

Vibrational Analysis, PDI Anti Conformer, CCSD(T)/cc-pVTZ

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NORMAL COORDINATE ANALYSIS IN THE HARMONIC APPROXIMATION  
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ATOMIC WEIGHTS (AMU)

1	H	1.00782
2	C	12.00000
3	C	12.00000
4	C	12.00000
5	N	14.00307
6	N	14.00307
7	H	1.00782
8	H	1.00782
9	H	1.00782
10	H	1.00782
11	H	1.00782
12	H	1.00782

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

ANALYZING SYMMETRY OF NORMAL MODES...

--- SYMMETRY FOR NORMAL MODES ---

INCLUDING TRANSLATION AND ROTATION

21\*A' 15\*A''

EXCLUDING TRANSLATION AND ROTATION (SAYVETZ < 0.01)

16\*A' 9\*A''

FREQUENCIES IN CM\*\*-1, IR INTENSITIES IN DEBYE\*\*2/AMU-ANGSTROM\*\*2,  
REDUCED MASSES IN AMU.

			1	2	3	4	5
	FREQUENCY:		16.91	16.67	13.51	5.06	4.07
	SYMMETRY:		A'	A''	A''	A'	A'
	REDUCED MASS:		3.81207	5.59135	1.76519	7.10812	7.04565
1	H	X	-0.05905091	0.00000000	-0.00000000	-0.06221565	0.09798814
		Y	0.23879053	-0.00000000	0.00000000	-0.01089376	0.02200768
		Z	0.00000000	0.06762440	0.19322832	0.00000000	0.00000000
2	C	X	-0.01026429	0.00000000	-0.00000000	-0.08360207	0.08350208
		Y	0.19699842	-0.00000000	0.00000000	0.00740260	0.03438725
		Z	0.00000000	0.10473587	0.02062237	0.00000000	0.00000000
3	C	X	-0.04310598	0.00000000	-0.00000000	-0.06910696	0.09335254
		Y	0.11342315	-0.00000000	0.00000000	0.04426441	0.05940624
		Z	0.00000000	0.08915257	0.13989932	-0.00000000	0.00000000
4	C	X	0.02545822	-0.00000000	-0.00000000	-0.09978719	0.07239387
		Y	0.05761027	-0.00000000	0.00000000	0.06922845	0.07644678
		Z	0.00000000	0.14211337	-0.10956398	0.00000000	-0.00000000
5	N	X	-0.00363689	0.00000000	-0.00000000	-0.08664951	0.08145471
		Y	-0.02337002	0.00000000	-0.00000000	0.10584122	0.10167907
		Z	0.00000000	0.12847975	-0.00737841	-0.00000000	-0.00000000
6	N	X	-0.02759285	0.00000000	-0.00000000	-0.07571187	0.08907676
		Y	-0.08100343	0.00000000	-0.00000000	0.13215933	0.12002002
		Z	0.00000000	0.11614186	0.07676723	-0.00000000	-0.00000000
7	H	X	0.02539161	0.00447917	0.00108727	-0.09924123	0.07287813
		Y	0.20821507	0.03596251	-0.18619091	0.00254625	0.03110928
		Z	0.00007368	0.12835864	-0.10682374	-0.00000645	0.00000897

8	H	X	0.02539161	-0.00447917	-0.00108727	-0.09924123	0.07287813
		Y	0.20821507	-0.03596251	0.18619091	0.00254625	0.03110928
		Z	-0.00007368	0.12835864	-0.10682374	0.00000645	-0.00000897
9	H	X	-0.07872635	-0.00444035	-0.00034099	-0.05329532	0.10410403
		Y	0.10318476	-0.03607213	0.18711835	0.04882903	0.06250118
		Z	0.00001679	0.06517180	0.26895462	0.00000336	-0.00000518
10	H	X	-0.07872635	0.00444035	0.00034099	-0.05329532	0.10410403
		Y	0.10318476	0.03607213	-0.18711835	0.04882903	0.06250118
		Z	-0.00001679	0.06517180	0.26895462	-0.00000336	0.00000518
11	H	X	0.06093467	0.00448942	-0.00218038	-0.11578595	0.06143564
		Y	0.06007517	0.03651029	-0.18794078	0.06813166	0.07567646
		Z	0.00001211	0.16694768	-0.23844604	-0.00000022	-0.00000422
12	H	X	0.06093467	-0.00448942	0.00218038	-0.11578595	0.06143564
		Y	0.06007517	-0.03651029	0.18794078	0.06813166	0.07567646
		Z	-0.00001211	0.16694768	-0.23844604	0.00000022	0.00000422

TRANS. SAYVETZ	X	-0.81645103	0.00000000	-0.00000000	-5.90705925	5.95826777
	Y	3.94425615	-0.00000000	0.00000000	5.01338920	5.51075419
	Z	0.00000000	8.25222658	1.62406478	-0.00000000	0.00000000
TOTAL		4.02787151	8.25222658	1.62406478	7.74773646	8.11599449

ROT. SAYVETZ	X	-0.00000000	-1.68880458	8.69835600	-0.00000000	0.00000000
	Y	0.00000000	2.02629677	-0.52887569	-0.00000000	-0.00000000
	Z	25.27884628	-0.00000000	0.00000000	-11.33937443	-7.77810130
TOTAL		25.27884628	2.63779064	8.71441947	11.33937443	7.77810130

	6	7	8	9	10
FREQUENCY:	9.26	97.95	158.64	232.92	316.64
SYMMETRY:	A''	A''	A'	A''	A'
REDUCED MASS:	4.66264	2.73078	4.65112	1.08469	3.29235

1	H	X	0.00000000	0.00000000	-0.11595224	-0.00000000	-0.02263788
		Y	-0.00000000	-0.00000000	0.17588242	0.00000000	0.19800115
		Z	0.21440182	0.07435559	-0.00000000	0.57723453	0.00000000
2	C	X	0.00000000	0.00000000	-0.01853877	-0.00000000	0.13210790
		Y	-0.00000000	-0.00000000	0.09191170	0.00000000	0.06300875
		Z	0.17362223	0.12048579	-0.00000000	0.01570242	-0.00000000
3	C	X	0.00000000	0.00000000	-0.07393756	-0.00000000	0.05243026
		Y	-0.00000000	0.00000000	-0.06415725	0.00000000	-0.10975562
		Z	0.07150343	-0.11027405	0.00000000	-0.07161033	-0.00000000
4	C	X	0.00000000	-0.00000000	-0.01337787	0.00000000	-0.04170411
		Y	-0.00000000	0.00000000	-0.11941408	0.00000000	-0.04449578
		Z	0.01455955	-0.12049108	0.00000000	0.02885205	0.00000000
5	N	X	0.00000000	0.00000000	0.01415741	0.00000000	-0.04700396
		Y	-0.00000000	0.00000000	-0.06278891	-0.00000000	0.08958908
		Z	-0.08275546	-0.01173800	-0.00000000	0.00208340	-0.00000000
6	N	X	0.00000000	0.00000000	0.09748305	0.00000000	-0.09482827
		Y	-0.00000000	0.00000000	0.13738989	0.00000000	-0.01966033
		Z	-0.15319151	0.11648286	-0.00000000	0.01407683	0.00000000
7	H	X	-0.06052842	-0.09880691	0.05195528	-0.21142508	0.24326601
		Y	0.00798879	0.13172389	0.11502435	-0.40491008	0.10358451
		Z	0.19190058	0.23122466	0.00033853	-0.21332893	0.00241162
8	H	X	0.06052842	0.09880691	0.05195528	0.21142508	0.24326601
		Y	-0.00798879	-0.13172389	0.11502435	0.40491008	0.10358451
		Z	0.19190058	0.23122466	-0.00033853	-0.21332893	-0.00241162
9	H	X	0.06070429	0.10023535	-0.13154151	0.02136327	0.03821755
		Y	-0.00677127	-0.07442168	-0.07672307	-0.06229464	-0.10185031
		Z	0.05478027	-0.18086281	0.00173003	-0.11834939	0.00695680
10	H	X	-0.06070429	-0.10023535	-0.13154151	-0.02136327	0.03821755
		Y	0.00677127	0.07442168	-0.07672307	0.06229464	-0.10185031

