
56	a	258.62	2.68677	YES	YES
57	a	263.50	0.99572	YES	YES
58	a	263.81	0.85826	YES	YES
59	a	295.97	2.60950	YES	YES
60	a	323.75	12.65305	YES	YES
61	a	393.03	1.90934	YES	YES
62	a	397.37	0.03975	YES	YES
63	a	397.64	0.23532	YES	YES
64	a	398.71	0.07904	YES	YES
65	a	399.60	0.50347	YES	YES
66	a	403.10	0.04859	YES	YES
67	a	404.56	1.55842	YES	YES
68	a	406.83	24.75834	YES	YES
69	a	413.17	0.17861	YES	YES
70	a	421.50	8.35195	YES	YES
71	a	430.46	0.75806	YES	YES
72	a	438.09	0.24426	YES	YES
73	a	441.87	20.09433	YES	YES
74	a	449.30	20.53627	YES	YES
75	a	469.26	0.25229	YES	YES
76	a	473.59	2.01739	YES	YES
77	a	488.86	11.11523	YES	YES
78	a	498.10	14.69672	YES	YES
79	a	500.65	15.71798	YES	YES
80	a	504.58	63.69480	YES	YES
81	a	507.76	45.97406	YES	YES
82	a	512.31	175.79488	YES	YES
83	a	515.75	8.38175	YES	YES
84	a	522.42	9.22102	YES	YES
85	a	579.90	15.77994	YES	YES
86	a	591.19	4.08465	YES	YES
87	a	600.36	5.14855	YES	YES
88	a	608.99	0.94586	YES	YES
89	a	609.27	1.48164	YES	YES
90	a	609.63	0.71107	YES	YES
91	a	609.94	1.62344	YES	YES
92	a	610.22	1.47135	YES	YES
93	a	610.45	0.37587	YES	YES
94	a	613.72	2.71288	YES	YES
95	a	650.36	24.31243	YES	YES
96	a	662.22	4.11094	YES	YES
97	a	673.19	39.37947	YES	YES
98	a	674.32	11.19913	YES	YES
99	a	676.06	4.71838	YES	YES
100	a	690.21	3.14046	YES	YES
101	a	691.87	1.73419	YES	YES
102	a	692.17	14.07624	YES	YES
103	a	693.11	13.79322	YES	YES
104	a	696.70	41.08625	YES	YES
105	a	698.42	51.08989	YES	YES
106	a	699.63	20.63912	YES	YES
107	a	700.86	24.90539	YES	YES
108	a	702.02	27.33310	YES	YES
109	a	702.59	25.77297	YES	YES
110	a	704.21	17.37232	YES	YES
111	a	738.87	5.56968	YES	YES
112	a	743.13	5.68550	YES	YES
113	a	744.09	5.12613	YES	YES
114	a	744.52	3.88279	YES	YES
115	a	745.44	9.48294	YES	YES
116	a	746.84	1.24656	YES	YES
117	a	747.12	7.40055	YES	YES
118	a	762.19	29.91717	YES	YES
119	a	820.38	4.45628	YES	YES
120	a	835.65	0.09464	YES	YES
121	a	836.64	0.14585	YES	YES
122	a	839.22	0.51538	YES	YES
123	a	841.58	0.12029	YES	YES
124	a	842.67	0.27387	YES	YES
125	a	845.24	0.36855	YES	YES
126	a	846.36	1.08039	YES	YES
127	a	906.21	4.36230	YES	YES
128	a	908.35	0.66590	YES	YES
129	a	912.30	1.33683	YES	YES
130	a	913.33	0.05547	YES	YES
131	a	919.40	0.31618	YES	YES
132	a	921.87	0.30109	YES	YES
133	a	924.34	0.95276	YES	YES
134	a	927.69	0.90573	YES	YES
135	a	946.02	14.81468	YES	YES
136	a	957.72	0.17654	YES	YES
137	a	958.78	0.04571	YES	YES
138	a	961.50	0.03071	YES	YES
139	a	962.32	0.25632	YES	YES
140	a	968.39	0.08299	YES	YES
141	a	971.02	0.06195	YES	YES
142	a	972.65	0.29057	YES	YES
143	a	979.85	2.55012	YES	YES
144	a	982.13	0.05404	YES	YES
145	a	982.52	0.27614	YES	YES
146	a	983.45	1.78207	YES	YES
147	a	983.55	1.78657	YES	YES
148	a	983.94	0.33955	YES	YES
149	a	984.46	1.72893	YES	YES
150	a	985.13	0.67414	YES	YES
151	a	985.71	0.15262	YES	YES
152	a	986.36	3.67715	YES	YES
153	a	987.12	0.03325	YES	YES
154	a	988.99	0.06150	YES	YES
155	a	989.60	6.81005	YES	YES
156	a	993.13	0.20937	YES	YES
157	a	999.26	0.77154	YES	YES
158	a	1008.32	2.62963	YES	YES
159	a	1018.43	11.24857	YES	YES
160	a	1023.38	1.44079	YES	YES
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162	a	1023.99	2.02269	YES	YES
163	a	1024.52	2.88680	YES	YES
164	a	1025.32	2.14175	YES	YES
165	a	1025.40	1.73275	YES	YES

