

Dianion Acepentalene

CAS(12/10)/cc-pVDZ

C3v

C	6.0	0.6562117423	-0.0000562218	0.0000000000
C	6.0	0.3755435877	1.3827402387	0.0000000000
C	6.0	0.3754291365	-0.6914453919	-1.1975477557
C	6.0	0.3754291365	-0.6914453919	1.1975477557
C	6.0	-0.0369617590	1.6154099738	-1.3821557157
C	6.0	-0.0369617590	1.6154099738	1.3821557157
C	6.0	-0.0370549394	0.3892390207	-2.0901073563
C	6.0	-0.0370549394	0.3892390207	2.0901073563
C	6.0	-0.0370254803	-2.0048210314	-0.7079396939
C	6.0	-0.0370254803	-2.0048210314	0.7079396939
H	1.0	-0.2266847713	2.5803964465	-1.8647371965
H	1.0	-0.2266847713	2.5803964465	1.8647371965
H	1.0	-0.2269705182	0.3247083339	-3.1670329143
H	1.0	-0.2269705182	0.3247083339	3.1670329143
H	1.0	-0.2266093334	-2.9052538814	-1.3023014092
H	1.0	-0.2266093334	-2.9052538814	1.3023014092

FREQUENCY: 215.48 324.34 324.53 546.40

REDUCED MASS: 3.90722 4.57934 4.59633 6.60092

IR INTENSITY: 0.24176 0.00736 0.00483 0.00240

1 C X 0.14905593 0.00134644 -0.00010957 -0.00001478

Y 0.00032481 -0.00745784 0.00055577 0.00026142

Z -0.00027337 0.00045618 0.00775431 -0.00374012

2 C X 0.08103205 0.12254336 -0.00866657 0.00008144

Y 0.00011027 0.01776776 -0.00123656 0.00031230

Z -0.00039313 0.00026726 0.00523805 0.00244593

3 C X 0.08361536 -0.05274966 0.10947905 0.00010389

Y 0.00011962 0.00003399 -0.00965647 0.00017815

Z -0.00079713 0.00883045 -0.01250406 -0.00391399

4 C X 0.08379656 -0.06760577 -0.10102058 -0.00014828

Y 0.00005114 0.00145981 0.00953053 -0.00002760

Z 0.00012623 -0.01068808 -0.01107933 -0.00421238

5 C X -0.04761773 0.03939239 -0.10453470 0.10791804

Y -0.02789975 0.02126489 -0.04126315 0.02601837

Z 0.03388465 0.02623978 0.02606506 -0.01960611

6 C X -0.04729079 0.05376433 0.09794663 -0.10785522

Y -0.02784558 0.02698389 0.03786457 -0.02621285

Z -0.03462764 -0.02260638 0.02963778 -0.01894604

7 C X -0.04578331 -0.11274182 -0.00146791 -0.10866381

Y -0.01678326 0.01057355 -0.03112983 -0.00357332

Z 0.04009225 0.04778419 0.01316383 0.02965162

8 C X -0.04535767 -0.11131792 0.01733115 0.10854306
Y -0.01671778 0.01500325 0.02930078 0.00296858
Z -0.04076750 -0.04568864 0.01986499 0.02969909

9 C X -0.04681114 0.06926501 0.08708107 0.10958760
Y 0.04396516 -0.04220893 -0.01174543 -0.03298307
Z 0.00617868 -0.00399234 -0.03903030 -0.00601430

10 C X -0.04671359 0.05635113 -0.09595225 -0.10954746
Y 0.04390335 -0.04010881 0.01754098 0.03317998
Z -0.00699230 -0.00168829 -0.03918562 -0.00607608

11 H X -0.16178725 0.04461601 -0.20100660 0.10569087
Y -0.03688849 0.02390207 -0.05613062 0.02394885
Z 0.06063851 0.02945055 0.03234817 -0.01712007

12 H X -0.16133748 0.07251410 0.19283663 -0.10482510
Y -0.03682661 0.03172511 0.05220395 -0.02445387
Z -0.06134448 -0.02498189 0.03638553 -0.01548738

13 H X -0.16038440 -0.20703540 -0.03332382 -0.10089557
Y -0.03650198 0.01393682 -0.03474262 0.00109712
Z 0.06170274 0.06372682 0.01886072 0.02528409

14 H X -0.15964812 -0.20008556 0.06224732 0.10036157
Y -0.03630465 0.01892377 0.03239976 -0.00243931
Z -0.06232426 -0.06065145 0.02777532 0.02521502

15 H X -0.16472335 0.15217158 0.14295779 0.11483679
Y 0.07196889 -0.05442856 -0.01731873 -0.03541228
Z -0.00062282 -0.00900673 -0.04678404 0.00192867

16 H X -0.16444194 0.13062906 -0.16288358 -0.11522106

Y 0.07182682 -0.05141069 0.02474842 0.03586911

Z -0.00026011 0.00222289 -0.04758637 0.00209505

FREQUENCY: 552.34 553.41 623.68 624.61 637.75

REDUCED MASS: 2.95972 2.90325 10.36398 10.43321 1.46398

IR INTENSITY: 1.14033 1.19738 0.29754 0.31549 1.02174

1 C X -0.00000443 -0.00029989 0.00011623 -0.00019024 -0.01222799

Y 0.08064451 -0.00153840 0.01821565 -0.00211101 0.00092780

Z -0.00178082 -0.08003865 -0.00190516 -0.01888289 -0.00006899

2 C X 0.01446796 -0.00010106 0.14086432 -0.01332534 0.05274799

Y 0.09188842 -0.00158133 0.07730689 -0.00776441 0.02129665

Z 0.00033251 0.00103832 0.00305354 0.02937909 0.00000478

3 C X -0.00728252 0.01152057 -0.05732472 0.12873068 0.05700507

Y 0.02011342 -0.03994586 -0.00794703 -0.04566004 -0.01037127

Z 0.03863598 -0.06628043 0.04105536 -0.05510485 -0.01926039

4 C X -0.00797958 -0.01113040 -0.08074772 -0.11461681 0.05818671

Y 0.02221634 0.03948469 0.00112875 0.04614039 -0.01052028

Z -0.04181800 -0.06566183 -0.05093066 -0.04572157 0.01931757

5 C X 0.01364048 -0.02168068 -0.09171949 0.06273900 -0.04906438

Y -0.02846977 0.04329693 -0.01735369 -0.01747272 -0.01025699

Z -0.09731421 0.03282915 0.03274313 0.00993981 0.00031200

6 C X 0.01475657 0.02109950 -0.10220277 -0.04441498 -0.04847679

Y -0.02898802 -0.04239423 -0.01320962 0.02059896 -0.01019079

Z 0.09814365 0.02909665 -0.03024389 0.01577700 -0.00043914

7	C	X	-0.02010296	0.01037342	0.08786919	-0.06613441	-0.05180794
		Y	-0.08981783	0.06212014	0.00659226	-0.01738744	0.00103979
		Z	-0.00939751	-0.03256691	0.00995787	0.03534916	0.00874440
8	C	X	-0.02082427	-0.00939876	0.09883187	0.04761789	-0.05221627
		Y	-0.09122804	-0.05908631	0.01027112	0.01636634	0.00102277
		Z	0.00754855	-0.03349952	-0.00304564	0.03668434	-0.00936549
9	C	X	0.00681825	0.01506055	-0.01051651	-0.10995419	-0.05672387
		Y	0.02867734	-0.06061795	-0.03274281	0.02259419	0.00913750
		Z	0.01071967	0.09185627	-0.00841006	-0.00501496	0.00706810
10	C	X	0.00767947	-0.01529757	0.01081022	0.10935581	-0.05767738
		Y	0.03076666	0.05970786	-0.03643988	-0.01597329	0.00955129
		Z	-0.00780429	0.09212504	0.00696701	-0.00649586	-0.00706111
11	H	X	0.13729169	-0.02783331	-0.02160475	0.03658928	0.29953762
		Y	-0.07408789	0.06069215	-0.02930959	-0.02631670	0.01241277
		Z	-0.24295075	0.06517433	-0.03005324	0.00195349	-0.10222275
12	H	X	0.13779299	0.02227276	-0.02880781	-0.03117501	0.29868967
		Y	-0.07500844	-0.05833030	-0.02311733	0.03200568	0.01232111
		Z	0.24400261	0.05626474	0.02937621	-0.00455068	0.10178380
13	H	X	-0.08318311	0.11909565	0.05345124	-0.00979895	0.29685587
		Y	-0.19522364	0.17670282	0.00094000	0.04434270	0.07690533
		Z	0.00774324	-0.06219514	0.01772146	0.01694990	-0.06224909
14	H	X	-0.08731262	-0.11658586	0.05515990	0.00222830	0.29628962
		Y	-0.20091540	-0.17051268	-0.00690877	-0.04195288	0.07698129
		Z	-0.01059261	-0.06273678	-0.01400929	0.02081504	0.06163006
15	H	X	-0.05734421	0.13480450	-0.01122415	-0.03921579	0.34227700

Y 0.06465983 -0.16221506 -0.00933517 -0.01786351 -0.10383684
Z -0.01925018 0.20687697 -0.03802415 0.02569715 0.04223843
16 H X -0.06036349 -0.13328218 -0.00238932 0.04377268 0.34208825
Y 0.07053802 0.16043511 -0.00605345 0.01802922 -0.10356084
Z 0.02659415 0.20642464 0.04176873 0.01741936 -0.04211653

FREQUENCY: 654.87 658.47 721.53 736.38 737.57
REDUCED MASS: 1.22711 1.22109 1.15350 2.43453 2.48191
IR INTENSITY: 0.06638 0.06814 0.00348 0.04060 0.03171

1 C X 0.00119659 -0.00005153 0.00000876 0.00149091 0.00513040
Y 0.00922569 0.00004477 0.00004289 0.00089258 0.03896892
Z -0.00000510 -0.00795727 -0.00255733 0.04105723 -0.00033924
2 C X -0.00383534 0.00002704 -0.00008521 -0.00176353 -0.04961446
Y 0.00229876 0.00008429 0.00005096 0.00077530 0.07819936
Z 0.00001899 -0.00624353 -0.00357917 -0.06239461 0.00051808
3 C X -0.00279865 -0.00019834 0.00203001 0.03690340 0.01849282
Y 0.00638774 0.00231111 -0.00825062 0.06277069 -0.02646095
Z -0.00041640 -0.00300316 -0.00095465 0.04786786 0.06431526
4 C X -0.00268905 0.00030393 -0.00201483 -0.03789461 0.01903569
Y 0.00638529 -0.00228230 0.00824415 -0.06303930 -0.02539820
Z 0.00043252 -0.00317069 -0.00113663 0.04542712 -0.06486479
5 C X 0.02307406 0.06445711 0.03665329 -0.01064190 0.04515686
Y -0.00610756 0.01439233 -0.01970600 0.05374998 0.04189523
Z -0.01640131 -0.01265099 0.00880179 -0.06143050 -0.00327821