		Z	0.05478027	-0.18086281	-0.00173003	-0.11834939	-0.00695680
11	H	X	-0.05988985	0.04553482	-0.00988114	0.00665885	-0.13457157
		Y	0.00570371	-0.03269825	-0.11584661	0.09745406	-0.04817846
		Z	0.02131031	-0.14444423	0.00174453	0.09545118	0.00242206
12	H	X	0.05988985	-0.04553482	-0.00988114	-0.00665885	-0.13457157
		Y	-0.00570371	0.03269825	-0.11584661	-0.09745406	-0.04817846
		Z	0.02131031	-0.14444423	-0.00174453	0.09545118	-0.00242206

TRANS.	SAYVETZ	X	0.00000000	0.00000000	-0.00413557	0.00000000	0.00122994
		Y	-0.00000000	0.00000000	-0.03431823	0.00000000	-0.00975940
		Z	0.56849640	0.02869771	-0.00000000	0.00722273	-0.00000000
		TOTAL	0.56849640	0.02869771	0.03456651	0.00722273	0.00983660

ROT.	SAYVETZ	X	-0.34314455	0.15609324	-0.00000000	0.03715468	-0.00000000
		Y	-27.91581034	0.27460837	0.00000000	-0.03815319	-0.00000000
		Z	0.00000000	-0.00000000	-0.15418336	0.00000000	-0.03591783
		TOTAL	27.91791925	0.31587159	0.15418336	0.05325538	0.03591783

			11	12	13	14	15
FREQUENCY:			345.29	472.58	669.25	755.36	877.62
SYMMETRY:			A'	A'	A'	A'	A'
REDUCED MASS:			4.38835	8.05801	6.72151	1.08099	1.18130

1	H	X	-0.00000000	-0.08009924	0.01032913	0.00000000	-0.00000000
		Y	0.00000000	0.01476604	-0.05086782	-0.00000000	0.00000000
		Z	0.05787970	-0.00000000	0.00000000	-0.07805990	0.19541425
2	C	X	0.00000000	-0.07494571	-0.05017301	0.00000000	-0.00000000
		Y	0.00000000	0.01202791	0.00470712	0.00000000	-0.00000000
		Z	0.01094849	-0.00000000	-0.00000000	0.00998559	-0.05286537
3	C	X	0.00000000	-0.05845455	-0.02692760	-0.00000000	0.00000000
		Y	-0.00000000	-0.04774606	-0.00423145	0.00000000	-0.00000000
		Z	-0.03260724	0.00000000	0.00000000	0.05514609	-0.03483780
4	C	X	-0.00000000	-0.05185621	0.21637192	-0.00000000	0.00000000
		Y	-0.00000000	-0.02169341	-0.09718167	0.00000000	0.00000000
		Z	-0.05008412	0.00000000	0.00000000	0.05036220	0.09024034
5	N	X	-0.00000000	0.14630605	-0.03589160	0.00000000	0.00000000
		Y	0.00000000	0.14908214	0.08702578	-0.00000000	-0.00000000
		Z	0.20380849	0.00000000	-0.00000000	-0.01975768	-0.03132215
6	N	X	-0.00000000	0.05377381	-0.07724434	0.00000000	0.00000000
		Y	0.00000000	-0.09186741	0.01480393	-0.00000000	-0.00000000
		Z	-0.12090592	-0.00000000	0.00000000	0.00397296	0.00637939
7	H	X	-0.04428662	-0.06832553	-0.09487710	0.17302048	-0.33687662
		Y	-0.01288604	0.01043372	-0.01626231	-0.10668494	0.15809831
		Z	0.01164226	-0.00201117	-0.00345943	-0.10368571	0.13397833
8	H	X	0.04428662	-0.06832553	-0.09487710	-0.17302048	0.33687662
		Y	0.01288604	0.01043372	-0.01626231	0.10668494	-0.15809831
		Z	0.01164226	0.00201117	0.00345943	-0.10368571	0.13397833
9	H	X	0.01060260	-0.09520910	-0.07743544	0.08548385	-0.33260825
		Y	0.00996779	-0.05029051	-0.03312611	-0.41793693	0.03943430
		Z	-0.02744924	0.00357652	-0.00832582	-0.25694100	0.05675366
10	H	X	-0.01060260	-0.09520910	-0.07743544	-0.08548385	0.33260825
		Y	-0.00996779	-0.05029051	-0.03312611	0.41793693	-0.03943430
		Z	-0.02744924	-0.00357652	0.00832582	-0.25694100	0.05675366
11	H	X	0.17252827	-0.08362112	0.12385101	-0.10164930	-0.06819829
		Y	-0.14961880	-0.02350324	-0.05672691	-0.33783960	-0.32272800
		Z	-0.16419298	0.00320026	0.02733704	-0.17865341	-0.13016122
12	H	X	-0.17252827	-0.08362112	0.12385101	0.10164930	0.06819829
		Y	0.14961880	-0.02350324	-0.05672691	0.33783960	0.32272800
		Z	-0.16419298	-0.00320026	-0.02733704	-0.17865341	-0.13016122

TRANS. SAYVETZ	X	-0.00000000	-0.00025086	-0.00026639	-0.00000000	0.00000000
	Y	0.00000000	-0.00058694	0.00029927	-0.00000000	-0.00000000
	Z	-0.00450825	0.00000000	-0.00000000	-0.00077857	0.00020350
	TOTAL	0.00450825	0.00063830	0.00040066	0.00077857	0.00020350

ROT. SAYVETZ	X	-0.00747727	-0.00000000	0.00000000	0.00159366	-0.00084312
	Y	0.02246073	0.00000000	0.00000000	-0.00338011	-0.00179008
	Z	0.00000000	-0.00405053	0.00058974	0.00000000	-0.00000000
	TOTAL	0.02367264	0.00405053	0.00058974	0.00373697	0.00197870

		16	17	18	19	20
FREQUENCY:		903.57	1028.66	1130.68	1174.28	1275.74
SYMMETRY:		A'	A'	A'	A''	A''
REDUCED MASS:		1.76933	3.26721	2.19305	1.57844	1.20176

1	H	X	0.47685121	-0.09229214	-0.31234801	-0.00000000	0.00000000
		Y	-0.28895087	0.02973911	0.17461036	0.00000000	0.00000000
		Z	0.00000000	-0.00000000	0.00000000	0.16745556	0.15346814
2	C	X	0.08670975	-0.13676180	-0.00369628	0.00000000	0.00000000
		Y	0.04882043	0.06921749	-0.10141152	-0.00000000	0.00000000
		Z	-0.00000000	-0.00000000	-0.00000000	-0.08003588	-0.07360467
3	C	X	0.01639189	0.18670430	-0.01499945	-0.00000000	-0.00000000
		Y	0.10512324	-0.00491144	0.15282232	0.00000000	-0.00000000
		Z	-0.00000000	0.00000000	0.00000000	0.11493127	0.07333832
4	C	X	-0.06237208	-0.02751033	-0.02689790	0.00000000	-0.00000000
		Y	-0.11696068	-0.06002536	-0.11631485	-0.00000000	-0.00000000
		Z	0.00000000	-0.00000000	0.00000000	-0.10363338	0.03190580
5	N	X	0.00413817	-0.00724162	0.01092307	-0.00000000	-0.00000000
		Y	0.01556394	-0.00684834	0.02657600	-0.00000000	0.00000000
		Z	-0.00000000	-0.00000000	0.00000000	0.04566268	-0.04867261
6	N	X	-0.00554903	-0.00644748	-0.00399869	0.00000000	-0.00000000
		Y	-0.00407206	0.00251799	-0.00590881	-0.00000000	0.00000000
		Z	-0.00000000	-0.00000000	0.00000000	-0.00757368	0.00747418
7	H	X	-0.19882416	-0.16652559	0.28170678	-0.23384149	-0.15797596
		Y	-0.09456480	0.06520067	0.08163646	0.14468332	0.12675853
		Z	-0.03184362	-0.00072141	0.06014160	0.07455704	0.05222615
8	H	X	-0.19882416	-0.16652559	0.28170678	0.23384149	0.15797596
		Y	-0.09456480	0.06520067	0.08163646	-0.14468332	-0.12675853
		Z	0.03184362	0.00072141	-0.06014160	0.07455704	0.05222615
9	H	X	-0.14870528	0.26346709	0.11208666	-0.03982186	0.28309229
		Y	0.06694306	0.01007447	0.16651664	-0.28216192	-0.07859248
		Z	0.00145662	-0.00274067	-0.01909040	-0.07456247	-0.03264663
10	H	X	-0.14870528	0.26346709	0.11208666	0.03982186	-0.28309229
		Y	0.06694306	0.01007447	0.16651664	0.28216192	0.07859248
		Z	-0.00145662	0.00274067	0.01909040	-0.07456247	-0.03264663
11	H	X	-0.12366410	-0.08929624	-0.01427248	-0.25792141	0.51567939
		Y	-0.12738121	-0.08560291	-0.09282440	0.21981184	-0.00991093
		Z	0.00101730	-0.00918862	0.01866491	0.06101831	0.00144714
12	H	X	-0.12366410	-0.08929624	-0.01427248	0.25792141	-0.51567939
		Y	-0.12738121	-0.08560291	-0.09282440	-0.21981184	0.00991093
		Z	-0.00101730	0.00918862	-0.01866491	0.06101831	0.00144714