166	a	1027.42	17.56211	YES	YES
167	a	1028.82	4.78626	YES	YES
168	a	1072.50	4.35875	YES	YES
169	a	1073.00	2.35470	YES	YES
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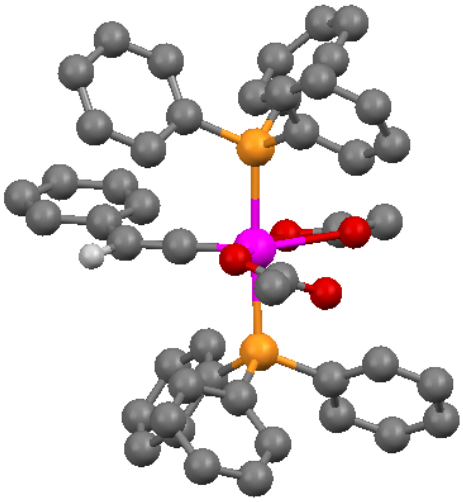
171	a	1074.08	7.68584	YES	YES
172	a	1074.88	0.33673	YES	YES
173	a	1075.87	2.20176	YES	YES
174	a	1076.58	11.64185	YES	YES
175	a	1078.86	18.12209	YES	YES
176	a	1079.46	21.84509	YES	YES
177	a	1080.39	24.69844	YES	YES
178	a	1080.74	10.38114	YES	YES
179	a	1085.04	17.61026	YES	YES
180	a	1085.58	5.27580	YES	YES
181	a	1136.68	1.43441	YES	YES
182	a	1140.70	0.35236	YES	YES
183	a	1141.77	0.65705	YES	YES
184	a	1142.04	0.32916	YES	YES
185	a	1142.27	0.31098	YES	YES
186	a	1143.06	0.40097	YES	YES
187	a	1143.32	0.59058	YES	YES
188	a	1152.17	26.89652	YES	YES
189	a	1167.78	4.47566	YES	YES
190	a	1168.58	2.30498	YES	YES
191	a	1168.95	3.43676	YES	YES
192	a	1169.71	11.59833	YES	YES
193	a	1170.80	0.61534	YES	YES
194	a	1171.58	8.74728	YES	YES
195	a	1178.20	5.97170	YES	YES
196	a	1234.24	2.34826	YES	YES
197	a	1291.45	84.81858	YES	YES
198	a	1292.90	63.18440	YES	YES

* zero point VIBRATIONAL energy : 0.7454454 Hartree *

Trans 5_bx



bp86-SVP SCF energy: -2931.4816175800
pbe-TZVPP SCF energy: -2931.025834284

XYZ Coordinates
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H	2.33887	0.00448	2.61860
C	3.67248	-0.40254	0.91380
C	3.85994	-0.52168	-0.49009
H	2.99602	-0.38330	-1.16081
C	5.12592	-0.79681	-1.02613
H	5.24321	-0.88311	-2.12016
C	6.24399	-0.95614	-0.18532
H	7.23809	-1.17009	-0.61133
C	6.07502	-0.83353	1.20512
H	6.94048	-0.95156	1.87902
C	4.81002	-0.56162	1.74686
H	4.69065	-0.47134	2.84006
C	-1.11395	3.29905	-1.43918
C	-2.41922	2.90331	-1.81679
H	-2.93364	2.11787	-1.24251
C	-3.04832	3.51962	-2.91176
H	-4.06698	3.20647	-3.19520
C	-2.38687	4.51854	-3.64806
H	-2.88373	4.99356	-4.51068
C	-1.08811	4.90891	-3.27999
H	-0.55998	5.69146	-3.84954
C	-0.45400	4.30547	-2.17987
H	0.56165	4.62397	-1.89881
C	-1.10912	3.23734	1.49670
C	-2.06170	4.27281	1.40147
H	-2.37411	4.64358	0.41260
C	-2.61640	4.83483	2.56440
H	-3.36057	5.64389	2.47634
C	-2.22390	4.37139	3.83133
H	-2.65840	4.81562	4.74247
C	-1.27653	3.33660	3.93281
H	-0.96512	2.96528	4.92356
C	-0.72650	2.76648	2.77318
H	0.00750	1.94916	2.85857
C	1.38546	3.22505	0.02876
C	1.72343	4.31438	0.86026
H	0.97890	4.73135	1.55642
C	3.01238	4.87334	0.80611
H	3.26483	5.72193	1.46379
C	3.97277	4.35396	-0.07786
H	4.98491	4.79044	-0.11494
C	3.64010	3.27085	-0.90997
H	4.39157	2.84874	-1.59699
C	2.35584	2.70603	-0.85740
H	2.09680	1.85573	-1.50854
C	-2.39185	-2.88198	0.15872
C	-3.39098	-2.22575	-0.59645
H	-3.11893	-1.38609	-1.25395
C	-4.72963	-2.64289	-0.50138
H	-5.50051	-2.12059	-1.09187
C	-5.08778	-3.70561	0.34552
H	-6.14094	-4.02452	0.42045
C	-4.09806	-4.35724	1.10086
H	-4.36853	-5.19119	1.77018
C	-2.75644	-3.94963	1.00882
H	-1.98949	-4.46837	1.60500
C	-0.04117	-3.21338	-1.53685
C	-0.88863	-4.02424	-2.32175
H	-1.94021	-4.16871	-2.02849
C	-0.39622	-4.65311	-3.47895
H	-1.06867	-5.28552	-4.08238
C	0.94501	-4.48319	-3.86126
H	1.33008	-4.97996	-4.76738
C	1.79451	-3.67620	-3.08343
H	2.84916	-3.53766	-3.37365
C	1.30400	-3.03708	-1.93374
H	1.97760	-2.40365	-1.33486
C	0.22563	-3.22977	1.36988
C	0.12631	-2.68066	2.66948
H	-0.42959	-1.73944	2.81729
C	0.72267	-3.33785	3.75742
H	0.63773	-2.90476	4.76833
C	1.43182	-4.53681	3.56203
H	1.90518	-5.04659	4.41793
C	1.53824	-5.08121	2.27165
H	2.09432	-6.01966	2.10993
C	0.93535	-4.43374	1.17854
H	1.02226	-4.87216	0.17184
C	-0.47041	0.04023	-2.65349
C	-0.36727	0.12086	-4.15729
H	-1.11109	-0.55673	-4.62427
H	0.65437	-0.13621	-4.50146
H	-0.60297	1.15969	-4.47950
C	-2.76640	0.34853	1.48416
C	-3.73474	0.25041	2.65486
H	-4.77573	0.37264	2.29547
H	-3.50952	1.05841	3.38581
H	-3.62421	-0.72184	3.17948
O	0.60063	0.14393	-1.93745
O	-1.57706	-0.08643	-2.05833
O	-1.55669	-0.07890	1.72837
O	-3.09756	0.81911	0.38245
P	-0.30861	2.47338	0.01494
P	-0.62555	-2.34238	-0.01249
Ru	-0.36041	0.06029	-0.01071