6	C	X	0.02312591	-0.06454229	-0.03661748	0.01100939	0.04503707
		Y	-0.00606098	-0.01446134	0.01973792	-0.05308041	0.04275434
		Z	0.01641139	-0.01271577	0.00871680	-0.06261999	0.00451148
7	C	X	0.04971396	0.04984957	-0.03332026	-0.04710862	-0.01025975
		Y	-0.00526915	0.01661740	-0.00174139	0.02527383	-0.01690907
		Z	-0.01522497	-0.00986049	-0.02077044	-0.00381317	0.09200787
8	C	X	0.04968190	-0.04987020	0.03335193	0.04785062	-0.01126115
		Y	-0.00523075	-0.01673332	0.00166877	-0.02631728	-0.01639793
		Z	0.01519542	-0.01008263	-0.02103474	-0.00731617	-0.09143224
9	C	X	-0.06370404	-0.01660441	0.04292630	-0.02994149	-0.03228370
		Y	0.01971587	0.00035461	0.01420712	0.06515989	-0.05567936
		Z	-0.00238146	0.01458905	0.01599032	0.03731699	0.00244101
10	C	X	-0.06378523	0.01645052	-0.04298188	0.02917434	-0.03283507
		Y	0.01974633	-0.00028631	-0.01423554	-0.06594642	-0.05464573
		Z	0.00234462	0.01455140	0.01597096	0.03716988	-0.00317647
11	H	X	-0.21528220	-0.45406747	-0.34471293	-0.16032333	-0.29920488
		Y	-0.02889383	-0.02479491	-0.04341853	0.04715721	-0.02826174
		Z	0.03453092	0.12402556	0.11618964	-0.00747533	0.00185061
12	H	X	-0.21552921	0.45486505	0.34488714	0.16474639	-0.30325386
		Y	-0.02886289	0.02469943	0.04338653	-0.04722919	-0.02754379
		Z	-0.03461727	0.12437353	0.11627439	-0.00562616	-0.00201103
13	H	X	-0.31722700	-0.40343541	0.31953688	0.22413589	0.27563004
		Y	-0.08368110	-0.06072909	0.08340170	-0.01828104	0.00140390
		Z	0.05868916	0.07827325	-0.09062057	-0.05130873	0.03567794
14	H	X	-0.31732459	0.40384443	-0.31929866	-0.22082856	0.28023797

Y -0.08363566 0.06055926 -0.08354764 0.01629574 0.00157517
Z -0.05872714 0.07812061 -0.09085447 -0.05440018 -0.03407683
15 H X 0.47389631 0.06811075 -0.39740820 0.31331125 0.03135876
Y -0.11945668 -0.02895145 0.13328546 0.01582891 -0.03534590
Z 0.02991608 0.02864362 -0.02086298 -0.00897604 -0.04481939
16 H X 0.47399202 -0.06717925 0.39760126 -0.30990527 0.03741485
Y -0.11948580 0.02881475 -0.13328737 -0.01639183 -0.03555732
Z -0.02997636 0.02863939 -0.02077505 -0.00756682 0.04452969

FREQUENCY: 762.08 764.62 766.85 847.18 869.52
REDUCED MASS: 1.91643 2.40286 3.01285 7.16282 4.33452
IR INTENSITY: 0.58302 0.65398 0.64970 0.04122 0.00042

1 C X 0.00790144 -0.10240595 0.12650009 0.16220311 0.00187832
Y 0.00079408 -0.00974354 -0.00909395 -0.00074921 0.00014987
Z 0.01356453 0.00137743 -0.00016114 0.00027560 -0.00047378
2 C X -0.00846616 0.11906477 -0.01488715 -0.01896993 0.00009275
Y -0.00266182 0.03567751 -0.04967755 0.03514050 0.00093291
Z -0.03112636 -0.00264440 0.00029521 0.00082940 -0.04970185
3 C X 0.06920185 0.03232387 -0.09636344 -0.01609098 0.00083390
Y 0.01775485 -0.00107002 0.03761174 -0.01961619 -0.04367940
Z -0.00091142 -0.04335589 0.02549076 -0.03054305 0.02401652
4 C X -0.07429507 0.02155506 -0.09537317 -0.01620896 -0.00111431
Y -0.01677342 -0.00528738 0.03819909 -0.02069360 0.04315896
Z -0.00739911 0.04353148 -0.02577002 0.02919270 0.02509757

5 C X -0.03769840 0.01590666 0.02188091 -0.01747956 -0.01997740
Y 0.05724877 -0.02264542 -0.04805177 0.05204164 0.09066488
Z -0.03997498 -0.04654627 0.01328611 -0.06870048 -0.04670180

6 C X 0.03523597 0.02143533 0.02137393 -0.01770103 0.01962675
Y -0.05437647 -0.03149478 -0.04717165 0.05405830 -0.08978995
Z -0.04639449 0.03836646 -0.01244460 0.06882601 -0.04482454

7 C X 0.01148243 -0.03766573 -0.02448439 -0.01658416 0.01911409
Y 0.04413081 0.00840386 -0.02665878 0.03426901 0.00540133
Z 0.00080730 -0.07944529 -0.02793437 -0.07884183 0.09834594

8 C X -0.00633595 -0.03768509 -0.02455725 -0.01569185 -0.01978643
Y -0.04539437 0.00149254 -0.02607153 0.03397658 -0.00458710
Z -0.01000725 0.07741389 0.02799051 0.07485268 0.10109324

9 C X 0.03931431 0.00975763 0.01478177 -0.01748572 -0.01932750
Y 0.03810238 0.01330565 0.06543413 -0.08836902 -0.08468499
Z 0.06287804 0.00269891 -0.00780843 -0.00991863 -0.05367772

10 C X -0.04009568 0.00445953 0.01519592 -0.01794063 0.01886041
Y -0.03838505 0.00597913 0.06634057 -0.09002425 0.08231501
Z 0.06257710 0.00751142 0.00686020 0.01154257 -0.05341883

11 H X 0.18764333 -0.35881429 -0.10479763 -0.01670360 -0.12561600
Y 0.07724065 -0.05739770 -0.03711094 0.04759894 0.04028198
Z -0.09200084 0.03214692 0.08821014 -0.08775616 -0.09640489

12 H X -0.13527783 -0.37712971 -0.10351396 -0.01879188 0.12417080
Y -0.06916839 -0.06852592 -0.03608357 0.04837071 -0.03991063
Z -0.08709243 -0.04554072 -0.08695215 0.08926020 -0.09361938

13 H X -0.25740972 0.11922581 0.29288410 -0.02730952 0.12501138

Y -0.02558506 0.06715278 0.00173788 0.05428549 -0.06428263
Z 0.05326749 -0.11346983 -0.08618936 -0.08301619 0.07986052
14 H X 0.24139297 0.14992472 0.29085872 -0.02355287 -0.12558492
Y 0.01559090 0.07069387 0.00111334 0.05191725 0.06641800
Z 0.03777644 0.11752320 0.08582357 0.07945119 0.08283059
15 H X -0.33201424 -0.07618766 0.14498510 -0.02156096 -0.13237377
Y 0.14154813 0.01664871 0.04578485 -0.09767931 -0.10075635
Z 0.02419144 0.02398133 -0.01987129 0.00124691 0.01808155
16 H X 0.34204736 -0.03618303 0.14238561 -0.02462231 0.13150517
Y -0.14164364 -0.00423814 0.04788850 -0.09883883 0.09807255
Z 0.02748892 -0.02026774 0.01983828 -0.00002780 0.01782680

FREQUENCY: 1065.75 1068.52 1071.05 1115.69 1116.30

REDUCED MASS: 1.79640 1.83566 1.44485 1.98035 2.05928

IR INTENSITY: 0.91596 0.80441 0.15155 0.62911 0.64309

1 C X -0.00075981 0.00180662 0.02585572 0.00054381 -0.00130395
Y 0.06092359 -0.00056986 0.00732488 -0.00800355 0.09335223
Z 0.00170668 0.06366260 -0.00442206 -0.09296099 -0.00774130
2 C X -0.04165473 -0.00154559 -0.03275053 0.00160480 -0.02116986
Y 0.05374203 0.00303688 0.05234395 -0.00544870 0.06676999
Z -0.00088823 -0.01097839 0.00045977 -0.00156088 -0.00100742
3 C X 0.02186113 0.03337828 -0.03288844 -0.02022613 0.01209583
Y 0.00385775 0.02756789 -0.02419821 -0.02951022 0.01841922
Z 0.02936614 0.03303282 -0.04158223 -0.05451785 0.02763836

4	C	X	0.01998255	-0.03928058	-0.02725446	0.01792559	0.01538712
		Y	0.00242944	-0.03148002	-0.01951784	0.02652920	0.02338191
		Z	-0.02739164	0.04105854	0.03594039	-0.04987038	-0.03627576
5	C	X	0.02828094	0.00027158	0.01721547	-0.00124847	0.01874830
		Y	-0.07901098	0.02096859	-0.05541120	0.05988716	-0.02250574
		Z	0.03973182	0.01906501	0.00443104	0.02771409	0.06518696
6	C	X	0.02806985	0.00113138	0.01700363	-0.00173816	0.01847395
		Y	-0.07956754	-0.02533326	-0.05080396	-0.05616667	-0.03132411
		Z	-0.03796143	0.01951299	-0.00728245	0.03844642	-0.05901011
7	C	X	-0.01397181	-0.02380939	0.01679977	0.01675499	-0.00959275
		Y	0.02066557	-0.01779204	0.02328242	-0.05955666	-0.03520462
		Z	-0.03540736	-0.07963330	0.04659284	0.03449739	-0.05934362
8	C	X	-0.01272653	0.02696362	0.01291778	-0.01507367	-0.01241953
		Y	0.02152143	0.01959750	0.01963629	0.06535415	-0.02509365
		Z	0.03123008	-0.08783317	-0.03366494	0.02453397	0.06481940
9	C	X	-0.01534416	-0.02265873	0.01663942	0.01701010	-0.00952655
		Y	-0.03437226	-0.06406188	0.02969365	0.06165336	-0.03125683
		Z	-0.05484712	-0.02276445	0.04913388	0.02354514	0.06037145
10	C	X	-0.01406926	0.02580107	0.01299337	-0.01521681	-0.01225639
		Y	-0.03093781	0.06986474	0.01974945	-0.05601771	-0.04126614
		Z	0.05336234	-0.03306115	-0.04504045	0.03235200	-0.05569474
11	H	X	0.06977057	0.07804224	-0.04931929	0.01958356	0.08892164
		Y	-0.08837739	0.18273128	-0.20631958	0.12349760	0.12178237
		Z	0.00355821	0.30573438	-0.26672680	0.14454746	0.32218594
12	H	X	0.06422162	-0.08797967	-0.03672991	-0.03422450	0.08334628

Y -0.09860263 -0.20743085 -0.17439168 -0.14409866 0.09996640
Z 0.01525334 0.34177260 0.21542299 0.19861479 -0.29228281
13 H X -0.10947249 -0.01563837 -0.05177599 0.08654594 -0.00940731
Y 0.30198748 -0.21741063 0.34967027 -0.36783906 -0.08206355
Z -0.03379421 -0.07019222 0.04082058 0.03946940 -0.05664440
14 H X -0.10788915 0.01333628 -0.05259997 -0.08505362 -0.02270222
Y 0.31198138 0.25219960 0.30729672 0.38144086 -0.02391689
Z 0.03021020 -0.07751703 -0.02946462 0.02987212 0.06300637
15 H X 0.03953146 -0.10958117 -0.04659449 0.06284181 -0.05550691
Y 0.13848696 -0.14722589 -0.12745545 0.14486026 -0.14620893
Z -0.33798166 0.13714717 0.30977807 -0.12236595 0.25338397
16 H X 0.04479537 0.09871931 -0.06257881 -0.05369213 -0.06573155
Y 0.14520905 0.11821144 -0.14702896 -0.12116332 -0.16901655
Z 0.34305955 0.06901562 -0.32509866 -0.08320778 -0.27130839

FREQUENCY: 1234.67 1265.40 1305.29 1306.27 1427.63

REDUCED MASS: 1.59630 7.38490 3.14885 3.16533 2.19099

IR INTENSITY: 0.00207 0.00679 0.12549 0.12804 0.00996

1 C X -0.00025467 0.01575649 -0.00048541 -0.00013818 0.00045232
Y 0.00058424 0.00070843 0.02549739 0.00954325 -0.07109686
Z -0.00006304 -0.00000284 -0.00860614 0.02611635 -0.01569397
2 C X 0.00000090 -0.02750474 -0.00333254 -0.00169150 -0.02403434
Y -0.00151802 0.13379655 -0.01331801 -0.00320288 0.04456513
Z 0.10538606 -0.00047759 -0.04959031 0.15121243 -0.01242849