TRANS. SAYVETZ	X	-0.00018017	-0.00010754	0.00002832	-0.00000000	-0.00000000
	Y	0.00107390	-0.00011522	-0.00037950	-0.00000000	0.00000000
	Z	-0.00000000	-0.00000000	0.00000000	0.00025344	-0.00017965
	TOTAL	0.00108891	0.00015761	0.00038056	0.00025344	0.00017965

ROT. SAYVETZ	X	-0.00000000	-0.00000000	-0.00000000	0.00195792	0.00044172
	Y	0.00000000	-0.00000000	0.00000000	0.00175095	0.00095334
	Z	0.00701863	-0.00119835	-0.00257767	0.00000000	-0.00000000

TOTAL 0.00701863 0.00119835 0.00257767 0.00262664 0.00105070

	21	22	23	24	25
FREQUENCY:	1315.45	1329.11	1369.80	1428.74	1462.63
SYMMETRY:	A'	A''	A'	A'	A'
REDUCED MASS:	1.24149	1.07678	1.33003	1.20248	1.07029

1	H	X	0.13863511	0.00000000	0.08303256	0.38109377	-0.02907057
		Y	-0.07117180	0.00000000	-0.02032027	-0.37589594	0.02992875
		Z	-0.00000000	0.05792230	0.00000000	0.00000000	-0.00000000
2	C	X	0.00869270	0.00000000	0.02466872	-0.11540422	0.00404948
		Y	0.04017523	0.00000000	0.03256116	0.03454300	0.00249720
		Z	0.00000000	-0.04795063	-0.00000000	-0.00000000	-0.00000000
3	C	X	-0.05721978	-0.00000000	-0.12681628	0.00360023	0.00540897
		Y	-0.03060137	-0.00000000	-0.00820516	-0.00373660	0.01063516
		Z	0.00000000	-0.02844024	0.00000000	-0.00000000	0.00000000
4	C	X	-0.08091475	-0.00000000	0.05967386	0.00977614	0.01507477
		Y	-0.05886828	-0.00000000	0.01405904	0.00764208	-0.06651680
		Z	-0.00000000	0.04610374	0.00000000	0.00000000	0.00000000
5	N	X	0.00326005	0.00000000	0.00138687	-0.00154766	-0.00166670
		Y	0.02661523	0.00000000	-0.00951102	-0.00459534	-0.01403250
		Z	0.00000000	0.02219102	-0.00000000	0.00000000	-0.00000000
6	N	X	-0.01718591	-0.00000000	0.01642477	0.00237997	0.01426527
		Y	0.00298471	0.00000000	-0.00530956	0.00011925	-0.00370694
		Z	-0.00000000	-0.00289422	0.00000000	-0.00000000	0.00000000
7	H	X	-0.01822813	-0.10688147	-0.05152484	0.48884612	-0.02290741
		Y	-0.05522596	0.07336811	-0.07422169	-0.01388041	-0.02584272
		Z	-0.05326858	0.02247317	-0.05416301	-0.14815044	-0.01378880
8	H	X	-0.01822813	0.10688147	-0.05152484	0.48884612	-0.02290741
		Y	-0.05522596	-0.07336811	-0.07422169	-0.01388041	-0.02584272
		Z	0.05326858	0.02247317	0.05416301	0.14815044	0.01378880
9	H	X	0.31400774	0.51886224	0.47020610	-0.02277433	0.00494606
		Y	0.05967570	0.21154825	0.05602016	-0.01307948	-0.06052429
		Z	-0.00752836	0.01528048	-0.06580783	0.00018236	-0.04605112
10	H	X	0.31400774	-0.51886224	0.47020610	-0.02277433	0.00494606
		Y	0.05967570	-0.21154825	0.05602016	-0.01307948	-0.06052429
		Z	0.00752836	0.01528048	0.06580783	-0.00018236	0.04605112
11	H	X	0.50221532	-0.33448178	-0.33103928	-0.05488133	-0.20097198
		Y	0.11905013	-0.12643955	-0.09729179	0.01729889	0.51254237
		Z	0.08543573	-0.02054678	-0.05081656	0.00825706	0.39165608
12	H	X	0.50221532	0.33448178	-0.33103928	-0.05488133	-0.20097198
		Y	0.11905013	0.12643955	-0.09729179	0.01729889	0.51254237
		Z	-0.08543573	-0.02054678	0.05081656	-0.00825706	-0.39165608

TRANS. SAYVETZ	X	-0.00010818	-0.00000000	0.00007108	0.00021263	0.00022625
	Y	0.00016089	-0.00000000	0.00017360	0.00039215	0.00016347
	Z	-0.00000000	-0.00017250	0.00000000	-0.00000000	0.00000000
TOTAL		0.00019388	0.00017250	0.00018759	0.00044609	0.00027913

ROT. SAYVETZ	X	-0.00000000	-0.00096814	0.00000000	-0.00000000	0.00000000
	Y	-0.00000000	0.00099070	-0.00000000	-0.00000000	0.00000000
	Z	0.00058037	-0.00000000	0.00112042	0.00366102	0.00005286
TOTAL		0.00058037	0.00138520	0.00112042	0.00366102	0.00005286

	26	27	28	29	30
FREQUENCY:	1499.25	1506.84	1514.20	2367.13	3052.25
SYMMETRY:	A'	A''	A'	A'	A'
REDUCED MASS:	1.04137	1.03572	1.09298	13.49355	1.03681