Vibrational Frequencies

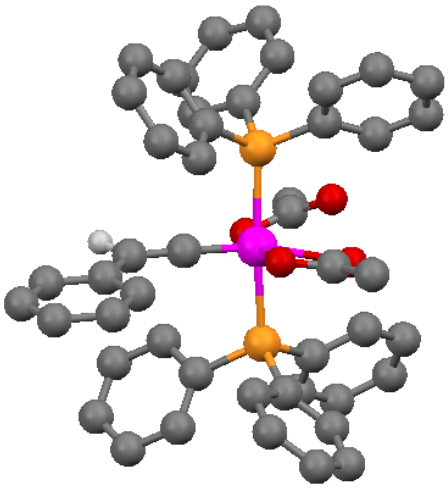
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.30	0.20858	YES	YES
8	a	17.90	0.15873	YES	YES
9	a	21.77	0.04110	YES	YES
10	a	23.89	0.02874	YES	YES
11	a	25.42	0.42545	YES	YES
12	a	32.14	0.21441	YES	YES
13	a	34.17	1.00740	YES	YES
14	a	41.24	0.25000	YES	YES
15	a	43.77	0.21316	YES	YES
16	a	45.70	0.08805	YES	YES

17	a	47.08	1.66134	YES	YES
18	a	52.03	0.10176	YES	YES
19	a	53.13	0.53334	YES	YES
20	a	54.68	0.29534	YES	YES
21	a	55.53	0.69100	YES	YES
22	a	57.10	0.11840	YES	YES
23	a	59.87	0.21651	YES	YES
24	a	63.58	4.16301	YES	YES
25	a	66.16	1.07184	YES	YES
26	a	67.55	0.65207	YES	YES
27	a	69.24	0.18097	YES	YES
28	a	75.03	1.92684	YES	YES
29	a	77.65	2.70798	YES	YES
30	a	78.73	0.81330	YES	YES
31	a	81.23	0.15490	YES	YES
32	a	83.29	0.52526	YES	YES
33	a	93.49	3.06633	YES	YES
34	a	100.25	0.16474	YES	YES
35	a	104.73	6.23031	YES	YES
36	a	117.59	0.62772	YES	YES
37	a	122.36	4.24109	YES	YES
38	a	127.20	1.83115	YES	YES
39	a	141.61	0.31143	YES	YES
40	a	151.11	4.43714	YES	YES
41	a	164.48	0.47577	YES	YES
42	a	180.45	1.37794	YES	YES
43	a	192.32	0.19420	YES	YES
44	a	194.49	0.11630	YES	YES
45	a	206.68	10.46446	YES	YES
46	a	209.45	1.32273	YES	YES
47	a	214.58	2.74565	YES	YES
48	a	217.19	1.47726	YES	YES
49	a	221.62	0.23731	YES	YES
50	a	237.65	5.68978	YES	YES
51	a	241.22	5.84528	YES	YES
52	a	242.45	0.67381	YES	YES
53	a	253.90	0.89793	YES	YES
54	a	255.37	0.54901	YES	YES
55	a	257.23	0.67870	YES	YES
56	a	260.83	0.15140	YES	YES
57	a	261.94	1.41023	YES	YES
58	a	266.35	2.10299	YES	YES
59	a	295.21	0.96722	YES	YES
60	a	313.05	13.76343	YES	YES
61	a	396.90	0.13872	YES	YES
62	a	397.83	0.46540	YES	YES
63	a	398.88	0.31859	YES	YES
64	a	398.96	0.12850	YES	YES
65	a	403.43	0.10071	YES	YES
66	a	403.67	0.04192	YES	YES
67	a	409.52	24.62112	YES	YES
68	a	412.89	1.73738	YES	YES
69	a	420.54	5.91189	YES	YES
70	a	426.46	2.46506	YES	YES
71	a	432.97	4.86553	YES	YES
72	a	437.91	0.41076	YES	YES
73	a	445.38	20.50483	YES	YES
74	a	445.71	15.98708	YES	YES
75	a	466.33	2.41599	YES	YES
76	a	473.06	1.76376	YES	YES
77	a	485.09	12.52216	YES	YES
78	a	492.57	2.33226	YES	YES
79	a	498.69	31.85054	YES	YES
80	a	500.23	2.41775	YES	YES
81	a	504.47	32.91791	YES	YES
82	a	506.64	75.72724	YES	YES
83	a	513.05	183.59830	YES	YES
84	a	521.56	13.71933	YES	YES
85	a	585.89	20.16499	YES	YES
86	a	592.92	5.78041	YES	YES
87	a	600.87	3.85792	YES	YES
88	a	609.43	0.20221	YES	YES
89	a	609.71	0.67125	YES	YES
90	a	609.87	2.65687	YES	YES
91	a	609.95	1.26104	YES	YES
92	a	610.03	1.07480	YES	YES
93	a	610.99	1.55996	YES	YES
94	a	614.42	3.84141	YES	YES
95	a	646.60	8.72214	YES	YES
96	a	669.79	44.37624	YES	YES
97	a	674.48	13.45533	YES	YES
98	a	675.62	12.35536	YES	YES
99	a	675.86	0.41370	YES	YES
100	a	689.91	3.26935	YES	YES
101	a	691.34	11.88782	YES	YES
102	a	692.52	0.76371	YES	YES
103	a	693.75	17.69064	YES	YES
104	a	695.53	28.77554	YES	YES
105	a	696.02	77.49374	YES	YES
106	a	698.49	5.75181	YES	YES
107	a	699.28	8.90627	YES	YES
108	a	699.86	44.65547	YES	YES
109	a	702.47	29.83871	YES	YES
110	a	704.43	17.43055	YES	YES
111	a	722.79	2.73384	YES	YES
112	a	742.84	7.62511	YES	YES
113	a	744.20	5.24128	YES	YES
114	a	744.47	3.81574	YES	YES
115	a	745.08	5.48000	YES	YES
116	a	747.45	10.40164	YES	YES
117	a	747.82	1.39915	YES	YES
118	a	758.77	30.78732	YES	YES
119	a	819.04	2.01571	YES	YES
120	a	831.67	0.28976	YES	YES
121	a	832.61	0.04951	YES	YES
122	a	838.02	0.12325	YES	YES
123	a	841.82	0.52587	YES	YES
124	a	842.71	0.57389	YES	YES
125	a	845.07	0.27622	YES	YES
126	a	845.18	1.68761	YES	YES
127	a	893.56	5.75653	YES	YES
128	a	904.57	0.51848	YES	YES
129	a	910.54	0.64145	YES	YES
130	a	918.14	0.66500	YES	YES
131	a	919.63	0.31755	YES	YES
132	a	920.01	0.20668	YES	YES
133	a	920.61	0.64436	YES	YES
134	a	932.03	6.50290	YES	YES
135	a	948.79	9.48335	YES	YES
136	a	952.92	0.42648	YES	YES
137	a	956.23	0.05069	YES	YES
138	a	961.20	0.13690	YES	YES
139	a	966.18	0.19658	YES	YES
140	a	966.97	0.47340	YES	YES
141	a	969.17	0.01120	YES	YES
142	a	969.41	0.19226	YES	YES
143	a	975.62	0.31121	YES	YES
144	a	979.49	1.89601	YES	YES
145	a	982.62	0.13923	YES	YES
146	a	982.87	0.81756	YES	YES
147	a	983.24	1.01356	YES	YES
148	a	983.46	0.87194	YES	YES
149	a	983.93	1.51854	YES	YES
150	a	984.51	1.08807	YES	YES
151	a	984.93	0.25994	YES	YES
152	a	986.91	0.42896	YES	YES
153	a	988.34	2.44201	YES	YES
154	a	988.87	2.62916	YES	YES
155	a	990.21	2.90175	YES	YES
156	a	991.44	0.69674	YES	YES
157	a	992.58	0.36177	YES	YES
158	a	992.88	0.89930	YES	YES
159	a	1022.80	5.41718	YES	YES
160	a	1023.93	6.26783	YES	YES
161	a	1023.95	0.12672	YES	YES
162	a	1024.55	3.35373	YES	YES
163	a	1024.99	2.00883	YES	YES
164	a	1025.12	2.15645	YES	YES