3	C	X	-0.00036284	-0.02802259	0.00195997	0.00435827	0.01630760
		Y	0.09153592	-0.06275230	0.13442593	-0.03261742	-0.02203374
		Z	-0.05161588	-0.12109510	-0.07440316	0.00784867	0.04727270
4	C	X	0.00109031	-0.02728384	0.00431560	-0.00293900	0.00686587
		Y	-0.09036485	-0.06544227	0.08863099	0.10491832	-0.04063635
		Z	-0.05520483	0.11727832	0.05422248	0.05280316	-0.03708870
5	C	X	0.00346260	0.00996459	0.01718319	-0.00467435	0.02059323
		Y	0.00082031	0.02282422	-0.06385756	0.04878667	0.00694381
		Z	0.00101879	0.05486553	0.02934735	0.00020380	0.09416880
6	C	X	-0.00346584	0.00955885	0.01079889	0.01431553	0.01437481
		Y	-0.00200143	0.02368022	-0.02226412	-0.07760434	0.02291451
		Z	0.00191173	-0.05381878	-0.02288902	-0.01827720	-0.07621818
7	C	X	-0.00324655	0.00952505	0.00624911	-0.01679381	-0.02214237
		Y	0.00499188	-0.05801092	0.02879673	-0.00063851	0.06357462
		Z	0.00275574	0.00715650	0.05063742	-0.06461357	-0.06152477
8	C	X	0.00313592	0.00902601	-0.00506821	0.01772992	-0.01827440
		Y	-0.00387651	-0.05792932	0.02321712	0.01601731	0.03629865
		Z	0.00283313	-0.00515019	-0.00213809	-0.08302871	0.06038548
9	C	X	0.00397958	0.00919867	-0.01291115	-0.01284012	-0.00190475
		Y	0.00086668	0.03322023	-0.05212595	-0.03934620	-0.00679397
		Z	-0.00260837	-0.05021900	-0.05771699	-0.01268246	0.05545247
10	C	X	-0.00418606	0.00865669	-0.01803555	0.00277522	0.00750638
		Y	-0.00153283	0.03189151	-0.06539839	0.00120444	0.02863764
		Z	-0.00428190	0.05030750	0.05357958	0.02527983	-0.03936957
11	H	X	-0.07901010	0.02116273	0.00257838	-0.07740274	-0.02573661

Y -0.14719743 0.04051140 -0.11829059 -0.07295213 -0.19989845
Z -0.26905801 0.07829526 -0.04886479 -0.24047879 -0.30543882
12 H X 0.07981668 0.02182864 -0.04411817 0.06567144 -0.02944279
Y 0.14743395 0.04388363 -0.13792870 -0.00861481 -0.14857521
Z -0.27092215 -0.08135322 0.18209681 -0.17170177 0.25848393
13 H X 0.07907892 0.02676498 0.07739091 0.00566779 0.00913830
Y -0.29609486 -0.11091069 -0.22850908 -0.12244412 -0.32186894
Z 0.01009576 0.00428561 0.06739718 -0.07097930 -0.04634252
14 H X -0.08101046 0.02386911 0.06543687 0.04102340 -0.00172833
Y 0.30356158 -0.10251841 -0.25564932 -0.03384689 -0.22932963
Z 0.01019203 -0.00189042 -0.01183301 -0.09790974 0.05196693
15 H X -0.07982207 0.01860997 -0.07168099 0.03568178 0.02885508
Y -0.15911098 0.03876626 -0.16222599 0.06679612 0.09531810
Z 0.26178805 -0.06984227 0.10342325 -0.19453184 -0.09798168
16 H X 0.07915830 0.02056138 -0.03605748 -0.07128172 0.02219441
Y 0.15773248 0.04386219 -0.09013568 -0.15015562 0.03539839
Z 0.25863346 0.08012521 0.03316219 -0.21730267 -0.03504314

FREQUENCY: 1429.56 1476.51 1479.27 1504.44 1512.30

REDUCED MASS: 2.24471 3.81039 3.79062 3.25036 3.29964

IR INTENSITY: 0.01451 4.36482 4.43426 0.54780 0.00649

1 C X -0.00006448 0.00076138 -0.00012101 0.01208570 0.00000422
Y -0.01412406 0.06066496 -0.00231954 -0.00426321 0.00005425
Z 0.07244887 0.00294580 0.05903910 0.00013700 -0.00365150

2 C X -0.00507137 0.01947225 -0.00112647 -0.01592127 -0.00027630
Y 0.00875837 -0.05960287 0.00260991 0.05076117 0.00026096
Z 0.05986272 0.00274409 0.07789316 -0.00051873 0.09630095

3 C X -0.01876305 -0.01219875 -0.01668959 -0.01400459 0.00092428
Y -0.05064280 0.03924814 -0.05934233 -0.02529359 0.08888158
Z -0.01185434 -0.06701836 -0.02677011 -0.03707921 -0.04845771

4 C X 0.02364695 -0.01061654 0.01777829 -0.01402217 -0.00091740
Y 0.03736910 0.04420925 0.05464204 -0.02559695 -0.08920470
Z -0.02959291 0.06362119 -0.03299819 0.03674080 -0.04834326

5 C X -0.01008623 -0.00199732 -0.01377760 0.00200916 -0.01286461
Y 0.04471488 0.03589166 -0.07257465 -0.07958841 -0.00082555
Z -0.01879284 0.02937539 -0.08774122 -0.06127701 -0.06865007

6 C X 0.01765471 -0.00094822 0.01436074 0.00186919 0.01319912
Y -0.03856472 0.04213258 0.06875222 -0.07995942 0.00077849
Z -0.05550807 -0.03620405 -0.08645248 0.06203800 -0.07000709

7 C X 0.00419653 0.01311181 -0.00585800 0.00148649 0.01373612
Y -0.05590633 -0.05617997 0.10543997 0.09286050 -0.06736073
Z -0.01407619 0.00000804 0.02817737 0.03877872 0.03283881

8 C X -0.01268919 0.01359738 0.00439441 0.00145878 -0.01382476
Y 0.07740877 -0.06548330 -0.09844798 0.09330198 0.06768511
Z 0.01161043 0.00246714 0.02870375 -0.03890114 0.03321552

9 C X 0.02240349 -0.01101462 0.00789405 0.00270305 -0.01429359
Y 0.08571761 -0.04066000 0.00904086 -0.00942077 -0.06402975
Z -0.02807294 0.12349611 -0.00364211 0.08519293 0.03966068

10 C X -0.02130986 -0.01152657 -0.00685764 0.00279272 0.01429385

		Y	-0.08140963	-0.04074562	-0.00533522	-0.00916060	0.06405742
		Z	-0.04922209	-0.12296180	0.00600112	-0.08499695	0.03918892
11	H	X	-0.01789614	-0.05170787	0.02990406	0.04486246	-0.00357232
		Y	0.07505088	-0.03426662	0.07296619	0.05093472	0.11517118
		Z	0.03055184	-0.09669189	0.20822922	0.20316286	0.15235025
12	H	X	0.00591187	-0.05397048	-0.02545947	0.04508871	0.00358371
		Y	-0.15007055	-0.03918938	-0.07305355	0.05183125	-0.11700855
		Z	0.15113820	0.11295115	0.20286358	-0.20482496	0.15439970
13	H	X	-0.02729722	0.01145940	0.06283787	0.04002113	0.00164008
		Y	0.15897707	0.09238487	-0.21380265	-0.19174727	0.20079012
		Z	-0.02799921	-0.01435373	0.04395024	0.05878395	0.02168558
14	H	X	0.02921774	0.00562493	-0.06310180	0.04021113	-0.00161199
		Y	-0.27698598	0.11265630	0.19829689	-0.19207967	-0.20323292
		Z	-0.00728630	0.01823826	0.04287405	-0.05895889	0.02197465
15	H	X	-0.01104899	0.05642299	0.03387926	0.03666840	-0.00426324
		Y	-0.12723340	0.17058276	0.00357839	0.13077291	0.08101438
		Z	0.30672997	-0.20183196	-0.00816573	-0.12658040	-0.18762659
16	H	X	0.02218471	0.05279646	-0.03817847	0.03662754	0.00447072
		Y	0.15620757	0.16831771	-0.01681814	0.13024570	-0.08035825
		Z	0.32149881	0.19763699	-0.02460076	0.12550292	-0.18709307

FREQUENCY: 1603.87 1607.85 3114.41 3116.43 3141.54
REDUCED MASS: 7.36944 7.49145 1.08235 1.08344 1.08032
IR INTENSITY: 1.44687 1.39148 1.33950 2.79691 0.88720

1	C	X	-0.00036934	-0.00003296	-0.00000027	-0.00004568	0.00000058
		Y	0.07111768	0.19579328	0.00000030	-0.00231753	0.00000136
		Z	0.19440235	-0.07191826	0.00119847	0.00000640	-0.00192347
2	C	X	0.00831451	0.02217957	0.00000073	0.00035576	-0.00000022
		Y	-0.03826252	-0.10329723	-0.00000131	0.00178306	0.00000012
		Z	-0.07944655	0.02807148	-0.00255992	-0.00002045	0.00099821
3	C	X	-0.02300211	-0.00404160	0.00025572	-0.00024453	-0.00016936
		Y	-0.04148831	-0.08107241	-0.00168661	0.00196158	-0.00117278
		Z	-0.10031371	0.02491686	-0.00001652	-0.00004906	0.00213037
4	C	X	0.01536079	-0.01815311	-0.00025522	-0.00024471	0.00016890
		Y	-0.02045738	-0.08922076	0.00168580	0.00196345	0.00117119
		Z	-0.09454723	0.04613163	-0.00001778	0.00004826	0.00213213
5	C	X	0.00581410	-0.00020072	0.00771901	-0.00714392	-0.00205563
		Y	0.01820663	-0.00468524	-0.03339692	0.03095884	0.00995170
		Z	0.03920494	-0.00140567	0.01691132	-0.01608868	-0.00420963
6	C	X	-0.00478480	0.00343037	-0.00771337	-0.00715040	0.00205533
		Y	-0.01694785	0.00788179	0.03336969	0.03098459	-0.00994902
		Z	0.03170088	-0.02336310	0.01689965	0.01610417	-0.00420953
7	C	X	-0.00073801	-0.00575011	-0.00808559	0.00863397	-0.00092978
		Y	0.00374165	0.04314172	-0.00208317	0.00264607	-0.00096868
		Z	-0.00372915	-0.00326115	-0.03980471	0.04250501	-0.00491291
8	C	X	-0.00329623	-0.00487352	0.00807822	0.00864137	0.00092878
		Y	0.02545960	0.03553114	0.00208084	0.00264786	0.00096825
		Z	-0.00063495	0.00485991	-0.03976906	-0.04254163	-0.00490762
9	C	X	-0.00278969	0.00512439	0.00073002	-0.00053079	0.01084124

Y -0.01371174 0.02124757 0.00295205 -0.00190434 0.04407114
Z 0.01357094 -0.03178656 0.00189917 -0.00176878 0.02893629
10 C X 0.00551531 0.00220138 -0.00072972 -0.00053162 -0.01084128
Y 0.02455808 0.00760584 -0.00295117 -0.00190799 -0.04407128
Z 0.03180873 0.01550582 0.00189834 0.00177116 0.02893641
11 H X -0.03172122 -0.01497226 -0.08358549 0.07912006 0.02303090
Y -0.06685258 -0.03348902 0.40898988 -0.38168919 -0.10742100
Z -0.10214080 -0.04292842 -0.20478704 0.19249766 0.05294261
12 H X 0.01443956 -0.03175392 0.08351399 0.07918494 -0.02302484
Y 0.02991132 -0.06747885 -0.40864791 -0.38200799 0.10739139
Z -0.05011350 0.09655676 -0.20461501 -0.19265894 0.05292850
13 H X 0.02012656 0.02800083 0.08798792 -0.09468104 0.00876595
Y -0.07361331 -0.10772914 0.02971265 -0.03097756 0.00488896
Z -0.00832212 -0.00552017 0.48185639 -0.50817668 0.05146192
14 H X 0.00259484 0.03450729 -0.08790802 -0.09476169 -0.00875521
Y -0.01344046 -0.12933949 -0.02968635 -0.03100559 -0.00488511
Z -0.00270909 0.00957924 0.48143065 0.50862091 0.05140385
15 H X 0.02889892 -0.01973574 -0.00718615 0.00531658 -0.11940079
Y 0.04484900 -0.03483096 -0.03831524 0.02214000 -0.54688634
Z -0.09778057 0.06714642 -0.02628779 0.01538996 -0.35891167
16 H X -0.03529491 0.00364329 0.00718333 0.00532553 0.11940129
Y -0.05849605 0.00196013 0.03830400 0.02218624 0.54688845
Z -0.12032125 0.01083013 -0.02628003 -0.01542180 -0.35891279