1	H	X	0.20325596	0.00000000	0.15886265	0.00000845	0.27552605
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		Y	-0.19498998	-0.00000000	-0.15617834	0.00027794	0.33960754
		Z	-0.00000000	0.68012236	-0.00000000	0.00000000	0.00000000
2	C	X	-0.00268413	0.00000000	-0.00248558	0.00001664	-0.04076636
		Y	-0.03734732	-0.00000000	-0.02835430	-0.00059499	0.02856224
		Z	0.00000000	-0.04456558	0.00000000	-0.00000000	-0.00000000
3	C	X	-0.02012472	-0.00000000	-0.01188496	-0.00467265	0.00311338
		Y	0.03164720	-0.00000000	-0.07658168	-0.00089755	-0.00741418
		Z	0.00000000	-0.02141003	0.00000000	0.00000000	0.00000000
4	C	X	-0.00743812	-0.00000000	0.01377937	-0.00161363	0.00039112
		Y	0.00810737	0.00000000	-0.00741412	0.00511684	0.00076076
		Z	-0.00000000	-0.00024433	0.00000000	0.00000000	-0.00000000
5	N	X	0.00026413	0.00000000	-0.00135678	0.17868210	-0.00020055
		Y	0.00058262	-0.00000000	-0.00315245	-0.07438888	-0.00012126
		Z	0.00000000	0.00216533	-0.00000000	0.00000000	-0.00000000
6	N	X	-0.00027050	0.00000000	0.00323227	-0.16955693	0.00006992
		Y	0.00003603	-0.00000000	-0.00054261	0.07035222	0.00000704
		Z	-0.00000000	-0.00041107	0.00000000	-0.00000000	0.00000000
7	H	X	-0.03831548	0.43488793	-0.03726391	0.00121733	0.09760801
		Y	0.40677981	0.23680362	0.30758988	0.00010813	-0.33735812
		Z	0.30046073	0.04684494	0.22927481	0.00034081	0.50643672
8	H	X	-0.03831548	-0.43488793	-0.03726391	0.00121733	0.09760801
		Y	0.40677981	-0.23680362	0.30758988	0.00010813	-0.33735812
		Z	-0.30046073	0.04684494	-0.22927481	-0.00034081	-0.50643672
9	H	X	0.08722930	-0.04160297	0.00236210	0.00539121	-0.01112582
		Y	-0.32839642	0.02354279	0.41161142	0.00175539	0.04042072
		Z	-0.25571909	-0.00031234	0.32156309	0.00020202	-0.06132889
10	H	X	0.08722930	0.04160297	0.00236210	0.00539121	-0.01112582
		Y	-0.32839642	-0.02354279	0.41161142	0.00175539	0.04042072
		Z	0.25571909	-0.00031234	-0.32156309	-0.00020202	0.06132889
11	H	X	0.02952865	-0.02279738	-0.05395987	-0.03267567	-0.00152318
		Y	0.00020491	-0.00497331	0.05335104	0.00445908	-0.00248937
		Z	-0.00861565	-0.00447463	0.04418685	0.01809538	0.00317446
12	H	X	0.02952865	0.02279738	-0.05395987	-0.03267567	-0.00152318
		Y	0.00020491	0.00497331	0.05335104	0.00445908	-0.00248937
		Z	0.00861565	-0.00447463	-0.04418685	-0.01809538	-0.00317446
TRANS. SAYVETZ		X	-0.00009388	-0.00000000	0.00016031	0.00001096	-0.00004197
		Y	-0.00055936	-0.00000000	-0.00014867	-0.00000978	0.00003179
		Z	-0.00000000	0.00014423	-0.00000000	0.00000000	0.00000000
		TOTAL	0.00056719	0.00014423	0.00021864	0.00001469	0.00005265
ROT. SAYVETZ		X	0.00000000	0.00035514	0.00000000	-0.00000000	0.00000000
		Y	0.00000000	-0.00039232	0.00000000	-0.00000000	-0.00000000
		Z	-0.00252229	-0.00000000	-0.00170109	0.00025030	0.00027094
		TOTAL	0.00252229	0.00052919	0.00170109	0.00025030	0.00027094
			31	32	33	34	35
	FREQUENCY:		3072.22	3089.88	3117.08	3136.46	3149.33
	SYMMETRY:		A'	A'	A''	A''	A'
	REDUCED MASS:		1.05894	1.05575	1.10623	1.10602	1.10156
1	H	X	0.06315336	-0.01434731	0.00000000	0.00000000	0.54998121
		Y	0.07917409	-0.01679123	0.00000000	0.00000000	0.64407526
		Z	-0.00000000	0.00000000	0.01485890	-0.01620605	-0.00000000
2	C	X	-0.00597674	0.00117805	-0.00000000	-0.00000000	-0.03699511
		Y	-0.00229371	0.00116135	-0.00000000	-0.00000000	-0.07968000
		Z	-0.00000000	0.00000000	0.05589167	-0.06874515	-0.00000000
3	C	X	-0.01672587	0.00424198	0.00000000	0.00000000	0.00078680
		Y	0.06217594	-0.01222366	-0.00000000	-0.00000000	-0.00471008
		Z	-0.00000000	0.00000000	-0.06884220	-0.05341478	0.00000000

4	C	X	-0.00009895	0.00357677	0.00000000	0.00000000	0.00066748
		Y	-0.01423602	-0.06257071	-0.00000000	-0.00000000	0.00000442
		Z	-0.00000000	-0.00000000	0.01515846	0.02231893	-0.00000000
5	N	X	0.00114376	0.00400610	0.00000000	0.00000000	0.00004579
		Y	0.00017002	-0.00133799	-0.00000000	-0.00000000	0.00019753
		Z	0.00000000	-0.00000000	-0.00010632	0.00003023	0.00000000
6	N	X	-0.00040161	-0.00283720	-0.00000000	-0.00000000	0.00005508
		Y	0.00003870	0.00085912	0.00000000	0.00000000	-0.00010666
		Z	-0.00000000	0.00000000	0.00005887	0.00006022	-0.00000000
7	H	X	0.00748627	-0.00209348	-0.06833932	0.08710447	-0.05671478
		Y	-0.02813234	0.00309003	0.23909024	-0.29245423	0.15325195
		Z	0.03880306	-0.00418866	-0.34110370	0.41722596	-0.25041853
8	H	X	0.00748627	-0.00209348	0.06833932	-0.08710447	-0.05671478
		Y	-0.02813234	0.00309003	-0.23909024	0.29245423	0.15325195
		Z	-0.03880306	0.00418866	-0.34110370	0.41722596	0.25041853
9	H	X	0.09939287	-0.01936259	0.07831344	0.06594629	-0.00816308
		Y	-0.36139801	0.07951145	-0.28705373	-0.22186115	0.02477239
		Z	0.54920618	-0.11679934	0.41131622	0.31810200	-0.03572605
10	H	X	0.09939287	-0.01936259	-0.07831344	-0.06594629	-0.00816308
		Y	-0.36139801	0.07951145	0.28705373	0.22186115	0.02477239
		Z	-0.54920618	0.11679934	0.41131622	0.31810200	0.03572605
11	H	X	-0.00785897	-0.03301764	-0.00652729	-0.01045198	0.00076919
		Y	0.07673429	0.36750123	0.06081734	0.08953479	0.00159180
		Z	-0.12012485	-0.56104709	-0.09047424	-0.13349061	-0.00229734
12	H	X	-0.00785897	-0.03301764	0.00652729	0.01045198	0.00076919
		Y	0.07673429	0.36750123	-0.06081734	-0.08953479	0.00159180
		Z	0.12012485	0.56104709	-0.09047424	-0.13349061	0.00229734

TRANS. SAYVETZ	X	0.00001110	0.00007031	0.00000000	-0.00000000	-0.00001334
	Y	-0.00001651	0.00002508	-0.00000000	-0.00000000	-0.00019708
	Z	-0.00000000	0.00000000	-0.00003456	-0.00006470	0.00000000
TOTAL		0.00001989	0.00007465	0.00003456	0.00006470	0.00019753

ROT. SAYVETZ	X	-0.00000000	0.00000000	-0.00002325	-0.00006582	-0.00000000
	Y	0.00000000	0.00000000	0.00003342	0.00031176	-0.00000000
	Z	-0.00000888	-0.00007507	-0.00000000	-0.00000000	-0.00115697
TOTAL		0.00000888	0.00007507	0.00004071	0.00031863	0.00115697

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FREQUENCY: 3162.74

SYMMETRY: A''

REDUCED MASS: 1.11137

1	H	X	-0.00000000
		Y	-0.00000000
		Z	-0.00033195
2	C	X	0.00000000
		Y	0.00000000
		Z	-0.00758486
3	C	X	0.00000000
		Y	-0.00000000
		Z	-0.02543348
4	C	X	-0.00000000
		Y	0.00000000
		Z	-0.08815248
5	N	X	-0.00000000
		Y	0.00000000
		Z	0.00049944
6	N	X	0.00000000
		Y	0.00000000

		Z	-0.00047100
7	H	X	0.01180968
		Y	-0.03307728
		Z	0.04668197
8	H	X	-0.01180968
		Y	0.03307728
		Z	0.04668197
9	H	X	0.02652553
		Y	-0.10626089
		Z	0.15031009
10	H	X	-0.02652553
		Y	0.10626089
		Z	0.15031009
11	H	X	0.02530825
		Y	-0.36338272
		Z	0.52437531
12	H	X	-0.02530825
		Y	0.36338272
		Z	0.52437531

TRANS. SAYVETZ	X	0.00000000
	Y	0.00000000
	Z	0.00003809
TOTAL		0.00003809

ROT. SAYVETZ	X	-0.00013054
	Y	0.00026981
	Z	0.00000000
TOTAL		0.00029973

REFERENCE ON SAYVETZ CONDITIONS - A. SAYVETZ, J.CHEM.PHYS., 7, 383-389(1939).