165	a	1025.33	2.73042	YES	YES
166	a	1027.14	4.56774	YES	YES
167	a	1028.46	15.21527	YES	YES
168	a	1070.52	6.08467	YES	YES
169	a	1073.04	6.51303	YES	YES
170	a	1073.58	8.89162	YES	YES
171	a	1074.23	3.81966	YES	YES
172	a	1074.75	1.68188	YES	YES
173	a	1075.40	3.85996	YES	YES
174	a	1075.89	0.33576	YES	YES
175	a	1076.44	15.29171	YES	YES
176	a	1079.53	24.46944	YES	YES
177	a	1080.65	20.15357	YES	YES
178	a	1081.18	22.58815	YES	YES
179	a	1084.97	16.40048	YES	YES
180	a	1085.64	5.89283	YES	YES
181	a	1136.14	2.02526	YES	YES
182	a	1141.16	0.45666	YES	YES
183	a	1141.59	0.61112	YES	YES
184	a	1141.81	0.95493	YES	YES
185	a	1142.25	0.46589	YES	YES
186	a	1142.51	0.38276	YES	YES
187	a	1142.77	0.49954	YES	YES
188	a	1147.98	30.26748	YES	YES
189	a	1163.39	3.50786	YES	YES
190	a	1166.88	3.52520	YES	YES
191	a	1168.76	1.37740	YES	YES
192	a	1170.40	4.64596	YES	YES
193	a	1171.26	10.81776	YES	YES
194	a	1172.37	12.46690	YES	YES
195	a	1174.20	7.64279	YES	YES
196	a	1243.33	0.64868	YES	YES
197	a	1291.86	5.72484	YES	YES
198	a	1292.91	7.73997	YES	YES

* zero point VIBRATIONAL energy : 0.7453586 Hartree *

Trans 5_by



bp86-SVP SCF energy: -2931.4816246870
pbe-TZVPP SCF energy: -2931.025768417

XYZ Coordinates
97

C	-0.90233	0.04991	-1.26067
C	-1.51897	0.14061	-2.45101
H	-2.62063	0.01232	-2.42547
C	-0.91597	0.41099	-3.76207
C	0.48778	0.53343	-3.94873
H	1.15745	0.40376	-3.08263
C	1.02482	0.79986	-5.21617
H	2.11872	0.88905	-5.33270
C	0.18513	0.94733	-6.33681
H	0.61169	1.15507	-7.33202
C	-1.20521	0.82212	-6.16863
H	-1.87849	0.93133	-7.03587
C	-1.74784	0.55860	-4.90214
H	-2.84088	0.46538	-4.78376
C	-0.16164	2.90089	2.30351
C	0.59261	2.24271	3.30224
H	1.24960	1.40282	3.02942
C	0.49743	2.65837	4.64145
H	1.08748	2.13497	5.41190
C	-0.34829	3.72211	5.00055
H	-0.42201	4.04129	6.05378
C	-1.10268	4.37553	4.01103
H	-1.77092	5.21003	4.28210
C	-1.01067	3.96905	2.66903
H	-1.60680	4.48877	1.90259
C	1.53559	3.23017	-0.04782
C	2.32181	4.04079	0.79863
H	2.02985	4.18563	1.85052
C	3.47898	4.66918	0.30542
H	4.08345	5.30081	0.97766
C	3.86044	4.49915	-1.03595
H	4.76631	4.99588	-1.42184
C	3.08174	3.69195	-1.88441
H	3.37122	3.55281	-2.93915
C	1.93199	3.05346	-1.39312
H	1.33260	2.42029	-2.06634
C	-1.37041	3.25264	-0.31536
C	-1.17729	4.45947	-1.01979
H	-0.17053	4.89873	-1.10133
C	-2.26837	5.10875	-1.62433
H	-2.10465	6.04929	-2.17622
C	-3.55886	4.56328	-1.52506
H	-4.41333	5.07441	-1.99942
C	-3.75617	3.36171	-0.82120
H	-4.76696	2.92759	-0.74175
C	-2.67009	2.70294	-0.22322
H	-2.82015	1.76014	0.32888
C	1.44281	-3.27847	1.02788
C	1.82362	-2.88169	2.33195
H	1.24906	-2.09786	2.84807
C	2.92146	-3.49543	2.95860
H	3.20646	-3.18149	3.97663
C	3.65819	-4.49313	2.29588
H	4.52271	-4.96652	2.79101
C	3.28755	-4.88411	0.99815
H	3.85710	-5.66621	0.46883
C	2.18484	-4.28306	0.36638
H	1.90231	-4.60241	-0.64847
C	-1.49541	-3.22143	1.02703
C	-1.39798	-4.24701	1.98992
H	-0.40862	-4.61443	2.30497
C	-2.55990	-4.80365	2.55235
H	-2.46983	-5.60544	3.30408
C	-3.82771	-4.34433	2.15795
H	-4.73802	-4.78341	2.59940
C	-3.93111	-3.31975	1.20020
H	-4.92252	-2.95090	0.88845
C	-2.77296	-2.75507	0.64212
H	-2.86014	-1.94501	-0.09965
C	-0.03108	-3.20854	-1.47023
C	0.85176	-2.68854	-2.44302
H	1.50244	-1.83744	-2.18596
C	0.90091	-3.25287	-3.72759
H	1.58522	-2.82990	-4.48105
C	0.06873	-4.33649	-4.05813
H	0.10289	-4.77229	-5.07060
C	-0.81172	-4.85727	-3.09538
H	-1.46920	-5.70656	-3.34617
C	-0.86213	-4.29873	-1.80613
H	-1.55570	-4.71640	-1.05968
C	-1.49311	-0.33670	2.66638
C	-2.63212	-0.19635	3.66467
H	-2.44943	0.70394	4.29254
H	-2.64572	-1.08002	4.33569
H	-3.61307	-0.08355	3.16111
C	2.65156	-0.01948	0.38577
C	4.15504	-0.10377	0.27758
H	4.46891	-1.15846	0.44446
H	4.62841	0.52132	1.06183
H	4.50087	0.21272	-0.72691
O	-1.74099	0.09490	1.46045
O	-0.38765	-0.80578	2.99124
O	1.93338	-0.12469	-0.68372
O	2.05940	0.10919	1.49371
P	0.00936	2.36164	0.53658
P	-0.01541	-2.45690	0.22402
Ru	0.00614	-0.04059	0.27407