FREQUENCY: 3152.10 3158.27 3183.50

REDUCED MASS: 1.09784 1.09698 1.09295

IR INTENSITY: 18.61256 11.05570 7.66142

1 C X -0.00000011 -0.00063088 0.00068576

Y -0.00000022 -0.00001785 -0.00013686

Z 0.00004673 -0.00002279 0.00002947

2 C X -0.00000128 -0.00154981 -0.00009275

Y 0.00000086 -0.00118320 0.00011093

Z 0.00368535 0.00000638 0.00001926

3 C X 0.00110341 -0.00012624 0.00105332

Y -0.00170604 0.00205801 0.00135205

Z 0.00004972 -0.00102972 -0.00172756

4 C X -0.00110337 -0.00012699 0.00105419

Y 0.00170576 0.00205726 0.00135336

Z 0.00004964 0.00103294 0.00172372

5 C X -0.00758401 0.00854886 -0.00169529

Y 0.03878233 -0.04085001 0.00831210

Z -0.01644620 0.01771231 -0.00376205

6 C X 0.00758481 0.00855002 -0.00169413

Y -0.03878170 -0.04085529 0.00830868

Z -0.01644944 -0.01771538 0.00375864

7 C X -0.00769026 0.00667245 -0.00231499

Y -0.00511623 0.00455638 -0.00102225

Z -0.04114545 0.03674328 -0.01075853

8 C X 0.00768951 0.00667289 -0.00231413

		Y	0.00511590	0.00455709	-0.00102170
		Z	-0.04114039	-0.03674621	0.01075468
9	C	X	-0.00235684	-0.00252022	-0.01066953
		Y	-0.00845656	-0.01150195	-0.04531408
		Z	-0.00560775	-0.00891802	-0.03407842
10	C	X	0.00235794	-0.00252104	-0.01066896
		Y	0.00846144	-0.01150527	-0.04531167
		Z	-0.00561174	0.00891986	0.03407736
11	H	X	0.08408180	-0.09054967	0.02019798
		Y	-0.41961374	0.44571640	-0.09513147
		Z	0.20324505	-0.21869300	0.04610928
12	H	X	-0.08407773	-0.09056286	0.02019335
		Y	0.41959864	0.44577812	-0.09510041
		Z	0.20323811	0.21872439	-0.04609462
13	H	X	0.08194364	-0.07445445	0.02321775
		Y	0.03226148	-0.03052528	0.00767770
		Z	0.45145645	-0.40575553	0.12272342
14	H	X	-0.08193314	-0.07446090	0.02321214
		Y	-0.03225777	-0.03052772	0.00767553
		Z	0.45139372	0.40579134	-0.12269557
15	H	X	0.02230323	0.02771179	0.11621119
		Y	0.10376927	0.13186835	0.53388287
		Z	0.06671169	0.08990141	0.35802369
16	H	X	-0.02231534	0.02772074	0.11620533
		Y	-0.10382470	0.13190568	0.53386038

Z 0.06674924 -0.08992525 -0.35800968

NOTE - THE MODES J,K ARE ORTHONORMALIZED ACCORDING TO
SUM ON I M(I) * (X(I,J)*X(I,K) + Y(I,J)*Y(I,K) + Z(I,J)*Z(I,K)) = DELTA(J,K)

THERMOCHEMISTRY AT T= 298.15 K

USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.

P= 1.01325E+05 PASCAL.

ALL FREQUENCIES ARE SCALED BY 1.00000

THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)

842.94225 842.97066 1626.90142

THE ROTATIONAL SYMMETRY NUMBER IS 1.0

THE ROTATIONAL CONSTANTS ARE (IN GHZ)

2.13904 2.13897 1.10830

THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000)

0.121605 HARTREE/MOLECULE 26689.106984 CM**-1/MOLECULE

76.308063 KCAL/MOL 319.272934 KJ/MOL

	Q	LN Q
ELEC.	1.00000E+00	0.000000
TRANS.	5.56227E+07	17.834102
ROT.	3.84882E+05	12.860691

VIB. 4.92901E+00 1.595137
TOT. 1.05521E+14 32.289931

	E	H	G	CV	CP	S
	KJ/MOL	KJ/MOL	KJ/MOL	J/MOL-K	J/MOL-K	J/MOL-K
ELEC.	0.000	0.000	0.000	0.000	0.000	0.000
TRANS.	3.718	6.197	-44.210	12.472	20.786	169.066
ROT.	3.718	3.718	-31.881	12.472	12.472	119.401
VIB.	328.460	328.460	315.319	89.911	89.911	44.077
TOTAL	335.897	338.376	239.228	114.855	123.169	332.543

	E	H	G	CV	CP	S
	KCAL/MOL	KCAL/MOL	KCAL/MOL	CAL/MOL-K	CAL/MOL-K	CAL/MOL-K
ELEC.	0.000	0.000	0.000	0.000	0.000	0.000
TRANS.	0.889	1.481	-10.566	2.981	4.968	40.408
ROT.	0.889	0.889	-7.620	2.981	2.981	28.537
VIB.	78.504	78.504	75.363	21.489	21.489	10.535
TOTAL	80.281	80.874	57.177	27.451	29.438	79.480

.....END OF NORMAL COORDINATE ANALYSIS.....

Neutral T₁³A₂ Acepentalene

CAS(10/10)/cc-pVDZ

C3v

C	6.0	0.8965275490	0.0000226863	0.0000000000
C	6.0	0.4772442752	1.3444454112	0.0000000000
C	6.0	0.4778570721	-0.6723006434	-1.1644370986
C	6.0	0.4778570721	-0.6723006434	1.1644370986
C	6.0	-0.0178758877	1.5891320106	-1.3744091881
C	6.0	-0.0178758877	1.5891320106	1.3744091881
C	6.0	-0.0173474891	0.3954195568	-2.0637081568
C	6.0	-0.0173474891	0.3954195568	2.0637081568
C	6.0	-0.0176117817	-1.9847730299	-0.6892303842
C	6.0	-0.0176117817	-1.9847730299	0.6892303842
H	1.0	-0.3377165507	2.5384976650	-1.7788051828
H	1.0	-0.3377165507	2.5384976650	1.7788051828
H	1.0	-0.3363981949	0.2708590916	-3.0883235912
H	1.0	-0.3363981949	0.2708590916	3.0883235912
H	1.0	-0.3377930801	-2.8094932209	-1.3092828017
H	1.0	-0.3377930801	-2.8094932209	1.3092828017

FREQUENCY: 248.62 272.42 272.49 462.30
REDUCED MASS: 3.61632 3.89715 3.90970 3.35083
IR INTENSITY: 0.20197 0.00008 0.00138 0.00002

1 C X 0.13818969 0.00256304 0.01332989 -0.00000108
Y 0.00094292 -0.00290115 -0.01369484 0.00004805
Z -0.00013136 0.01382655 -0.00299862 -0.00166860

2 C X 0.06425550 0.02360586 0.11136769 0.00004385
Y -0.00892624 0.00538412 0.02501911 0.00004944
Z -0.00025840 0.00860646 -0.00191011 0.00547133

3 C X 0.08124342 0.07986609 -0.06383727 -0.00094376
Y 0.00191008 -0.01427381 0.00364889 0.00405547
Z 0.00295049 -0.01355154 0.01844755 -0.00356619

4 C X 0.08106626 -0.09930432 -0.02562754 0.00093976
Y 0.00191036 0.01447196 -0.00245607 -0.00402060
Z -0.00349427 -0.01983681 -0.01146753 -0.00360093

5 C X -0.04944444 -0.08380992 0.06259083 0.09371349
Y -0.03504889 -0.03924577 0.03884723 0.03279967
Z 0.04134300 0.04059367 0.02049572 -0.02602109

6 C X -0.04877848 0.10223982 0.02301579 -0.09370163
Y -0.03480286 0.05184228 0.01949733 -0.03283900
Z -0.04169223 0.02897028 -0.03548777 -0.02583849

7 C X -0.03449418 -0.02945232 -0.10633293 -0.09434732
Y -0.02604573 -0.03218298 0.01757024 -0.00575169
Z 0.04242384 0.02826323 0.05813747 0.04001902

8	C	X	-0.03405037	-0.01628511	-0.10904314	0.09429717
		Y	-0.02582097	0.03664966	0.00298085	0.00562732
		Z	-0.04279562	0.00235390	-0.06479928	0.04005966
9	C	X	-0.04788379	0.09855988	0.03320451	0.09442508
		Y	0.05672492	-0.03181153	-0.03687166	-0.04041171
		Z	0.00363085	-0.04518930	0.01034968	-0.01207044
10	C	X	-0.04810574	-0.07626519	0.07047638	-0.09442138
		Y	0.05674167	0.01376547	-0.04657882	0.04046237
		Z	-0.00445313	-0.04548407	0.00882826	-0.01207538
11	H	X	-0.16399031	-0.19010412	0.10933092	0.18510250
		Y	-0.05502189	-0.06494211	0.05566528	0.05176728
		Z	0.08620149	0.06493000	0.02238951	-0.05356183
12	H	X	-0.16266560	0.21887197	0.02231308	-0.18500987
		Y	-0.05463348	0.08224914	0.02438218	-0.05183756
		Z	-0.08636050	0.05064725	-0.04719010	-0.05323967
13	H	X	-0.13339305	-0.08245162	-0.22355768	-0.17863276
		Y	-0.05645985	-0.04304294	0.01716625	-0.01806689
		Z	0.07763215	0.04638813	0.09538651	0.06785425
14	H	X	-0.13249295	-0.01522251	-0.23769711	0.17854404
		Y	-0.05606732	0.04652571	-0.00179300	0.01780430
		Z	-0.07784777	0.00388855	-0.10620588	0.06786898
15	H	X	-0.17108945	0.20113162	0.08611489	0.18684153
		Y	0.10989613	-0.05809195	-0.05584142	-0.07590742
		Z	-0.00463837	-0.06224696	0.00934404	-0.01083426
16	H	X	-0.17151759	-0.14782762	0.16051218	-0.18691205