NOTE - THE MODES J,K ARE ORTHONORMALIZED ACCORDING TO  

$$\text{SUM ON I } M(I) * (X(I,J)*X(I,K) + Y(I,J)*Y(I,K) + Z(I,J)*Z(I,K)) = \text{DELTA}(J,K)$$



Vibrational Analysis, PDI Gauche Conformer, CCSD(T)/cc-pVTZ

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 NORMAL COORDINATE ANALYSIS IN THE HARMONIC APPROXIMATION  
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ATOMIC WEIGHTS (AMU)

1	H	1.00782
2	C	12.00000
3	C	12.00000
4	C	12.00000
5	N	14.00307
6	N	14.00307
7	H	1.00782
8	H	1.00782
9	H	1.00782
10	H	1.00782
11	H	1.00782
12	H	1.00782

MODES 1 TO 6 ARE TAKEN AS ROTATIONS AND TRANSLATIONS.

ANALYZING SYMMETRY OF NORMAL MODES...

FREQUENCIES IN CM\*\*<sup>-1</sup>, IR INTENSITIES IN DEBYE\*\*<sup>2</sup>/AMU-ANGSTROM\*\*<sup>2</sup>,  
 REDUCED MASSES IN AMU.

			1	2	3	4	5
	FREQUENCY:		9.44	7.78	2.62	3.42	8.18
	SYMMETRY:		A	A	A	A	A
	REDUCED MASS:		3.25590	4.22515	5.78733	8.46353	4.34120
1	H	X	0.03392277	0.01754462	-0.12752324	-0.00429544	0.15491497
		Y	-0.05988480	0.03793821	-0.12825045	-0.02630855	-0.00600405
		Z	0.18239115	0.15494465	-0.05078809	-0.06147125	0.03688848
2	C	X	-0.02154427	0.00024771	-0.07317874	0.02008513	0.14099087
		Y	-0.06076017	0.05766805	-0.10391458	-0.03820961	-0.00272264
		Z	0.13958439	0.10203306	-0.05524831	-0.01836709	0.01920097
3	C	X	0.03956304	0.05086995	-0.06273734	0.02997295	0.11178557
		Y	-0.07143641	0.06668659	-0.03901795	0.02634243	-0.06330418
		Z	-0.00763193	-0.00907692	-0.03982998	-0.00187463	0.04960959
4	C	X	-0.03973872	0.02415871	0.01026079	0.06245043	0.09541513
		Y	-0.07388721	0.09709626	0.00208530	0.01244671	-0.06163690
		Z	-0.08026452	-0.09057053	-0.04391883	0.05509844	0.03058615
5	N	X	-0.02562069	0.06192667	0.07049109	0.09475283	0.05166976
		Y	-0.06835553	0.07481082	-0.04676039	-0.00141001	-0.04119514
		Z	0.01042941	-0.05873521	-0.06922140	0.11176341	-0.03671245
6	N	X	-0.01254994	0.09107010	0.11340335	0.11779168	0.01934414
		Y	-0.06424156	0.05721600	-0.08436375	-0.01113981	-0.02609271
		Z	0.07950508	-0.03318299	-0.08773468	0.15201532	-0.08624169
7	H	X	-0.13600303	-0.08293901	-0.06682810	0.01510803	0.17923456
		Y	-0.05778154	0.08872721	-0.08890594	-0.08733233	0.02947279
		Z	0.13288188	0.10172228	-0.05248393	-0.02643354	0.02668229
8	H	X	-0.00672159	0.02854884	-0.03494456	0.04112524	0.11133289
		Y	-0.05658983	0.03868596	-0.14478460	-0.04944035	0.01425386
		Z	0.21688550	0.13567826	-0.07407588	0.01884862	-0.02840330
9	H	X	0.15427046	0.13400273	-0.06956071	0.03466748	0.07354451
		Y	-0.07415137	0.03594297	-0.05337807	0.07581919	-0.09634007
		Z	-0.00281192	-0.00989477	-0.04228948	0.00576190	0.04290322

10	H	X	0.02671916	0.02335132	-0.10234732	0.00828329	0.14140677
		Y	-0.07581531	0.08487447	0.00079115	0.03790435	-0.07991957
		Z	-0.08323256	-0.04073816	-0.02078799	-0.03984974	0.09763477
11	H	X	0.00425502	0.06205038	0.02086790	0.07108030	0.07188565
		Y	-0.08186164	0.10263226	0.04728283	0.05834094	-0.10502551
		Z	-0.18254889	-0.16958890	-0.03406035	0.06980624	0.05037521
12	H	X	-0.15534424	-0.05741565	0.02214417	0.06048678	0.13190414
		Y	-0.07099523	0.12862379	0.01721341	-0.03708126	-0.02822487
		Z	-0.08688741	-0.09352122	-0.04234081	0.05209723	0.03467644

TRANS. SAYVETZ	X	-0.87466429	3.17186335	0.70622842	4.55460555	6.04369753
	Y	-4.81058467	5.02766533	-3.87907793	-0.19709948	-2.74811540
	Z	2.05767458	-1.17929254	-4.18513810	4.13089899	-0.26617740
TOTAL		5.30478908	6.06043453	5.74990305	6.15204083	6.64449159

ROT. SAYVETZ	X	1.80480898	8.59410614	2.92590566	-13.41792435	9.10276096
	Y	10.45510697	7.45218919	-1.26575402	-0.35816920	-2.78954548
	Z	-2.34272494	6.46730361	18.27249120	9.37058712	-10.71259429
TOTAL		10.86530982	13.08509839	18.54850376	16.36999945	14.33183511

		6	7	8	9	10
FREQUENCY:		10.76	105.42	171.07	255.56	323.01
SYMMETRY:		A	A	A	A	A
REDUCED MASS:		3.77852	2.49088	2.14496	1.40184	4.62445

1	H	X	-0.09457317	0.02537100	-0.15923669	-0.22109983	0.08154034
		Y	-0.04739412	0.06674510	-0.23700076	-0.26246516	0.10758888
		Z	0.15465867	0.09663369	0.18141321	0.35294316	0.09967881
2	C	X	-0.05547928	0.03638825	0.00219342	-0.00821019	-0.05919340
		Y	-0.01561319	0.13827433	-0.06951292	-0.00572693	0.08779133
		Z	0.12320576	-0.03646496	-0.01977892	0.01613321	0.02124408
3	C	X	-0.06795564	-0.03856720	-0.02212654	0.04494423	-0.05202566
		Y	-0.01121012	-0.02538910	-0.06985312	0.06358304	-0.03169972
		Z	0.15467722	0.03445411	0.03614491	-0.06593553	-0.05414378
4	C	X	-0.01414842	-0.06758254	0.03821395	0.00064725	0.03122671
		Y	0.03733861	0.00285793	0.00742759	-0.01185615	-0.03365609
		Z	0.11830008	-0.04407788	-0.05376905	0.03323468	-0.00273315
5	N	X	0.00772859	-0.00954771	0.04319620	-0.03228879	0.14418032
		Y	0.00515287	-0.03510105	0.01896524	0.00400818	-0.09285705
		Z	0.02679002	-0.00394421	-0.03998278	0.07162398	0.06961700
6	N	X	0.02260913	0.07879655	-0.05406374	-0.00485618	-0.06590889
		Y	-0.02047904	-0.09266845	0.12012742	-0.04483483	0.04823752
		Z	-0.04007736	0.05424463	0.07629804	-0.05693999	-0.04449625
7	H	X	-0.02085254	0.15903385	0.10859352	-0.01372569	-0.11948069
		Y	0.03887371	0.33642027	0.22201143	0.40528695	0.14129661
		Z	0.13397602	0.00311884	0.03370699	0.08280701	0.02707453
8	H	X	-0.04294685	-0.01343432	0.06671466	0.14929192	-0.12937419
		Y	-0.04295967	0.13100067	-0.20226806	-0.23263814	0.16104837
		Z	0.05813391	-0.26544492	-0.31699944	-0.29874069	0.04143097
9	H	X	-0.10288906	-0.12936877	-0.08876919	0.12667885	-0.03569070
		Y	-0.06538460	-0.13580668	-0.19906892	0.17411885	-0.02176494
		Z	0.14495014	0.01437536	0.01454046	-0.04597481	-0.05099886
10	H	X	-0.08148198	0.03093158	-0.04491590	0.02568142	-0.03361166
		Y	0.01487771	-0.05713645	-0.02092616	0.05218353	-0.04525427
		Z	0.22015500	0.18012913	0.17818291	-0.20300548	-0.05028764
11	H	X	-0.02210121	-0.03071913	0.05834430	-0.01728814	0.07343969
		Y	0.03915177	0.01346637	0.01605993	-0.01252091	0.12512680
		Z	0.13708002	-0.11610441	-0.09255452	0.07174448	0.01761025
12	H	X	0.02379455	-0.14215967	0.00269707	0.01996882	0.02422385
		Y	0.09265986	0.03174032	0.05902455	-0.10347577	-0.11535152