Vibrational Frequencies

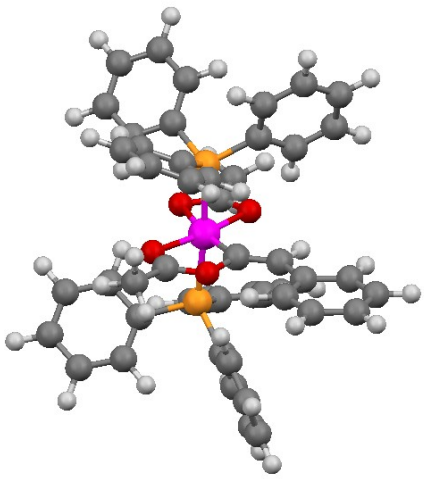
mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.91	0.23536	YES	YES
8	a	17.99	0.13603	YES	YES
9	a	21.87	0.04092	YES	YES
10	a	23.72	0.04066	YES	YES
11	a	25.37	0.48924	YES	YES
12	a	32.16	0.06878	YES	YES
13	a	33.71	1.16556	YES	YES
14	a	38.59	0.16742	YES	YES
15	a	42.16	0.51272	YES	YES
16	a	43.76	0.17209	YES	YES
17	a	45.95	0.11951	YES	YES

18	a	46.58	2.01618	YES	YES
19	a	51.96	0.22139	YES	YES
20	a	52.74	0.39071	YES	YES
21	a	54.77	0.22261	YES	YES
22	a	57.23	0.04339	YES	YES
23	a	58.79	0.40840	YES	YES
24	a	60.22	0.90776	YES	YES
25	a	63.86	0.79356	YES	YES
26	a	65.46	4.26403	YES	YES
27	a	67.20	0.02663	YES	YES
28	a	70.81	0.96909	YES	YES
29	a	73.70	0.05164	YES	YES
30	a	75.49	1.92308	YES	YES
31	a	77.50	3.11592	YES	YES
32	a	80.46	0.31070	YES	YES
33	a	93.58	3.13771	YES	YES
34	a	100.85	0.15577	YES	YES
35	a	104.13	6.02319	YES	YES
36	a	117.58	0.86799	YES	YES
37	a	122.35	4.04243	YES	YES
38	a	126.51	2.10096	YES	YES
39	a	141.52	0.32012	YES	YES
40	a	151.42	4.20767	YES	YES
41	a	163.93	0.48933	YES	YES
42	a	181.47	1.89386	YES	YES
43	a	192.22	0.14854	YES	YES
44	a	194.41	0.12744	YES	YES
45	a	205.55	10.94618	YES	YES
46	a	209.44	1.19478	YES	YES
47	a	214.54	2.82583	YES	YES
48	a	216.90	1.25860	YES	YES
49	a	221.52	0.30250	YES	YES
50	a	238.15	4.58797	YES	YES
51	a	241.02	6.72568	YES	YES
52	a	242.01	0.12825	YES	YES
53	a	254.76	0.88933	YES	YES
54	a	255.31	0.84418	YES	YES
55	a	256.97	0.77102	YES	YES
56	a	260.73	0.17397	YES	YES
57	a	261.87	1.31962	YES	YES
58	a	266.95	2.02568	YES	YES
59	a	294.82	0.85770	YES	YES
60	a	313.05	14.48572	YES	YES
61	a	396.86	0.15245	YES	YES
62	a	398.04	0.43618	YES	YES
63	a	398.89	0.31941	YES	YES
64	a	398.95	0.15969	YES	YES
65	a	403.28	0.07516	YES	YES
66	a	403.63	0.10779	YES	YES
67	a	409.22	25.07014	YES	YES
68	a	412.97	1.22794	YES	YES
69	a	420.16	5.84522	YES	YES
70	a	426.19	2.54840	YES	YES
71	a	433.02	4.85896	YES	YES
72	a	437.70	0.43599	YES	YES
73	a	445.34	19.80956	YES	YES
74	a	445.55	16.57422	YES	YES
75	a	466.26	2.18154	YES	YES
76	a	473.06	1.79378	YES	YES
77	a	484.86	11.34130	YES	YES
78	a	488.73	3.29879	YES	YES
79	a	498.45	31.77325	YES	YES
80	a	500.11	3.07238	YES	YES
81	a	504.40	32.36707	YES	YES
82	a	506.46	76.50535	YES	YES
83	a	512.93	183.67853	YES	YES
84	a	521.38	13.47224	YES	YES
85	a	585.98	22.04289	YES	YES
86	a	595.24	2.63709	YES	YES
87	a	600.85	5.07033	YES	YES
88	a	609.44	0.24513	YES	YES
89	a	609.67	0.57356	YES	YES
90	a	609.88	2.48935	YES	YES
91	a	609.93	1.07097	YES	YES
92	a	610.04	1.36775	YES	YES
93	a	610.99	1.59021	YES	YES
94	a	614.40	3.75133	YES	YES
95	a	646.55	8.52498	YES	YES
96	a	670.81	47.98082	YES	YES
97	a	674.28	13.47620	YES	YES
98	a	675.61	1.53605	YES	YES
99	a	677.09	8.36938	YES	YES
100	a	689.78	3.76736	YES	YES
101	a	691.17	11.32939	YES	YES
102	a	692.38	1.29299	YES	YES
103	a	693.58	17.53718	YES	YES
104	a	695.42	27.99984	YES	YES
105	a	695.95	78.64882	YES	YES
106	a	698.42	5.23071	YES	YES
107	a	699.23	7.47362	YES	YES
108	a	699.76	45.30386	YES	YES
109	a	701.84	30.12721	YES	YES
110	a	704.33	17.11692	YES	YES
111	a	723.13	2.77471	YES	YES
112	a	742.57	7.24243	YES	YES
113	a	744.09	5.29159	YES	YES
114	a	744.41	2.74230	YES	YES
115	a	744.95	6.47449	YES	YES
116	a	747.60	10.83293	YES	YES
117	a	747.99	1.17984	YES	YES
118	a	758.84	30.84609	YES	YES
119	a	818.93	1.96627	YES	YES
120	a	831.42	0.29612	YES	YES
121	a	831.96	0.03435	YES	YES
122	a	837.83	0.13344	YES	YES
123	a	841.90	0.52397	YES	YES
124	a	842.55	0.50075	YES	YES
125	a	844.27	0.46216	YES	YES
126	a	845.09	1.47062	YES	YES
127	a	893.13	5.68359	YES	YES
128	a	904.07	0.46791	YES	YES
129	a	910.49	0.64811	YES	YES
130	a	918.49	0.70608	YES	YES
131	a	919.24	0.33025	YES	YES
132	a	919.44	0.25327	YES	YES
133	a	920.28	0.66655	YES	YES
134	a	933.34	6.13750	YES	YES
135	a	948.80	9.48760	YES	YES
136	a	952.79	0.43270	YES	YES
137	a	955.82	0.04907	YES	YES
138	a	961.10	0.13362	YES	YES
139	a	966.54	0.20170	YES	YES
140	a	966.85	0.45182	YES	YES
141	a	968.44	0.05464	YES	YES
142	a	969.27	0.17377	YES	YES
143	a	975.29	0.30562	YES	YES
144	a	979.47	1.91422	YES	YES
145	a	982.52	0.12381	YES	YES
146	a	982.89	0.85464	YES	YES
147	a	983.33	0.95126	YES	YES
148	a	983.52	0.95704	YES	YES
149	a	983.96	1.20577	YES	YES
150	a	984.50	1.08455	YES	YES
151	a	984.88	0.26508	YES	YES
152	a	986.87	0.44175	YES	YES
153	a	988.15	0.33255	YES	YES
154	a	989.30	1.60649	YES	YES
155	a	989.74	3.01815	YES	YES
156	a	990.80	1.57340	YES	YES
157	a	992.29	0.30397	YES	YES
158	a	992.59	0.78085	YES	YES
159	a	1023.82	1.76918	YES	YES
160	a	1023.99	0.86493	YES	YES
161	a	1024.42	2.35958	YES	YES
162	a	1024.65	2.74421	YES	YES
163	a	1025.06	3.63413	YES	YES
164	a	1025.20	2.63934	YES	YES
165	a	1025.43	9.48719	YES	YES