Y 0.10991415 0.02977986 -0.07456033 0.07600526

Z 0.00370716 -0.06070224 0.01672158 -0.01081427

FREQUENCY: 516.01 517.39 634.29 637.10 685.58

REDUCED MASS: 3.43386 3.42855 5.40293 5.57908 5.96951

IR INTENSITY: 0.12146 0.12434 0.12492 0.12929 0.05322

1 C X 0.00046557 -0.00016609 0.00130982 0.00022058 0.00030034

Y -0.07576579 0.00025451 0.02904081 0.00197261 0.00153005

Z 0.00005623 -0.07551571 -0.00181472 0.02967216 0.01424743

2 C X -0.00889657 0.00003294 0.08497586 0.00424000 -0.01341885

Y -0.05979250 0.00013333 0.13572227 0.00799599 0.00361303

Z -0.00032016 -0.01210259 0.00300046 -0.04723917 -0.05760293

3 C X 0.00467970 0.00745038 -0.03891111 -0.07968046 0.12855324

Y -0.02329136 -0.02048762 -0.00688844 0.07912842 0.03940099

Z -0.01984683 -0.04642671 0.07515437 0.09439018 0.01850611

4 C X 0.00446405 -0.00734766 -0.04694609 0.07476970 -0.11671450

Y -0.02375214 0.02096320 0.00236327 -0.07941993 -0.04530508

Z 0.02028149 -0.04715657 -0.08545523 0.08486516 0.00969041

5 C X -0.03306111 -0.03382128 -0.04843792 -0.07292457 -0.00542423

Y 0.03386353 0.04795014 -0.00122766 0.02236894 0.06698383

Z 0.10897098 0.01917002 0.00702432 -0.04272762 -0.06043317

6 C X -0.03260656 0.03409860 -0.05649005 0.06745985 0.01126946

Y 0.03286173 -0.04834239 0.00189890 -0.02237471 -0.05583465

Z -0.10864480 0.01970458 -0.00194678 -0.04304824 -0.06011135

7	C	X	0.04482380	0.01495136	0.08702880	0.01673350	-0.03183462
		Y	0.09043588	0.07442100	-0.02272517	0.01556220	0.03360135
		Z	0.01657620	-0.03869768	0.03674823	-0.02047403	0.01822536
8	C	X	0.04478604	-0.01520252	0.08819759	-0.00692810	0.03079378
		Y	0.08932364	-0.07524932	-0.02032605	-0.01857758	-0.03538204
		Z	-0.01633948	-0.03907572	-0.03432241	-0.02508352	-0.00121025
9	C	X	-0.01186001	0.04225254	-0.04049513	0.07988004	-0.02190375
		Y	-0.04383695	-0.06069783	-0.04444302	0.01728823	0.06829325
		Z	-0.00264000	0.09919643	0.00361461	-0.00006696	0.05781232
10	C	X	-0.01264414	-0.04219546	-0.03127204	-0.08391122	0.01806940
		Y	-0.04367887	0.06120678	-0.04189752	-0.02210963	-0.07748592
		Z	0.00349475	0.09909653	-0.00395570	-0.00052933	0.05647522
11	H	X	-0.12597703	-0.00088037	-0.13869886	0.03455167	-0.08790874
		Y	0.05144342	0.06876792	-0.05898633	0.04413364	0.05199916
		Z	0.22437283	0.03804504	-0.05856990	-0.07770009	-0.03326802
12	H	X	-0.12587945	0.00166036	-0.13479340	-0.04841836	0.10610344
		Y	0.05012215	-0.06938715	-0.05304873	-0.05071070	-0.04389790
		Z	-0.22357890	0.03942402	0.06661858	-0.06909636	-0.01632600
13	H	X	0.05908247	0.11208994	0.02351910	0.14040160	-0.11846156
		Y	0.17059638	0.15589164	-0.07599085	-0.05605643	-0.05103051
		Z	0.00336296	-0.08044446	0.06409018	-0.04992474	0.05477414
14	H	X	0.05811898	-0.11256012	0.03856959	-0.13672914	0.12793781
		Y	0.16926349	-0.15764078	-0.08165807	0.04624608	0.04537487
		Z	-0.00343812	-0.08104295	-0.05835254	-0.05741038	0.03786147
15	H	X	0.07087138	0.10591057	0.10716883	0.10077983	-0.04191713

Y -0.08691447 -0.14323178 -0.06990499 0.06309352 0.11360344
Z 0.01111006 0.17808936 -0.03724112 -0.07110384 0.00546448
16 H X 0.06937250 -0.10665195 0.11793523 -0.08875749 0.01909896
Y -0.08646785 0.14435359 -0.06196762 -0.06998764 -0.11066021
Z -0.01022995 0.17832900 0.04481495 -0.06622470 0.01057930

FREQUENCY: 687.54 729.66 733.89 743.82 763.30
REDUCED MASS: 5.90727 1.40927 1.37750 2.12207 2.48551
IR INTENSITY: 0.05670 0.01444 0.00013 0.98910 1.47606

1 C X -0.00057387 0.00520904 0.00012509 0.13069696 -0.04268865
Y -0.01272127 -0.00838614 0.00003462 0.00134757 0.00058264
Z 0.00129602 0.00000447 0.00968538 -0.00001482 0.00003846
2 C X 0.14355021 -0.05922500 -0.00000541 -0.05329203 0.08879005
Y -0.03474874 -0.01774547 0.00004395 -0.05671719 0.06339185
Z -0.00533727 -0.00001270 -0.00404615 0.00004136 0.00003603
3 C X -0.05833666 0.03495924 -0.05205172 -0.06027437 0.08446015
Y 0.03797357 -0.00142634 0.00942093 0.02951931 -0.03120642
Z -0.04073987 -0.01217645 0.01253689 0.04759076 -0.05308918
4 C X -0.08060490 0.03489699 0.05192898 -0.05985813 0.08408380
Y 0.02967558 -0.00148320 -0.00942293 0.03003328 -0.03164662
Z 0.04351449 0.01217153 0.01251419 -0.04762357 0.05289970
5 C X -0.03206823 0.04845633 0.04571260 -0.01718924 -0.05707108
Y -0.05759640 0.01080775 0.01778042 -0.02538755 0.00113586
Z -0.00250754 -0.03105249 -0.01409472 0.03389778 -0.01282836

6 C X -0.03002947 0.04848477 -0.04576391 -0.01740972 -0.05679996
Y -0.06899629 0.01076451 -0.01782045 -0.02512374 0.00099940
Z -0.00921125 0.03096317 -0.01409821 -0.03319523 0.01216992

7 C X 0.00578862 0.00681237 0.06627424 -0.01594028 -0.05432077
Y 0.00891933 -0.00701061 0.01895588 -0.01607758 0.01194234
Z -0.10165136 -0.00633242 -0.03191725 0.03466583 -0.00817302

8 C X 0.01165138 0.00684133 -0.06627501 -0.01613003 -0.05398116
Y 0.00246473 -0.00704525 -0.01898770 -0.01587228 0.01174877
Z 0.10258601 0.00626571 -0.03189936 -0.03412273 0.00743222

9 C X 0.01946135 -0.06922261 0.02154843 -0.01174319 -0.04945194
Y 0.05835116 0.03532711 -0.01694655 0.04031198 -0.01617815
Z -0.00168866 0.00510411 0.00856658 0.00335962 0.00578580

10 C X 0.02269322 -0.06923311 -0.02157309 -0.01159151 -0.04955542
Y 0.04475188 0.03527223 0.01694608 0.04081417 -0.01658419
Z 0.01246084 -0.00503880 0.00857027 -0.00386633 -0.00528369

11 H X -0.10304838 -0.16583839 -0.40815194 0.27010115 0.21361003
Y -0.04391189 -0.03512066 -0.06737375 0.04365282 0.04700249
Z 0.08418780 0.03242437 0.14742511 -0.02875119 -0.12685556

12 H X -0.08544130 -0.16573371 0.40848736 0.26932963 0.21370018
Y -0.05299194 -0.03515551 0.06738774 0.04383691 0.04676595
Z -0.08966035 -0.03248112 0.14761130 0.02926900 0.12620880

13 H X -0.05919139 -0.22986719 -0.37110365 0.27069927 0.21833959
Y 0.01927299 -0.06696523 -0.06225986 0.00711514 0.09025813
Z -0.08404722 0.07526210 0.11560387 -0.05638777 -0.10590201

14 H X -0.03705848 -0.22974236 0.37141301 0.26967492 0.21885891

Y 0.02847572 -0.06692172 0.06228612 0.00660822 0.09041069
Z 0.09177439 -0.07529241 0.11572971 0.05660604 0.10522564
15 H X 0.12522090 0.46645217 0.03590950 0.24097974 0.16949524
Y -0.00292987 -0.17727144 -0.03093011 -0.03796976 -0.11770526
Z 0.02593474 0.00998718 0.02048444 -0.02152002 0.02437331
16 H X 0.13026696 0.46642973 -0.03562875 0.24117766 0.16922230
Y -0.02391226 -0.17734267 0.03082301 -0.03722187 -0.11815663
Z -0.02448068 -0.00995153 0.02050758 0.02137683 -0.02403216

FREQUENCY: 844.88 872.44 885.13 893.29 895.59
REDUCED MASS: 7.70274 3.69656 1.45981 1.27441 1.26538
IR INTENSITY: 0.26543 0.00018 0.00015 0.00173 0.00254

1 C X 0.18256847 0.00125649 -0.00069950 -0.00010066 -0.00050820
Y -0.00118838 0.00016517 -0.00010006 0.00002187 -0.01506024
Z 0.00033011 0.00184898 0.00489064 0.01576645 -0.00001771
2 C X -0.01733975 0.00006546 -0.00005007 -0.00005093 -0.01450884
Y 0.00893118 0.00043346 -0.00026053 0.00006064 -0.01615357
Z 0.00063627 -0.04743696 0.03341964 -0.00949917 0.00008727
3 C X -0.01625533 -0.00067727 -0.00200174 -0.01143844 0.00764860
Y -0.00559705 -0.03873792 0.03424833 0.01004910 0.00173122
Z -0.00769505 0.02442889 -0.01455579 0.01156605 -0.01043724
4 C X -0.01648937 0.00063742 0.00196750 0.01145053 0.00758934
Y -0.00662521 0.03859130 -0.03419258 -0.01010311 0.00166972
Z 0.00671150 0.02481597 -0.01479380 0.01171520 0.01026041

5	C	X	-0.01745574	-0.05123425	-0.02728688	0.04695112	-0.06311719
		Y	0.04413748	0.07757321	-0.04310508	0.00417247	-0.00570751
		Z	-0.07155358	-0.03495535	0.02477852	-0.01555423	0.02121987
6	C	X	-0.01758647	0.05084707	0.02760753	-0.04729473	-0.06285572
		Y	0.04527513	-0.07721960	0.04296011	-0.00433488	-0.00538778
		Z	0.07129450	-0.03391525	0.02422360	-0.01582788	-0.02091220
7	C	X	-0.01727653	0.05015982	0.02639900	-0.05058288	0.06135434
		Y	0.04036553	0.00897408	0.00077832	-0.00968054	0.01591457
		Z	-0.07406529	0.08226657	-0.05049652	0.00757901	-0.01732421
8	C	X	-0.01621672	-0.05042040	-0.02631913	0.05102527	0.06105260
		Y	0.04020505	-0.00837404	-0.00115480	0.00968968	0.01585024
		Z	0.07142141	0.08376126	-0.05142938	0.00763602	0.01698223
9	C	X	-0.01656556	-0.06482334	-0.04952271	-0.05634601	0.00171421
		Y	-0.08565404	-0.06303779	0.05198142	0.02363051	0.00209058
		Z	-0.00134742	-0.05018422	0.02236954	-0.00526845	0.00048867
10	C	X	-0.01694253	0.06442468	0.04977273	0.05637939	0.00137414
		Y	-0.08675632	0.06160284	-0.05113833	-0.02350929	0.00202681
		Z	0.00251209	-0.05016613	0.02236738	-0.00525960	-0.00032429
11	H	X	-0.05846935	0.04169966	0.26768240	-0.29282359	0.41657297
		Y	0.04272937	0.06627290	0.02686627	-0.05820660	0.09620876
		Z	-0.05445823	-0.13964972	-0.04449354	0.10976425	-0.12168311
12	H	X	-0.05951948	-0.04175775	-0.26834618	0.29558318	0.41391656
		Y	0.04310721	-0.06595656	-0.02714507	0.05861873	0.09585574
		Z	0.05515819	-0.13807055	-0.04562179	0.11060123	0.12126135
13	H	X	-0.06007236	-0.04069002	-0.26606318	0.31463378	-0.40676960

Y 0.02745624 -0.09263077 -0.03224497 0.04384208 -0.07161845
Z -0.06433079 0.12513999 0.04482951 -0.11371787 0.14062986
14 H X -0.05875028 0.03865064 0.26792340 -0.31732557 -0.40406248
Y 0.02617589 0.09339911 0.03184706 -0.04419942 -0.07156012
Z 0.06153453 0.12618336 0.04440476 -0.11469438 -0.14001622
15 H X -0.06509966 0.12632266 0.40985531 0.38279328 -0.01140649
Y -0.06609016 -0.18637690 -0.10786275 -0.13797265 -0.00258712
Z -0.00778116 0.01500537 -0.00304720 -0.01780355 0.01307783
16 H X -0.06672783 -0.12712906 -0.40940296 -0.38278631 -0.00975868
Y -0.06695149 0.18498772 0.10870315 0.13799121 -0.00346908
Z 0.00859561 0.01495984 -0.00299663 -0.01794465 -0.01297220