		Z	0.12375015	-0.04669715	-0.05243117	0.02804858	-0.00902126
TRANS.	SAYVETZ	X	-1.56989787	0.03142780	0.01017612	-0.00151680	-0.00390847
		Y	-0.05837181	-0.01079390	-0.00053916	0.00095076	-0.00013459
		Z	5.54844832	0.01625766	0.00512312	-0.00546382	0.00025103
		TOTAL	5.76656443	0.03699360	0.01140573	0.00574960	0.00391883
ROT.	SAYVETZ	X	13.79062993	0.04282982	0.04395761	-0.01574250	0.00221828
		Y	-3.11542077	0.02838210	-0.00218746	-0.01719492	0.00155874
		Z	8.53590655	-0.07958805	0.03887007	0.00675049	0.02039624
		TOTAL	16.51511492	0.09473223	0.05871915	0.02427057	0.02057565
			11	12	13	14	15
	FREQUENCY:		356.88	508.77	613.61	784.30	858.96
	SYMMETRY:		A	A	A	A	A
	REDUCED MASS:		2.38908	4.16583	3.63558	1.31969	2.21397
1	H	X	-0.02555817	0.11778439	0.03492220	-0.20916699	-0.14638580
		Y	-0.02151327	0.02660599	0.00864798	-0.08225152	0.03029778
		Z	-0.14585820	0.07549250	0.03224060	0.01645961	-0.04176908
2	C	X	0.04545941	-0.02239300	-0.01411809	0.02268550	-0.10642845
		Y	-0.04986754	0.00329907	0.00379729	0.02421060	0.04192634
		Z	-0.02921965	0.00577730	0.00120709	-0.00445242	-0.04193583
3	C	X	0.01929272	-0.01645803	0.00564745	0.02983154	0.04490003
		Y	0.00535169	-0.09594295	-0.00715297	0.09603769	0.06150903
		Z	0.05370558	-0.05044282	-0.02926303	-0.02457551	0.06371057
4	C	X	-0.05680909	0.00602776	0.15208328	-0.06939701	0.11197427
		Y	0.03767132	-0.09357754	0.12959961	-0.04865453	-0.10626709
		Z	-0.05511067	-0.01794831	-0.06263076	-0.01541226	0.01652599
5	N	X	0.02636100	-0.04335852	-0.07800715	0.03557097	-0.01705012
		Y	0.01238956	0.14942905	-0.02627794	-0.02069935	0.00849452
		Z	0.14767447	0.07905076	0.05459067	-0.00777940	-0.01493203
6	N	X	-0.02351860	0.08023705	-0.04511561	-0.00202045	0.00406457
		Y	0.00329240	0.03721158	-0.07585972	0.01167545	-0.00562342
		Z	-0.08612671	-0.04140725	0.00275820	-0.00013156	0.00227023
7	H	X	0.12727645	-0.08977122	-0.09859575	-0.25574219	-0.14598385
		Y	-0.14561211	0.04759668	-0.00022501	-0.09932633	0.03427387
		Z	-0.04075853	0.00934013	-0.00367533	-0.03751514	-0.04627080
8	H	X	0.05580629	-0.09760964	-0.00691941	0.30023748	-0.07489469
		Y	-0.05985858	0.08277245	0.01424655	-0.19274479	0.01719667
		Z	-0.02755615	0.03861262	0.07026954	0.22931860	-0.00999682
9	H	X	0.00270910	-0.09062231	-0.10723104	-0.31286943	-0.06898418
		Y	-0.04727934	-0.22206124	-0.23470903	-0.21858223	0.08239285
		Z	0.04488160	-0.06960190	-0.06524230	-0.08144983	0.06275223
10	H	X	0.01319903	-0.02673190	-0.05058064	0.22315321	0.01260353
		Y	0.01743180	-0.06267007	0.10739056	0.00576400	0.09482778
		Z	0.09433389	0.11042546	0.26057024	0.41725291	0.10317662
11	H	X	0.08518878	-0.02893153	0.06907786	-0.10510668	0.21660225
		Y	0.08744093	-0.07946310	0.05340616	0.00571032	-0.30896168
		Z	-0.33676857	0.07748671	0.05819718	0.10759727	-0.34998984
12	H	X	-0.39202381	0.09417212	0.16003508	0.09479401	-0.21314278
		Y	0.02948610	-0.16795858	-0.03328638	-0.14569860	0.04392013
		Z	-0.07838581	-0.01928966	-0.06844430	-0.01254167	0.00117600
TRANS.	SAYVETZ	X	0.00067257	-0.00012913	-0.00003110	0.00047881	0.00003924
		Y	-0.00353803	0.00077115	-0.00050420	-0.00005595	0.00012357
		Z	0.00041392	-0.00003453	0.00095707	0.00006288	-0.00081522
		TOTAL	0.00362510	0.00078265	0.00108220	0.00048615	0.00082547
ROT.	SAYVETZ	X	0.00843660	0.00313348	0.00321896	0.00179067	-0.00078759

Y	0.00353180	-0.00133730	0.00004285	-0.00086034	0.00083042
Z	-0.00305771	-0.00297800	-0.00119999	-0.00188028	0.00001582
TOTAL	0.00964362	0.00452499	0.00343562	0.00273534	0.00114462

	16	17	18	19	20
FREQUENCY:	895.06	1033.56	1117.54	1158.70	1275.16
SYMMETRY:	A	A	A	A	A
REDUCED MASS:	1.39111	1.72364	2.06264	1.75834	1.16946

1	H	X	-0.28710907	0.34978789	0.27405133	0.04788158	-0.01882398
		Y	0.10009417	-0.00434134	0.00883057	-0.10525822	0.07580930
		Z	-0.28172606	0.11305366	0.08192682	0.17471207	-0.10906717
2	C	X	-0.05273577	0.07883065	-0.08213592	0.02900975	-0.01859579
		Y	0.03276457	-0.07714502	-0.06914704	0.01002760	-0.00709944
		Z	0.04600530	0.03097256	-0.06422361	-0.07755888	0.06014651
3	C	X	0.00454831	-0.07634185	0.14023710	-0.03632826	0.01818756
		Y	0.04894290	0.11782003	0.02302874	-0.01337135	-0.00136391
		Z	0.06205237	-0.00323343	0.03565902	0.12567953	-0.06091952
4	C	X	0.00342529	0.00675870	-0.08068065	0.00634800	-0.01319197
		Y	-0.04768901	-0.05983432	0.04066187	-0.01004450	0.00606021
		Z	-0.09971323	-0.03305959	0.00326744	-0.11174802	-0.02798345
5	N	X	0.00799450	0.00670702	0.02540708	0.00507367	0.02382356
		Y	-0.00213403	-0.00883333	-0.01874934	0.00295505	-0.01056474
		Z	0.02024331	-0.00692043	0.00177395	0.03944908	0.04718840
6	N	X	-0.00065183	-0.00247753	-0.00374360	-0.00164026	-0.00535614
		Y	-0.00135432	-0.00229986	0.00503749	-0.00311253	-0.00051811
		Z	-0.00511409	0.00106104	0.00004069	-0.00682877	-0.00667886
7	H	X	0.35552045	0.13363953	-0.11677546	-0.31533741	0.17431105
		Y	-0.13733032	0.11006214	0.20385308	0.07384078	-0.04856267
		Z	0.03835866	0.06742397	-0.02493164	-0.08153889	0.06074199
8	H	X	-0.04925755	-0.12207858	-0.34324189	0.10107126	-0.05001684
		Y	-0.02790233	0.11858358	0.18355918	0.00097193	-0.02282733
		Z	-0.20409498	-0.00020580	-0.06942711	0.20109401	-0.14448799
9	H	X	0.28834428	-0.21760596	0.14740218	-0.01708898	-0.30633262
		Y	-0.11245334	0.06979129	-0.16591220	0.30758414	0.10199662
		Z	0.05368309	-0.01704087	0.01198358	0.17283070	-0.06702472
10	H	X	-0.06057943	-0.33992710	0.07072614	0.00160844	0.09047670
		Y	0.08932286	0.35813747	0.11232303	-0.11122846	-0.05143849
		Z	-0.01885491	0.07377636	0.16267847	-0.20352866	0.01759965
11	H	X	-0.11325573	-0.00033338	-0.16134929	-0.13454689	-0.18376176
		Y	-0.00408143	-0.11545166	-0.07051311	-0.11290494	-0.46640814
		Z	0.19925587	-0.04985609	0.10010115	0.12852455	0.00079393
12	H	X	0.29730174	0.02687075	0.09729486	0.28027840	0.19996652
		Y	-0.26393927	-0.15398285	-0.01687318	0.10902806	0.59424905
		Z	-0.09592199	-0.04205025	0.01369360	-0.08784659	0.02082046