166	a	1027.03	4.62083	YES	YES
167	a	1027.99	15.55247	YES	YES
168	a	1070.30	6.17567	YES	YES
169	a	1072.95	10.43450	YES	YES
170	a	1073.46	7.48313	YES	YES
171	a	1074.17	4.35626	YES	YES
172	a	1074.55	1.30228	YES	YES
173	a	1075.18	3.69334	YES	YES
174	a	1075.76	0.28891	YES	YES
175	a	1076.12	12.83876	YES	YES
176	a	1079.36	24.06430	YES	YES
177	a	1080.49	20.21030	YES	YES
178	a	1081.12	22.84278	YES	YES
179	a	1084.83	16.29177	YES	YES
180	a	1085.49	6.07248	YES	YES
181	a	1136.09	2.12058	YES	YES
182	a	1141.29	0.46947	YES	YES
183	a	1141.56	0.58415	YES	YES
184	a	1141.84	1.02069	YES	YES
185	a	1142.26	0.46375	YES	YES
186	a	1142.44	0.37132	YES	YES
187	a	1142.67	0.52483	YES	YES
188	a	1147.81	30.32987	YES	YES
189	a	1163.22	3.51209	YES	YES
190	a	1166.72	3.42612	YES	YES
191	a	1168.71	1.45789	YES	YES
192	a	1170.30	4.56431	YES	YES
193	a	1171.22	11.11967	YES	YES
194	a	1172.21	11.91570	YES	YES
195	a	1174.20	7.84581	YES	YES
196	a	1243.09	0.67544	YES	YES
197	a	1291.55	5.59485	YES	YES
198	a	1292.83	7.97818	YES	YES