FREQUENCY: 1081.64 1082.53 1127.83 1164.64 1165.20

REDUCED MASS: 3.37939 3.41539 1.38057 1.25634 1.24200

IR INTENSITY: 0.02184 0.02392 0.09134 0.03891 0.03259

1 C X 0.00202481 -0.00005482 -0.03916446 0.00256487 0.00017919
Y 0.12179629 -0.01432660 0.00161687 -0.05195491 -0.00147122
Z 0.01478355 0.12306900 0.00045111 0.00137642 -0.05108811
2 C X -0.04984221 0.00549898 0.03024487 0.00834567 0.00022082
Y 0.07039244 -0.00755055 -0.04699807 -0.02735215 -0.00082097
Z -0.00143738 -0.00228127 0.00085791 0.00083216 -0.00350967
3 C X 0.02727541 0.03857501 0.03314764 -0.00716013 -0.00858657
Y 0.01572137 0.02872317 0.02441986 -0.01847996 -0.00178398
Z 0.03447760 0.04491960 0.04363928 -0.01069789 -0.02949952

4 C X 0.01740876 -0.04499221 0.03230533 -0.00756203 0.00827981
Y 0.00903630 -0.03289159 0.02293250 -0.01929402 0.00111524
Z -0.02248711 0.05327197 -0.04288351 0.01165271 -0.02915927

5 C X 0.04490231 -0.00801580 -0.01331542 -0.00893141 -0.00036401
Y -0.08288392 0.00195807 0.03950409 -0.01041840 0.04998145
Z 0.06447642 -0.01175970 -0.00399750 -0.02919738 0.02682137

6 C X 0.04519568 -0.00229458 -0.01319130 -0.00881021 -0.00008044
Y -0.08033205 0.01699140 0.03908045 -0.00798445 -0.05092351
Z -0.06433915 0.00291495 0.00355918 0.02732466 0.02857005

7 C X -0.02360754 -0.03730260 -0.01598872 0.00606974 0.00735489
Y 0.00415895 0.01738860 -0.01465226 0.02940892 -0.04846773
Z -0.06280874 -0.07856134 -0.04180840 0.03256005 -0.00873912

8 C X -0.01416691 0.04236828 -0.01539673 0.00643467 -0.00705862
Y -0.00031903 -0.01824463 -0.01440110 0.02693807 0.05040577
Z 0.04246897 -0.09220443 0.04045676 -0.03195805 -0.01058117

9 C X -0.02807009 -0.03311034 -0.01599885 0.00499231 0.00765455
Y -0.05701649 -0.07757153 -0.02932196 0.01068886 0.01617310
Z -0.01477336 -0.03509429 -0.03904139 -0.06112296 0.00930693

10 C X -0.01954000 0.03929228 -0.01530976 0.00538730 -0.00739123
Y -0.03736437 0.08994280 -0.02777438 0.01166085 -0.01568010
Z 0.00606902 -0.03778046 0.03847422 0.06064284 0.01199876

11 H X 0.09039325 0.05933974 0.06081527 -0.06642096 0.07184750
Y -0.04513141 0.10443747 0.18473775 -0.13650188 0.20675319
Z 0.13225490 0.16871925 0.26555981 -0.27709191 0.32776591

12 H X 0.07174066 -0.07944090 0.06057857 -0.06146747 -0.07579056

Y -0.06937274 -0.09344558 0.18259488 -0.12443676 -0.21535254
Z -0.08508445 0.19793134 -0.26254015 0.25683343 0.34443611
13 H X -0.11195644 -0.02440101 0.05674318 -0.04354739 0.09714377
Y 0.23763336 -0.06350696 -0.31881512 0.24590811 -0.46109127
Z -0.06622438 -0.07903133 -0.03239828 0.02418612 0.01162233
14 H X -0.10182008 0.04951980 0.05579984 -0.03913481 -0.10000962
Y 0.24343393 0.00997766 -0.31255034 0.22304576 0.47657624
Z 0.04583385 -0.09330653 0.03117862 -0.02469499 0.01025600
15 H X 0.00345214 -0.11828380 0.06796440 0.09783453 0.01021618
Y 0.00894601 -0.17203222 0.15126960 0.23568038 0.03666099
Z -0.12567458 0.13129995 -0.33130580 -0.41526973 -0.01874817
16 H X 0.03032355 0.11368313 0.07039647 0.09889374 -0.00575110
Y 0.04809661 0.16379258 0.15475399 0.23819064 -0.02569362
Z 0.15144053 0.09401611 0.33411721 0.41712339 0.00031735

FREQUENCY: 1189.27 1291.93 1292.89 1312.22 1381.05

REDUCED MASS: 2.30963 5.14692 5.08545 6.38549 3.18100

IR INTENSITY: 0.00033 0.22396 0.20225 0.05540 0.15146

1 C X -0.00009946 0.00463237 0.00126036 0.05292562 -0.00095737
Y 0.00097644 0.09292147 0.01076507 -0.00804595 0.14541505
Z 0.00295792 -0.00907286 0.09143097 0.00113592 0.06203200
2 C X -0.00050882 0.01104402 0.00010524 -0.04595898 0.03812391
Y 0.00018833 -0.05340475 -0.00339337 0.13153257 -0.08446999
Z 0.12796520 -0.01568315 0.15314701 -0.00459315 -0.02551963

3 C X -0.00008119 -0.01011527 -0.01480142 -0.04502959 -0.03213396
Y 0.10944514 0.10116407 -0.08698861 -0.07136132 -0.06775142
Z -0.06237120 -0.10206556 -0.02217187 -0.10350661 -0.04293018

4 C X 0.00022692 -0.01253540 0.01054904 -0.04346755 -0.00411352
Y -0.10938353 0.08162825 0.10205331 -0.07471110 -0.05854697
Z -0.06316796 0.10348877 0.00259488 0.09850071 -0.02374169

5 C X -0.00323301 0.00913546 -0.02401116 0.01127272 -0.03214778
Y 0.00265515 -0.02665542 0.06929790 0.03091855 0.02596514
Z -0.02265480 0.01385705 -0.03065986 0.04632062 -0.06165315

6 C X 0.00387876 0.00403303 0.02589580 0.01077218 -0.01948247
Y -0.00388662 -0.01220011 -0.07231998 0.03315700 0.02081092
Z -0.02361366 -0.00706987 -0.03477058 -0.04506510 0.04278239

7 C X 0.00334137 0.02169325 -0.01518476 0.01058912 0.03187843
Y -0.01208780 -0.00004320 -0.00967277 -0.05562206 -0.03997987
Z 0.01756570 0.06229024 -0.05295901 -0.00598564 0.05058907

8 C X -0.00331916 0.01802356 0.02005660 0.00905879 0.01882909
Y 0.01201790 -0.00167246 0.00681838 -0.05524280 -0.02109245
Z 0.01760828 -0.05007984 -0.06481626 0.01016707 -0.02256909

9 C X -0.00309815 -0.02413894 0.00495261 0.01435897 0.01237581
Y -0.02187298 -0.06409986 0.01116714 0.03207078 0.03463304
Z 0.00530285 -0.05389974 0.00281214 -0.04471787 -0.00006902

10 C X 0.00302812 -0.02280169 -0.00921142 0.01320293 -0.01266279
Y 0.02179341 -0.06081127 -0.02253420 0.03025777 -0.01619793
Z 0.00425900 0.05211397 0.01531548 0.04504057 -0.00571593

11 H X -0.09102837 -0.01829384 -0.05354706 0.02657982 0.02949330

Y -0.11520793 -0.07771911 0.02339643 0.06725581 0.17632537
Z -0.23521018 -0.06543164 -0.15035047 0.10964216 0.23125369
12 H X 0.09239831 -0.02890172 0.05087928 0.02350043 -0.00079022
Y 0.11468964 -0.07155058 -0.03429818 0.06671772 0.10745697
Z -0.23762974 0.09483564 -0.14231266 -0.10222340 -0.13282795
13 H X 0.08128180 0.05995045 0.00212564 0.01962391 -0.03467928
Y -0.20312182 -0.15976233 -0.06180805 -0.10319091 0.28129088
Z 0.01965552 0.08082535 -0.06408599 -0.00688492 0.03554392
14 H X -0.08284281 0.05884727 0.00994103 0.01757662 -0.03923146
Y 0.20874253 -0.16845760 0.02854771 -0.10493387 0.17027139
Z 0.01989089 -0.06599689 -0.07920720 0.01141122 -0.01686528
15 H X -0.08906165 -0.03726437 0.04735949 0.02426298 0.01013323
Y -0.13551755 -0.11069285 0.09428407 0.05583763 -0.03667257
Z 0.19778831 -0.00908511 -0.13011421 -0.08511785 0.10269488
16 H X 0.08774764 -0.02684409 -0.05278065 0.02639017 0.03440480
Y 0.13249360 -0.08915693 -0.11264909 0.06119520 0.04634473
Z 0.19208174 0.03584667 -0.12247292 0.09675356 0.09926743

FREQUENCY: 1381.44 1460.53 1478.96 1479.78 1562.95

REDUCED MASS: 3.25404 1.98819 2.45161 2.45290 3.74514

IR INTENSITY: 0.15861 0.00073 0.79628 0.80904 0.02074

1 C X -0.00095721 0.00004725 -0.00027667 -0.00036058 -0.00769190
Y -0.06187075 -0.00073882 0.10792792 -0.05235502 0.00650657
Z 0.14699570 -0.00422493 0.05091645 0.10695043 0.00024729

2 C X -0.01515203 -0.00031422 0.01616383 -0.00736663 0.01238848
Y 0.03315229 0.00060043 -0.05774861 0.02708717 -0.03242316
Z -0.05665328 0.06657016 -0.03959504 -0.08309748 -0.00002959

3 C X -0.02415659 0.00068915 -0.01427364 -0.00927526 0.01711350
Y 0.01616196 0.05575190 -0.07009396 0.04987152 -0.00225131
Z -0.07142222 -0.02990680 -0.01940629 -0.06816595 0.05421303

4 C X 0.04149854 -0.00062640 -0.00154599 0.01751078 0.01721224
Y 0.03994856 -0.05479725 -0.08295493 0.02493581 -0.00200170
Z -0.08446806 -0.02960683 -0.04189961 -0.05883460 -0.05440624

5 C X -0.00419309 -0.02142848 0.01468595 0.00366138 -0.00256203
Y -0.00332206 -0.00185844 0.01387715 -0.03048844 0.04958945
Z -0.00048077 -0.07096283 0.07137274 0.00075596 0.03444092

6 C X 0.02579359 0.02157293 0.00615916 -0.01405387 -0.00252115
Y -0.01768123 0.00148808 0.03219536 0.00765649 0.05016471
Z -0.04343940 -0.07098814 -0.04340806 0.05752889 -0.03486908

7 C X 0.00367644 0.02141509 -0.01497045 0.00177349 -0.00812226
Y -0.00759150 -0.06230267 0.06586747 0.02322434 -0.04522661
Z 0.01582203 0.03334387 -0.02726170 0.02377885 -0.03275809

8 C X -0.02594078 -0.02134824 -0.01083865 0.01057889 -0.00808434
Y 0.03655822 0.06181818 0.02364856 -0.06544446 -0.04602539
Z 0.04714510 0.03314747 0.03551054 -0.00681674 0.03302822

9 C X 0.02920474 -0.02155214 -0.00490823 -0.01559372 0.00074226
Y 0.05529491 -0.06021321 -0.01531285 -0.05860579 0.02102803
Z -0.00692640 0.03529502 0.05015528 0.02811044 -0.14822922