TRANS. SAYVETZ	X	0.00001098	-0.00077840	0.00025988	0.00001587	0.00048031
	Y	0.00029614	-0.00001653	-0.00022031	0.00043680	0.00021742
	Z	0.00026816	0.00034136	0.00002965	-0.00011605	-0.00016979
	TOTAL	0.00039966	0.00085012	0.00034199	0.00045223	0.00055389

ROT. SAYVETZ	X	0.00149842	0.00136426	0.00061457	-0.00139203	-0.00047820
	Y	0.00011038	0.00102765	0.00013663	0.00038013	-0.00046894
	Z	0.00037505	0.00156465	-0.00067279	0.00062485	-0.00090736
	TOTAL	0.00154858	0.00231633	0.00092141	0.00157248	0.00112778

	21	22	23	24	25
FREQUENCY:	1292.78	1351.61	1383.77	1436.39	1461.69
SYMMETRY:	A	A	A	A	A
REDUCED MASS:	1.20738	1.19580	1.35113	1.23232	1.07512

1	H	X	0.11931344	-0.09255335	0.12361399	0.39319328	-0.07675837
		Y	0.03686097	-0.01071790	-0.03537839	0.03501923	-0.04119736
		Z	-0.04621194	-0.03815426	0.08886891	0.34520528	0.00479278
2	C	X	-0.02735027	0.01585526	0.00593762	-0.10881532	0.02000122
		Y	-0.06347594	0.01431290	-0.02092782	0.03959353	-0.00195850
		Z	0.02703292	-0.00626379	-0.03433395	-0.04234124	0.00263883
3	C	X	-0.01026487	0.05107003	-0.10833949	0.02959776	-0.00512041
		Y	0.06003433	-0.00651726	0.08784494	-0.01029251	0.00358258
		Z	0.01130187	-0.00073805	-0.01059560	0.00584560	-0.00206020
4	C	X	0.03474150	-0.00439593	0.02397143	-0.01327865	-0.05799089
		Y	-0.04187860	-0.09968200	-0.03009216	-0.01124897	0.00090443
		Z	-0.04008850	-0.01848947	0.01231317	-0.00224856	0.03643724
5	N	X	-0.02476523	-0.01454844	0.00093435	-0.00417245	-0.01095545
		Y	0.01322559	0.00362943	0.00122845	0.00212287	0.00524681
		Z	-0.00398382	0.00905058	0.01377242	0.00053022	0.00868460
6	N	X	-0.00276326	-0.01114981	-0.00290729	-0.00238463	-0.00803121
		Y	-0.01159105	-0.01695528	-0.00471652	-0.00345675	-0.01323712
		Z	0.00192339	0.00236088	-0.00126319	0.00057494	0.00123878
7	H	X	0.12994650	-0.12298915	0.07325732	0.47515459	-0.05655308
		Y	0.09972084	0.00485671	0.08372601	-0.20097032	-0.02690346
		Z	0.06283939	-0.02158167	-0.00819566	-0.03300375	-0.00410029
8	H	X	-0.20213686	-0.00782107	0.05309696	0.30646996	-0.07137943
		Y	0.07963910	0.03034347	-0.00883164	-0.29174113	0.07220014
		Z	-0.08666760	-0.01252555	0.16165454	0.16696051	-0.02734655
9	H	X	-0.24847546	0.03535144	0.51143376	-0.08216838	0.02103996
		Y	0.21661082	-0.10254715	-0.43493387	0.05051036	-0.04742262
		Z	0.02654885	-0.01589190	-0.05755916	0.01140078	-0.00919147
10	H	X	0.49129129	-0.28430443	0.21039951	-0.04946371	0.00812682
		Y	-0.37189974	0.28647808	-0.18995893	0.05826660	-0.01699412
		Z	0.04680946	0.01077638	0.00503376	-0.00123527	-0.02156682
11	H	X	0.13406932	0.09292721	0.00364067	0.05332518	0.28688065
		Y	0.43787304	0.51350697	-0.12163449	0.12360044	0.13911533
		Z	0.08550276	0.19208602	-0.00905535	-0.04816264	-0.59044022
12	H	X	-0.00713417	-0.00816904	-0.01359876	0.09582413	0.66575941
		Y	0.01775865	0.55671373	0.31703312	0.02891533	0.00201894
		Z	-0.03922705	0.03085697	0.03366378	0.00478337	0.06930003

TRANS. SAYVETZ	X	0.00016917	-0.00009329	0.00057727	-0.00010868	0.00000428
	Y	-0.00034836	-0.00060007	0.00002609	0.00000988	-0.00009731
	Z	0.00008517	0.00060474	-0.00014027	-0.00001698	0.00006843
TOTAL		0.00039652	0.00085703	0.00059464	0.00011044	0.00011904

ROT. SAYVETZ	X	-0.00021762	0.00049092	-0.00002347	-0.00041546	0.00023231
	Y	-0.00016263	-0.00015997	-0.00052625	-0.00042400	-0.00029841
	Z	-0.00007285	-0.00008954	-0.00098477	0.00006517	0.00025660
TOTAL		0.00028127	0.00052404	0.00111681	0.00059719	0.00045701

	26	27	28	29	30
FREQUENCY:	1481.79	1503.87	1513.34	2368.52	3043.73
SYMMETRY:	A	A	A	A	A
REDUCED MASS:	1.06911	1.05918	1.03609	13.47250	1.03980

1	H	X	0.07284256	-0.25814704	-0.35014909	-0.00269946	0.11597015
		Y	-0.01051786	-0.01675310	-0.36994155	0.00024490	-0.31813477
		Z	0.08090814	-0.22407501	0.44674429	-0.00072749	-0.16275528
2	C	X	0.00647305	-0.01284741	0.02536203	-0.00003076	-0.04632906
		Y	0.00841756	-0.03288561	0.02115200	0.00037060	-0.00734493
		Z	0.00560248	-0.02812080	-0.03032250	0.00007761	-0.02275992
3	C	X	-0.03941895	0.00680765	0.01069930	0.00025263	0.00651412