* zero point VIBRATIONAL energy : 0.7452452 Hartree *

Trans 6_y



bp86-SVP SCF energy: -2931.4834924360
pbe-TZVPP SCF energy: -2931.031632190

XYZ Coordinates
97

C	1.49680	0.29643	0.10003
C	2.49604	0.49429	-0.81796
H	2.12283	0.42009	-1.85442
C	3.93000	0.78355	-0.71592
C	4.66972	0.94025	0.49256
H	4.15219	0.85185	1.45697
C	6.04567	1.21294	0.47298
H	6.58475	1.32755	1.42948
C	6.74258	1.34236	-0.74201
H	7.82414	1.55667	-0.74899
C	6.03342	1.19485	-1.94797
H	6.55776	1.29322	-2.91398
C	4.65964	0.92253	-1.93227
H	4.11871	0.80996	-2.88767
C	-2.65373	2.68382	0.06082
C	-3.47315	1.90839	0.91311
H	-3.03234	1.06350	1.46626
C	-4.84171	2.19547	1.04000
H	-5.46743	1.58380	1.71087
C	-5.41604	3.24286	0.29817
H	-6.49358	3.46011	0.38874
C	-4.61301	4.00353	-0.56790
H	-5.05749	4.82059	-1.16067
C	-3.23883	3.72909	-0.68494
H	-2.62153	4.33386	-1.36780
C	-0.13302	3.15749	1.44071
C	-0.91461	3.53285	2.55411
H	-1.99837	3.33683	2.55843
C	-0.32442	4.17225	3.65895
H	-0.95317	4.46568	4.51630
C	1.05359	4.44738	3.66639
H	1.51296	4.95882	4.52890
C	1.84172	4.07107	2.56346
H	2.92409	4.28195	2.55511
C	1.25593	3.42753	1.46084
H	1.88707	3.13792	0.60487
C	-0.21665	3.28923	-1.43524
C	0.00501	4.67865	-1.28912
H	-0.16849	5.16864	-0.31744
C	0.45352	5.44662	-2.37636
H	0.62421	6.52860	-2.24653
C	0.68708	4.83820	-3.62186
H	1.04421	5.44128	-4.47341
C	0.46864	3.45907	-3.77367
H	0.65330	2.97413	-4.74689
C	0.02134	2.68465	-2.68871
H	-0.15711	1.60396	-2.80910
C	-1.08680	-3.17432	1.52682
C	-2.34350	-2.62184	1.87084
H	-2.77504	-1.82630	1.24135
C	-3.03644	-3.08960	2.99912
H	-4.01819	-2.65605	3.25360
C	-2.47949	-4.09582	3.80876
H	-3.02157	-4.45471	4.69978
C	-1.22701	-4.63909	3.47904
H	-0.78079	-5.42663	4.10928
C	-0.53448	-4.18479	2.34244
H	0.44509	-4.62195	2.09241
C	-1.04586	-3.32507	-1.39661
C	-2.20799	-4.11244	-1.26744
H	-2.66336	-4.26398	-0.27619
C	-2.78805	-4.71592	-2.39831
H	-3.69378	-5.33412	-2.28079
C	-2.21426	-4.53854	-3.66834
H	-2.66710	-5.01604	-4.55347
C	-1.05914	-3.74669	-3.80551
H	-0.60467	-3.59734	-4.79905
C	-0.48273	-3.13721	-2.68008
H	0.41744	-2.51277	-2.79756
C	1.41232	-3.39793	0.05931
C	2.55228	-2.81265	0.65031
H	2.50169	-1.79756	1.06551
C	3.77143	-3.51092	0.70265
H	4.65274	-3.02695	1.15468
C	3.87028	-4.80519	0.16744
H	4.82893	-5.34927	0.20259
C	2.74016	-5.40055	-0.41933
H	2.80451	-6.41729	-0.84191
C	1.52211	-4.70322	-0.47537
H	0.64743	-5.18310	-0.94183
C	-2.23779	-0.43574	-1.85634
C	-3.19803	-0.62214	-3.00731
H	-4.22381	-0.33267	-2.70082
H	-3.21079	-1.69616	-3.29968
H	-2.87751	-0.02964	-3.88846
C	1.00871	0.22167	2.41312
C	1.42082	0.36788	3.84805
H	1.53208	1.45012	4.08665
H	2.40006	-0.12208	4.03027
H	0.64451	-0.06686	4.50724
O	-0.99529	-0.18204	-2.09186
O	-2.61436	-0.54459	-0.64770
O	-0.17585	-0.02005	2.07436
O	1.96151	0.38314	1.51281
P	-0.84644	2.25258	-0.02555
P	-0.21279	-2.48453	0.03760
Ru	-0.42779	-0.08180	-0.01911

Vibrational Frequencies

mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	11.28	0.02340	YES	YES
8	a	14.64	0.04632	YES	YES
9	a	19.18	0.03192	YES	YES
10	a	19.90	0.11797	YES	YES
11	a	27.92	0.09150	YES	YES
12	a	31.81	0.09041	YES	YES
13	a	35.29	0.04045	YES	YES
14	a	38.32	0.31378	YES	YES
15	a	40.21	0.04443	YES	YES