10 C X -0.02950660 0.02154367 0.00950466 0.01326505 0.00070317

			Y	-0.06405089	0.06010155	0.03726040	0.04773930	0.02100352
			Z	-0.00673141	0.03577349	-0.00896295	0.05595790	0.14826689
11	H	X	0.02722883	0.03078831	-0.05552536	0.02393764	-0.02413649	
		Y	0.01718835	0.15187555	-0.16887770	-0.02112008	-0.01713659	
		Z	0.02949773	0.23772667	-0.29199965	0.02539640	-0.12632236	
12	H	X	-0.04087636	-0.03011095	-0.05319712	0.02844254	-0.02442686	
		Y	-0.14155846	-0.15130483	-0.08872400	0.14568802	-0.01712557	
		Z	0.19063164	0.23580853	0.20169952	-0.21333074	0.12721014	
13	H	X	0.02124372	-0.03003912	0.04935917	0.03107563	-0.02859326	
		Y	0.03067978	0.27365031	-0.32372216	-0.05379331	0.09432434	
		Z	0.00933077	0.01244573	-0.00465359	0.03105603	-0.05317044	
14	H	X	0.01046636	0.02983503	0.00660160	-0.05787064	-0.02900365	
		Y	-0.22416320	-0.27186142	-0.16011676	0.28728973	0.09561678	
		Z	0.03152466	0.01239971	0.02700218	0.01535364	0.05364908	
15	H	X	-0.03783890	0.02922427	0.05064178	0.03558071	-0.06305119	
		Y	-0.09916703	0.12233042	0.11721713	0.12887203	-0.20442792	
		Z	0.23629748	-0.24016657	-0.14774569	-0.25941184	0.15739519	
16	H	X	0.01849386	-0.02966191	0.00307764	-0.06152316	-0.06316250	
		Y	0.09419486	-0.12294804	-0.03008426	-0.17090747	-0.20458311	
		Z	0.23538479	-0.24039569	-0.11556913	-0.27526476	-0.15756629	

FREQUENCY:	1572.93	1575.98	3341.50	3341.94	3362.38
REDUCED MASS:	4.47539	4.69793	1.08972	1.09062	1.09866
IR INTENSITY:	0.06279	0.06519	0.09608	0.14802	0.38313

1	C	X	0.00359619	0.00008271	-0.00000003	-0.00006915	0.00000001
		Y	0.01113731	0.00012752	0.00000029	-0.00044121	0.00000008
		Z	-0.00032493	-0.00974592	0.00033464	-0.00000201	-0.00045866
2	C	X	-0.01380022	-0.00026844	-0.00000008	0.00050993	0.00000044
		Y	0.03808866	0.00046378	0.00000029	-0.00057914	-0.00000011
		Z	-0.00031173	0.06946157	-0.00132165	-0.00001798	-0.00288618
3	C	X	-0.00387387	-0.00672611	0.00037317	-0.00036965	-0.00042435
		Y	-0.05405820	-0.04076348	-0.00062316	0.00070994	0.00168513
		Z	0.01996073	0.00115441	0.00071994	-0.00079412	-0.00086921
4	C	X	-0.00404196	0.00651420	-0.00037241	-0.00037038	0.00042419
		Y	-0.05463187	0.03990867	0.00062216	0.00071086	-0.00168463
		Z	-0.01971621	0.00133011	0.00071828	0.00079551	-0.00086865
5	C	X	0.00282943	-0.01059112	0.01172303	-0.01128705	0.01158166
		Y	-0.08285338	-0.09140887	-0.03327338	0.03179079	-0.03672398
		Z	-0.05692892	-0.09042383	0.01502691	-0.01457682	0.01303823
6	C	X	0.00268177	0.01081454	-0.01170350	-0.01130641	-0.01157744
		Y	-0.08411894	0.08992248	0.03321763	0.03184411	0.03670898
		Z	0.05811349	-0.08990935	0.01500215	0.01460285	0.01303464
7	C	X	-0.00778052	-0.00449577	-0.01334327	0.01378552	0.00988490
		Y	0.10930456	0.11578547	-0.00452604	0.00488821	0.00650327
		Z	0.03116303	0.04142718	-0.04184982	0.04335812	0.03290017
8	C	X	-0.00785437	0.00440164	0.01331960	0.01380963	-0.00987906
		Y	0.11098636	-0.11395173	0.00451762	0.00489682	-0.00649996
		Z	-0.03174778	0.04088382	-0.04177539	-0.04343402	0.03288096
9	C	X	0.00954148	0.00675591	0.00043626	-0.00027621	-0.00900984

Y 0.02547691 0.01234015 0.00116738 -0.00073529 -0.02283259
Z -0.08233342 -0.00539600 0.00082996 -0.00070769 -0.01662485
10 C X 0.00963225 -0.00661105 -0.00043603 -0.00027702 0.00900814
Y 0.02558488 -0.01207899 -0.00116669 -0.00073746 0.02282832
Z 0.08231899 -0.00511497 0.00082917 0.00070921 -0.01662115
11 H X 0.04792470 0.04464932 -0.13277281 0.12706718 -0.13046869
Y 0.00850036 0.03167774 0.39112813 -0.37354439 0.38580846
Z 0.15668080 0.18667961 -0.16845644 0.16171896 -0.16208984
12 H X 0.04855414 -0.04381654 0.13254892 0.12728134 0.13041317
Y 0.00880000 -0.03205202 -0.39047038 -0.37417557 -0.38564550
Z -0.15903358 0.18435694 -0.16817187 -0.16199154 -0.16202167
13 H X 0.03766752 0.05207371 0.15072509 -0.15529599 -0.11011527
Y -0.17388493 -0.16028342 0.05786679 -0.05926593 -0.04554179
Z 0.06327579 0.07149130 0.48035996 -0.49459037 -0.35180471
14 H X 0.03848173 -0.05132520 -0.15045870 -0.15556970 0.11004865
Y -0.17634072 0.15671857 -0.05776523 -0.05937163 0.04551452
Z -0.06428727 0.07036012 0.47951164 0.49546334 -0.35159309
15 H X -0.03128243 0.00700549 -0.00576863 0.00338701 0.10345002
Y -0.08281949 -0.00540656 -0.01505125 0.00854539 0.26674321
Z 0.07182298 0.02006818 -0.01191048 0.00671968 0.19890618
16 H X -0.03110485 -0.00708869 0.00576518 0.00339749 -0.10343144
Y -0.08266280 0.00548869 0.01504237 0.00857284 -0.26669584
Z -0.07174351 0.02001403 -0.01190337 -0.00674144 0.19886999

FREQUENCY: 3363.12 3363.61 3384.36

REDUCED MASS: 1.10269 1.09164 1.09953

IR INTENSITY: 0.44179 0.66281 0.62280

1 C X -0.00076785 0.00000015 0.00054511
Y 0.00048433 0.00000012 0.00061877
Z -0.00001714 -0.00073899 0.00001627

2 C X -0.00143259 0.00000024 -0.00013597
Y 0.00042446 0.00000004 -0.00001863
Z 0.00000705 -0.00165067 0.00001403

3 C X -0.00049971 -0.00081345 0.00095370
Y 0.00129655 -0.00030229 0.00202084
Z -0.00090907 -0.00033952 -0.00088371

4 C X -0.00050050 0.00081329 0.00095397
Y 0.00129698 0.00030231 0.00202141
Z 0.00091091 -0.00033893 0.00088264

5 C X 0.01392420 0.00652692 -0.00015047
Y -0.04348064 -0.02081649 0.00065721
Z 0.01538033 0.00734388 -0.00017303

6 C X 0.01393072 -0.00652484 -0.00014852
Y -0.04350131 0.02080900 0.00065255
Z -0.01538814 0.00734215 0.00017001

7 C X 0.01118098 0.00648740 -0.00070626
Y 0.00746474 0.00404081 -0.00038071
Z 0.03743782 0.02138382 -0.00183323

8 C X 0.01118614 -0.00648436 -0.00070495

		Y	0.00746856	-0.00403911	-0.00038023
		Z	-0.03745539	0.02137384	0.00182926
9	C	X	-0.00048320	0.01525860	-0.01773269
		Y	-0.00147747	0.03795012	-0.04453495
		Z	-0.00111295	0.02777697	-0.03853924
10	C	X	-0.00048366	-0.01525984	-0.01773246
		Y	-0.00147899	-0.03795322	-0.04453427
		Z	0.00111374	0.02777975	0.03853897
11	H	X	-0.15485285	-0.07385132	0.00293281
		Y	0.45692260	0.21919170	-0.00743739
		Z	-0.19296923	-0.09160018	0.00273316
12	H	X	-0.15492714	0.07382328	0.00291702
		Y	0.45714278	-0.21910943	-0.00739041
		Z	0.19306250	-0.09156586	-0.00271376
13	H	X	-0.12601101	-0.07156894	0.00659914
		Y	-0.05223895	-0.02883579	0.00203257
		Z	-0.40038679	-0.22812174	0.02041805
14	H	X	-0.12607015	0.07153406	0.00658774
		Y	-0.05226296	0.02882150	0.00202785
		Z	0.40057610	-0.22801108	-0.02038263
15	H	X	0.00551768	-0.17140068	0.19891505
		Y	0.01487315	-0.44368860	0.51128500
		Z	0.01208712	-0.32929967	0.38657320
16	H	X	0.00552405	0.17141440	0.19891270
		Y	0.01488918	0.44372362	0.51127863

Z -0.01209904 -0.32932631 -0.38656877

THERMOCHEMISTRY AT T= 298.15 K

USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.

P= 1.01325E+05 PASCAL.

ALL FREQUENCIES ARE SCALED BY 1.00000

THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)

836.48315 836.70017 1574.98015

THE ROTATIONAL SYMMETRY NUMBER IS 1.0

THE ROTATIONAL CONSTANTS ARE (IN GHZ)

2.15556 2.15500 1.14483

THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000)

0.125423 HARTREE/MOLECULE 27527.207847 CM**-1/MOLECULE

78.704316 KCAL/MOL 329.298857 KJ/MOL

	Q	LN Q
ELEC.	3.00000E+00	1.098612
TRANS.	5.56227E+07	17.834102
ROT.	3.75831E+05	12.836895
VIB.	5.27624E+00	1.663214
TOT.	3.30895E+14	33.432824

	E	H	G	CV	CP	S
	KJ/MOL	KJ/MOL	KJ/MOL	J/MOL-K	J/MOL-K	J/MOL-K
ELEC.	0.000	0.000	-2.723	0.000	0.000	9.134
TRANS.	3.718	6.197	-44.210	12.472	20.786	169.066
ROT.	3.718	3.718	-31.822	12.472	12.472	119.203
VIB.	338.452	338.452	325.176	87.293	87.293	44.529
TOTAL	345.889	348.368	246.421	112.237	120.551	341.932

	E	H	G	CV	CP	S
	KCAL/MOL	KCAL/MOL	KCAL/MOL	CAL/MOL-K	CAL/MOL-K	CAL/MOL-K
ELEC.	0.000	0.000	-0.651	0.000	0.000	2.183
TRANS.	0.889	1.481	-10.566	2.981	4.968	40.408
ROT.	0.889	0.889	-7.606	2.981	2.981	28.490
VIB.	80.892	80.892	77.719	20.864	20.864	10.643
TOTAL	82.669	83.262	58.896	26.825	28.812	81.724

.....END OF NORMAL COORDINATE ANALYSIS.....