		Y	-0.03037821	-0.03964223	0.00910117	-0.00403810	0.00456565
		Z	-0.04817243	-0.02642596	-0.01508847	-0.00084344	0.00397324
4	C	X	-0.00606261	-0.00712363	0.00553289	-0.00452196	-0.00024176
		Y	-0.01279259	0.00155913	0.00188083	0.00012134	-0.00001132
		Z	-0.00833580	0.00147184	-0.00213278	0.00271432	-0.00025769
5	N	X	0.00065694	0.00027755	0.00179837	0.11798105	-0.00018828
		Y	-0.00073511	-0.00045526	-0.00171781	0.15009949	-0.00014004
		Z	0.00125671	0.00098302	-0.00022970	-0.03138518	0.00001276
6	N	X	0.00008557	0.00037853	0.00059039	-0.11193120	0.00014398
		Y	0.00072641	0.00073271	0.00066473	-0.14253241	0.00011666
		Z	-0.00021938	-0.00009695	-0.00012987	0.02963436	-0.00003104
7	H	X	-0.09042280	0.34195363	0.27135233	-0.00013370	-0.04650837
		Y	-0.16369433	0.51391946	-0.36049848	-0.00010735	-0.09268354
		Z	-0.02968575	0.08952521	-0.05843894	-0.00036052	0.55402111
8	H	X	-0.01113232	0.03486340	-0.33798780	0.00117285	0.46630575
		Y	-0.02007685	0.08330817	0.38056080	0.00053740	0.50398710
		Z	-0.16463420	0.58814473	0.15416520	0.00061894	-0.12615477
9	H	X	0.42185905	0.04475958	-0.05740230	0.00080799	0.00273040
		Y	0.50256918	0.19542417	-0.00010336	0.00651602	0.01032970
		Z	0.06887272	0.01249589	-0.02285737	-0.00015590	-0.05680263
10	H	X	0.04020562	-0.05436850	0.03765102	-0.00313128	-0.06276058
		Y	0.05961709	0.05862831	-0.00735193	-0.01093831	-0.07193867
		Z	0.64134560	0.17533937	0.00334060	0.00011547	0.01579964
11	H	X	-0.00705440	0.00370179	-0.03108084	-0.00532096	0.00304834
		Y	0.00017511	-0.00134514	-0.02664885	-0.03288542	0.00066739
		Z	-0.00161789	-0.02575678	0.05343230	0.01641396	0.00275350
12	H	X	0.02776541	0.03474576	-0.06076837	-0.02354134	-0.00121641
		Y	0.04561328	0.00794878	0.01594594	-0.02624652	0.00129888
		Z	-0.00338260	0.00408108	-0.00524589	-0.01478402	0.00020839

TRANS. SAYVETZ	X	-0.00008850	-0.00011069	0.00006073	0.00001252	0.00000556
	Y	-0.00023810	-0.00002691	-0.00005581	0.00003715	-0.00002616
	Z	0.00009377	0.00011264	0.00004919	-0.00000582	0.00005846
	TOTAL	0.00027077	0.00016020	0.00009603	0.00003963	0.00006428

ROT. SAYVETZ	X	0.00046721	0.00040251	0.00028812	0.00004571	0.00009087
	Y	0.00048375	0.00038317	-0.00062472	0.00000457	-0.00000565
	Z	0.00019427	-0.00024875	0.00020823	0.00009791	-0.00015250
	TOTAL	0.00070003	0.00060886	0.00071878	0.00010815	0.00017762

	31	32	33	34	35
FREQUENCY:	3065.92	3089.06	3106.09	3125.01	3148.07
SYMMETRY:	A	A	A	A	A
REDUCED MASS:	1.06124	1.05876	1.10042	1.10289	1.10033

1	H	X	0.02935600	0.00373749	-0.03841268	0.06636618	-0.28846006
		Y	-0.07998018	-0.00486090	0.06518520	-0.14101041	0.71839437
		Z	-0.04318863	-0.00423457	0.04961123	-0.08645336	0.36043484
2	C	X	-0.00434487	0.00259001	-0.02362514	0.02311492	0.01800253
		Y	0.00430183	0.00447208	-0.03742941	0.04527451	-0.06256855
		Z	-0.00095159	-0.00528123	0.04275624	-0.03676598	-0.05784879
3	C	X	-0.03957679	-0.00598867	0.02189097	0.02419853	0.00052054
		Y	-0.04028923	-0.00606965	0.02907983	0.03115301	0.00064918
		Z	-0.03639304	0.01510211	-0.04852987	-0.04739249	-0.00747649
4	C	X	0.00270938	0.04802220	0.01322651	0.00888372	0.00119756
		Y	-0.00269473	-0.01252425	-0.00259604	-0.00170386	-0.00014242
		Z	0.00265701	-0.03902647	-0.00240815	0.00457931	0.00214124
5	N	X	0.00089434	0.00250025	0.00016407	0.00006364	-0.00008631
		Y	0.00178615	0.00379418	-0.00013051	-0.00056770	0.00002670
		Z	-0.00001924	-0.00049538	-0.00016771	-0.00020288	-0.00002771

6	N	X	-0.00034997	-0.00164725	-0.00018882	-0.00018671	0.00004407
		Y	-0.00062499	-0.00249231	-0.00030014	-0.00013575	0.00004078
		Z	0.00003658	0.00029487	0.00008458	0.00008073	-0.00001519
7	H	X	-0.00494762	-0.00297509	0.03259569	-0.02590796	-0.02510174
		Y	-0.00935633	-0.00911544	0.06888430	-0.06260112	-0.07191820
		Z	0.06846452	0.06080461	-0.48851684	0.44982266	0.36931280
8	H	X	0.03649630	-0.03447934	0.29020338	-0.31761656	0.10399070
		Y	0.03870863	-0.03804164	0.31323945	-0.33532994	0.09693707
		Z	-0.00819835	0.00804907	-0.06887228	0.07565833	-0.03814602
9	H	X	-0.03795303	0.00589446	-0.02764386	-0.02169094	-0.00214085
		Y	-0.09310120	0.02540460	-0.07492546	-0.07449428	-0.01321967
		Z	0.55528951	-0.16051222	0.52801058	0.50682504	0.08433469
10	H	X	0.50208294	0.05420039	-0.23946508	-0.26746761	-0.00078066
		Y	0.57502836	0.05944217	-0.27655529	-0.30069400	-0.00146976
		Z	-0.13097133	-0.01087593	0.04990116	0.05526874	-0.00014866
11	H	X	-0.04312860	-0.53615518	-0.14997544	-0.10065689	-0.02182876
		Y	0.01086376	0.17177359	0.04708980	0.03076061	0.00711117
		Z	-0.02278844	-0.25864503	-0.07147869	-0.04581340	-0.00918748
12	H	X	0.00126244	-0.03342837	-0.00381230	-0.00047575	0.00003839
		Y	0.00220643	-0.05456137	-0.00661464	0.00348957	0.00213986
		Z	-0.00584343	0.71595271	0.10000093	-0.00603856	-0.01371528

TRANS. SAYVETZ	X	0.00002456	-0.00002920	-0.00001702	-0.00002965	-0.00006008
	Y	-0.00007902	-0.00001653	-0.00000806	0.00006883	-0.00004714
	Z	-0.00001483	0.00000679	0.00008260	0.00003720	-0.00003287
TOTAL		0.00008406	0.00003423	0.00008472	0.00008367	0.00008314

ROT. SAYVETZ	X	-0.00030712	0.00010553	-0.00006305	0.00006504	-0.00019065
	Y	-0.00005787	-0.00007808	0.00007354	0.00000978	-0.00004244
	Z	-0.00026624	-0.00002113	-0.00013445	0.00014975	0.00002232
TOTAL		0.00041056	0.00013296	0.00016571	0.00016356	0.00019659

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FREQUENCY: 3162.17  
 SYMMETRY: A  
 REDUCED MASS: 1.11142

1	H	X	-0.00364525
		Y	0.00887234
		Z	0.00464982
2	C	X	0.00135560
		Y	0.00003388
		Z	-0.00209766
3	C	X	0.00202153
		Y	0.00307748
		Z	-0.01025821
4	C	X	-0.04776953
		Y	0.02032778
		Z	-0.07522491
5	N	X	0.00012280
		Y	-0.00032566
		Z	0.00035950
6	N	X	-0.00017396
		Y	0.00020287
		Z	-0.00039959
7	H	X	0.00031653
		Y	-0.00431709
		Z	0.02209966
8	H	X	-0.00735294
		Y	-0.00792789

		Z	0.00128965
9	H	X	-0.00732744
		Y	-0.01418305
		Z	0.11373342
10	H	X	-0.01990598
		Y	-0.02278980
		Z	0.00398227
11	H	X	0.60857537
		Y	-0.20040396
		Z	0.27558548
12	H	X	-0.04138985
		Y	-0.03665221
		Z	0.62199757

TRANS. SAYVETZ	X	-0.00001328
	Y	-0.00002203
	Z	-0.00002892
TOTAL		0.00003871

ROT. SAYVETZ	X	-0.00002963
	Y	0.00000130
	Z	0.00010879
TOTAL		0.00011276

REFERENCE ON SAYVETZ CONDITIONS - A. SAYVETZ, J.CHEM.PHYS., 7, 383-389(1939).

NOTE - THE MODES J,K ARE ORTHONORMALIZED ACCORDING TO  

$$\text{SUM ON I } M(I) * (X(I,J)*X(I,K) + Y(I,J)*Y(I,K) + Z(I,J)*Z(I,K)) = \text{DELTA}(J,K)$$