16	a	43.30	0.07414	YES	YES
17	a	45.55	0.23036	YES	YES
18	a	48.28	0.21685	YES	YES
19	a	53.30	0.11457	YES	YES
20	a	55.36	0.37843	YES	YES
21	a	57.84	0.08059	YES	YES
22	a	62.63	0.28000	YES	YES
23	a	64.88	0.11723	YES	YES
24	a	68.73	0.11165	YES	YES
25	a	71.58	0.17977	YES	YES
26	a	75.31	2.09844	YES	YES
27	a	77.08	1.70604	YES	YES
28	a	81.12	0.23067	YES	YES
29	a	83.95	0.04933	YES	YES
30	a	90.56	0.57520	YES	YES
31	a	94.64	0.34056	YES	YES
32	a	97.18	0.25520	YES	YES
33	a	104.13	0.96061	YES	YES
34	a	114.00	0.34419	YES	YES
35	a	121.73	1.47575	YES	YES
36	a	140.94	0.46520	YES	YES
37	a	160.58	1.68168	YES	YES
38	a	169.20	2.24082	YES	YES
39	a	180.42	4.29916	YES	YES
40	a	186.48	7.60382	YES	YES
41	a	191.86	0.37300	YES	YES
42	a	195.40	0.12404	YES	YES
43	a	197.40	1.27715	YES	YES
44	a	206.80	0.07736	YES	YES
45	a	209.71	4.31329	YES	YES
46	a	223.22	0.65350	YES	YES
47	a	224.87	1.59878	YES	YES
48	a	231.82	2.49840	YES	YES
49	a	240.49	2.10209	YES	YES
50	a	242.42	0.72882	YES	YES
51	a	247.80	0.24068	YES	YES
52	a	250.59	0.73180	YES	YES
53	a	257.42	0.53784	YES	YES
54	a	262.43	1.33565	YES	YES
55	a	265.17	0.57826	YES	YES
56	a	270.17	6.28653	YES	YES
57	a	286.06	0.63849	YES	YES
58	a	288.36	0.73112	YES	YES
59	a	330.41	1.18741	YES	YES
60	a	364.45	7.19160	YES	YES
61	a	396.59	0.38595	YES	YES
62	a	398.10	0.15531	YES	YES
63	a	399.06	0.21680	YES	YES
64	a	400.45	0.39423	YES	YES
65	a	403.03	3.57591	YES	YES
66	a	405.77	43.83888	YES	YES
67	a	406.48	13.77282	YES	YES
68	a	408.12	0.46971	YES	YES
69	a	422.87	14.12706	YES	YES
70	a	426.52	3.43712	YES	YES
71	a	434.70	17.68835	YES	YES
72	a	440.18	10.65123	YES	YES
73	a	453.36	15.86683	YES	YES
74	a	467.74	3.19217	YES	YES
75	a	479.64	6.54986	YES	YES
76	a	491.86	20.81283	YES	YES
77	a	494.56	9.80017	YES	YES
78	a	502.71	53.49283	YES	YES
79	a	504.98	57.89796	YES	YES
80	a	508.13	70.12923	YES	YES
81	a	513.75	154.51506	YES	YES
82	a	524.39	23.90657	YES	YES
83	a	556.36	18.82270	YES	YES
84	a	575.36	0.79078	YES	YES
85	a	596.65	5.50756	YES	YES
86	a	608.99	0.35570	YES	YES
87	a	609.33	1.04617	YES	YES
88	a	609.72	1.87979	YES	YES
89	a	609.97	0.33589	YES	YES
90	a	610.10	1.21581	YES	YES
91	a	610.85	0.56802	YES	YES
92	a	611.29	1.70333	YES	YES
93	a	622.19	2.17402	YES	YES
94	a	632.98	5.20391	YES	YES
95	a	669.33	39.74337	YES	YES
96	a	672.06	17.01128	YES	YES
97	a	673.66	1.71610	YES	YES
98	a	684.68	6.78950	YES	YES
99	a	685.88	10.71706	YES	YES
100	a	687.04	11.03578	YES	YES
101	a	689.07	12.02277	YES	YES
102	a	693.30	28.95610	YES	YES
103	a	696.75	46.00052	YES	YES
104	a	697.31	26.93257	YES	YES
105	a	699.10	38.00879	YES	YES
106	a	700.87	8.43084	YES	YES
107	a	702.67	12.21229	YES	YES
108	a	703.29	57.23859	YES	YES
109	a	704.87	15.38074	YES	YES
110	a	741.29	0.79636	YES	YES
111	a	742.06	15.87966	YES	YES
112	a	744.01	1.33046	YES	YES
113	a	744.73	3.88034	YES	YES
114	a	746.83	4.97714	YES	YES
115	a	749.09	6.45158	YES	YES
116	a	750.66	9.97416	YES	YES
117	a	779.97	26.18364	YES	YES
118	a	815.95	7.80664	YES	YES
119	a	816.94	10.20950	YES	YES
120	a	833.90	0.12705	YES	YES
121	a	836.73	0.04671	YES	YES
122	a	837.65	0.77847	YES	YES
123	a	838.54	8.61166	YES	YES
124	a	842.35	0.71636	YES	YES
125	a	845.17	4.43964	YES	YES
126	a	846.60	0.31204	YES	YES
127	a	895.48	8.26886	YES	YES
128	a	908.52	0.23161	YES	YES
129	a	909.01	0.98884	YES	YES
130	a	910.75	0.41227	YES	YES
131	a	915.29	0.09629	YES	YES
132	a	915.75	0.27291	YES	YES
133	a	922.93	0.95820	YES	YES
134	a	942.08	10.76960	YES	YES
135	a	951.86	0.00940	YES	YES
136	a	958.92	0.34464	YES	YES
137	a	959.77	0.22824	YES	YES
138	a	960.32	0.17052	YES	YES
139	a	965.78	0.69031	YES	YES
140	a	967.41	0.42774	YES	YES
141	a	971.05	0.29912	YES	YES
142	a	971.47	0.46376	YES	YES
143	a	979.03	2.77381	YES	YES
144	a	980.28	10.16534	YES	YES
145	a	981.19	0.26737	YES	YES
146	a	981.39	0.13406	YES	YES
147	a	982.57	0.18241	YES	YES
148	a	982.98	0.76818	YES	YES
149	a	983.31	1.69020	YES	YES
150	a	983.82	2.98363	YES	YES
151	a	984.30	1.08321	YES	YES
152	a	985.00	0.39003	YES	YES
153	a	985.92	0.11161	YES	YES
154	a	986.13	2.68411	YES	YES
155	a	986.29	1.50086	YES	YES
156	a	987.30	0.12900	YES	YES
157	a	998.34	1.57663	YES	YES
158	a	1001.93	16.05234	YES	YES
159	a	1021.63	10.31004	YES	YES
160	a	1023.28	9.09619	YES	YES
161	a	1023.37	1.49693	YES	YES
162	a	1024.12	2.41035	YES	YES
163	a	1024.21	0.46859	YES	YES

164	a	1025.08	3.67230	YES	YES
165	a	1025.31	1.25343	YES	YES
166	a	1025.72	17.44040	YES	YES
167	a	1029.94	7.69415	YES	YES
168	a	1071.15	11.21260	YES	YES
169	a	1071.78	7.37514	YES	YES
170	a	1073.86	2.20087	YES	YES
171	a	1074.49	0.44854	YES	YES
172	a	1074.65	9.67838	YES	YES
173	a	1075.17	11.73642	YES	YES
174	a	1075.58	9.91434	YES	YES
175	a	1076.45	14.97703	YES	YES
176	a	1077.34	10.74581	YES	YES
177	a	1078.24	15.63111	YES	YES
178	a	1079.24	6.13324	YES	YES
179	a	1083.09	20.29123	YES	YES
180	a	1083.65	4.01129	YES	YES
181	a	1136.83	0.15888	YES	YES
182	a	1141.33	0.31681	YES	YES
183	a	1141.44	0.21261	YES	YES
184	a	1141.55	0.26350	YES	YES
185	a	1142.26	0.51794	YES	YES
186	a	1142.75	0.41664	YES	YES
187	a	1142.95	0.34357	YES	YES
188	a	1166.50	2.66084	YES	YES
189	a	1166.88	4.50937	YES	YES
190	a	1167.76	3.32665	YES	YES
191	a	1169.91	3.52887	YES	YES
192	a	1170.31	2.89698	YES	YES
193	a	1173.37	15.80127	YES	YES
194	a	1174.19	3.84931	YES	YES
195	a	1203.32	10.56550	YES	YES
196	a	1231.82	35.87161	YES	YES
197	a	1289.46	7.78901	YES	YES
198	a	1291.73	3.89467	YES	YES

* zero point VIBRATIONAL energy : 0.7477542 Hartree *