CPU TIME: STEP = 0.00 , TOTAL = 11886.6 SECONDS (198.1 MIN)
WALL CLOCK TIME: STEP = 0.01 , TOTAL = 11901.7 SECONDS (198.4 MIN)
CPU UTILIZATION: STEP = 0.00%, TOTAL = 99.87%
111640217 WORDS OF DYNAMIC MEMORY USED

Neutral S₂ 2¹A₁ Acepentalene

CAS(10/10)/cc-pVDZ

C3v

C	6.0	0.7615141090	-0.0000735727	0.0000000000
C	6.0	0.4077648153	1.3481440845	0.0000000000
C	6.0	0.4076207339	-0.6741565764	-1.1675879663
C	6.0	0.4076207339	-0.6741565764	1.1675879663
C	6.0	0.0045853953	1.6175776755	-1.3744762956
C	6.0	0.0045853953	1.6175776755	1.3744762956
C	6.0	0.0044325951	0.3815078475	-2.0880978972
C	6.0	0.0044325951	0.3815078475	2.0880978972
C	6.0	0.0045942737	-1.9992580546	-0.7136636127
C	6.0	0.0045942737	-1.9992580546	0.7136636127
H	1.0	-0.3018431791	2.5637909502	-1.7946161071
H	1.0	-0.3018431791	2.5637909502	1.7946161071
H	1.0	-0.3022444277	0.2723439359	-3.1175328945
H	1.0	-0.3022444277	0.2723439359	3.1175328945
H	1.0	-0.3017848534	-2.8362655557	-1.3229680990
H	1.0	-0.3017848534	-2.8362655557	1.3229680990

FREQUENCY: 195.37 305.08 305.25 489.46
REDUCED MASS: 3.85217 4.11470 4.10685 2.87646
IR INTENSITY: 0.27286 0.02874 0.02631 0.00004

1 C X 0.16227193 -0.00323796 0.00057826 0.00000129
 Y -0.00099657 0.01022632 -0.00169605 -0.00001787
 Z -0.00054244 -0.00163021 -0.01118887 0.00072093

2 C X 0.07146589 -0.11496145 0.01869358 -0.00001390
 Y -0.01152564 -0.01202960 0.00192552 -0.00002111
 Z -0.00068110 -0.00066164 -0.00532775 -0.00176480

3 C X 0.07582503 0.03956650 -0.10687529 0.00191816
 Y 0.00352388 0.00123147 0.00708453 -0.00057303
 Z 0.00765054 -0.00585366 0.00828736 0.00085464

4 C X 0.07612832 0.07130346 0.08897225 -0.00192068
 Y 0.00349513 -0.00120527 -0.00706587 0.00055909
 Z -0.00884459 0.00852006 0.00587595 0.00087001

5 C X -0.04564882 -0.03002032 0.11127017 -0.09295004
 Y -0.02872932 -0.01449779 0.04256448 -0.02763561
 Z 0.03574897 -0.02265975 -0.01775220 0.02046466

6 C X -0.04506165 -0.06380474 -0.09602927 0.09295075
 Y -0.02857738 -0.02746554 -0.03576122 0.02765143
 Z -0.03702316 0.01639106 -0.02423849 0.02039686

7 C X -0.04245932 0.11647113 -0.00802950 0.09261516
 Y -0.02119970 -0.01173111 0.02407049 0.00413579

Z 0.03978634 -0.04561871 -0.00807354 -0.03347290

8 C X -0.04169210 0.11284929 -0.02930654 -0.09260414

Y -0.02100595 -0.01906117 -0.01906017 -0.00408860

Z -0.04095388 0.04114406 -0.02232868 -0.03349064

9 C X -0.04422401 -0.07961551 -0.08292037 -0.09356167

Y 0.04394306 0.03559120 0.00861936 0.03325421

Z 0.00377909 0.01275174 0.03396036 0.01211033

10 C X -0.04405081 -0.04930538 0.10383640 0.09356467

Y 0.04390774 0.03095852 -0.01937563 -0.03327250

Z -0.00508458 -0.00107235 0.03620200 0.01211437

11 H X -0.15569799 -0.05326111 0.21526332 -0.20569906

Y -0.04599417 -0.02862447 0.06957722 -0.05144763

Z 0.07803886 -0.03668899 -0.03370544 0.04903146

12 H X -0.15478793 -0.11888770 -0.18742572 0.20566461

Y -0.04578562 -0.04949643 -0.05691263 0.05147723

Z -0.07920456 0.02474481 -0.04390524 0.04890613

13 H X -0.14949526 0.22569879 -0.01248170 0.20376054

Y -0.05037131 -0.01563977 0.04264937 0.01587087

Z 0.07536199 -0.07837287 -0.00857249 -0.06800470

14 H X -0.14818558 0.21766088 -0.05986144 -0.20373428

Y -0.04997329 -0.02879262 -0.03545325 -0.01576856

Z -0.07636504 0.07198648 -0.03323785 -0.06801279

15 H X -0.15857022 -0.15767957 -0.15908002 -0.21204469

Y 0.09110973 0.06129626 0.01933701 0.07295006

Z -0.00454537 0.01556912 0.05763719 0.01564605

16 H X -0.15820769 -0.09928348 0.20068588 0.21206301

Y 0.09102341 0.05189918 -0.03760497 -0.07298236

Z 0.00325461 0.00366167 0.05959718 0.01563897

FREQUENCY: 534.21 535.03 590.63 592.85 712.03

REDUCED MASS: 3.02162 2.98548 5.51061 5.40454 1.23807

IR INTENSITY: 0.01187 0.01130 0.78621 0.76944 0.07375

1 C X -0.00013174 -0.00021791 -0.00023394 0.00021671 0.00484647

Y 0.06562652 -0.00433407 -0.00495547 0.04277914 -0.00381551

Z -0.00433247 -0.06523863 -0.04221986 -0.00549384 -0.00041549

2 C X -0.05424575 0.00319893 -0.01901687 0.16130341 0.01101218

Y 0.05487692 -0.00359078 -0.00748102 0.06452355 -0.00185259

Z 0.00024055 0.00043815 -0.02225583 -0.00230726 0.00067375

3 C X 0.02368523 -0.05003793 0.14852277 -0.06412142 -0.00344877

Y 0.01140537 -0.02471980 -0.02071383 0.02937787 0.00366918

Z 0.02102761 -0.04076947 -0.05384697 0.01116062 -0.00473918

4 C X 0.03022114 0.04720230 -0.12958866 -0.09653843 -0.00370066

Y 0.01478376 0.02311775 0.01346193 0.03415631 0.00489015

Z -0.02638263 -0.03822816 -0.05021270 -0.02461007 0.00368394

5 C X 0.04374825 -0.03028471 0.00818952 -0.04603392 0.01639021

Y -0.01227926 0.04151758 0.04998265 -0.05858860 -0.01200329

Z -0.10133009 0.03229991 -0.01006733 -0.02513526 -0.01921964

6 C X 0.04709318 0.02471575 0.00294100 -0.04676793 0.01623782

Y -0.01675920 -0.03948917 -0.03535296 -0.06801942 -0.01075283

		Z	0.10441547	0.01902550	-0.01567236	0.02193408	0.02023282
7	C	X	-0.04354336	0.03121765	-0.04115673	0.01962175	0.03892829
		Y	-0.08089994	0.06604754	0.04414687	-0.02942409	-0.00118978
		Z	-0.00422134	-0.04485444	0.02338674	-0.05647802	-0.02785781
8	C	X	-0.04719021	-0.02554215	0.03542071	0.02873551	0.03938999
		Y	-0.08795792	-0.05536879	-0.03655625	-0.03851517	-0.00050947
		Z	-0.00197297	-0.04578199	0.00927947	0.05925230	0.02799801
9	C	X	0.00363080	0.05017585	-0.04058214	0.01694375	-0.06362787
		Y	0.03370284	-0.07192209	0.02430712	0.02242497	0.03414058
		Z	0.01483236	0.07953547	0.07630424	0.00118958	-0.00498809
10	C	X	-0.00259477	-0.05037375	0.03564344	0.02608471	-0.06304248
		Y	0.04275779	0.06717551	-0.02859748	0.01692618	0.03499879
		Z	-0.00508643	0.08073765	0.07447404	0.01652490	0.00430672
11	H	X	0.16308304	-0.06830499	0.10461775	-0.09684721	-0.19128475
		Y	-0.02759359	0.05026180	0.07591063	-0.08152081	-0.05591912
		Z	-0.22267484	0.07622469	-0.02359881	-0.04491183	0.03441581
12	H	X	0.17048375	0.04735803	-0.07896340	-0.11849334	-0.19550699
		Y	-0.03286304	-0.04627897	-0.05545705	-0.09626344	-0.05530129
		Z	0.23003264	0.04729505	-0.03294107	0.03783563	-0.03492866
13	H	X	-0.12243544	0.12809362	-0.06700128	0.13421558	-0.26475860
		Y	-0.16654109	0.15461247	0.06994546	-0.03761313	-0.05249230
		Z	0.02734336	-0.08414716	0.02608428	-0.08999983	0.06832687
14	H	X	-0.13750735	-0.11274724	0.03353441	0.14620793	-0.26723746
		Y	-0.18417926	-0.13279733	-0.06010820	-0.05338751	-0.05379726
		Z	-0.03821035	-0.08115801	0.00393478	0.09235262	-0.06928532

15 H X -0.02867063 0.17670128 -0.13591934 -0.05107397 0.49837586
Y 0.05466357 -0.17512310 0.03326969 0.04991574 -0.16178702
Z 0.00307710 0.16075545 0.10777959 -0.00067696 -0.01874166
16 H X -0.05058802 -0.17171507 0.14352730 -0.01832619 0.49973738
Y 0.07670608 0.16705201 -0.04332741 0.04248723 -0.16046497
Z 0.01702418 0.16004468 0.10479859 0.02670442 0.01908996

FREQUENCY: 715.71 734.66 735.25 739.47 755.22

REDUCED MASS: 1.23886 5.66389 6.00934 1.37861 8.52662

IR INTENSITY: 0.05463 0.21641 0.17164 1.94583 0.27193

1 C X -0.00020004 0.01870796 -0.00945648 0.08851897 0.15781764
Y 0.00000910 0.04210266 -0.01216062 -0.00788658 -0.00063957
Z -0.00841965 -0.01237140 -0.04422051 -0.00092343 -0.00063496
2 C X 0.00005473 0.01085751 -0.00124434 -0.01195711 -0.10900272
Y 0.00016988 0.10126038 -0.02684220 -0.04029316 -0.06686626
Z 0.00921803 0.02288504 0.08155865 0.00167012 0.00120008
3 C X -0.00499759 -0.00707485 0.02144562 -0.00583917 -0.10901036
Y -0.00877243 -0.05516121 -0.07511562 0.01495031 0.03193202
Z -0.00507857 0.06893874 -0.08644179 -0.00286880 0.05275359
4 C X 0.00530409 -0.01583753 -0.01029523 -0.00657309 -0.10949475
Y 0.00855408 -0.00887671 0.09090611 0.01851435 0.03487521
Z -0.00525752 -0.10297614 -0.03643403 0.00010256 -0.05469177
5 C X -0.05699660 -0.01841564 0.05820426 -0.03279677 0.03560723
Y -0.02416461 0.01781473 -0.07850563 -0.02590966 -0.00115238

Z 0.02884370 0.02103692 0.06011465 0.01893144 -0.00309208

6 C X 0.05668846 -0.04623878 -0.04052380 -0.03477079 0.03407196

Y 0.02451425 0.05666314 0.06013430 -0.02304648 0.00103311

Z 0.02866275 0.01336979 0.06300570 -0.01634584 0.00534939

7 C X -0.04570374 0.04660130 -0.01044745 -0.05178927 0.03293538

Y -0.02516234 -0.01585621 -0.02233176 -0.00602048 0.00330059

Z 0.01704755 0.10662420 -0.01364776 0.00328939 -0.00527459

8 C X 0.04547067 0.04514472 -0.01468099 -0.05173730 0.03292050

Y 0.02523298 -0.00154941 0.02822535 -0.00505833 0.00395544

Z 0.01644959 -0.09820240 0.04315838 -0.00277946 0.00618643

9 C X 0.01091517 -0.04681184 -0.04047564 -0.03192758 0.03322179

Y -0.01053620 -0.07714718 -0.04587921 0.03460628 -0.00288314

Z -0.02031681 -0.01840433 -0.04107999 0.00617239 0.00094754

10 C X -0.01047255 -0.01895074 0.05951003 -0.02976465 0.03502453

Y 0.00993890 -0.04314563 0.07659575 0.03731335 -0.00050862

Z -0.02034401 -0.00557429 -0.04446839 -0.00793132 -0.00260811

11 H X 0.44698707 -0.00898522 -0.01329038 0.34950100 -0.06217399

Y 0.07377790 -0.02758151 -0.09085701 0.06563657 -0.00950269

Z -0.11948263 -0.08784049 0.08859224 -0.05419121 0.05253490

12 H X -0.44550278 -0.00225476 0.00637131 0.34937440 -0.06235140

Y -0.07315334 0.02397611 0.09190343 0.06925122 -0.00673372

Z -0.11896335 0.12105816 0.02943958 0.05658971 -0.05042920

13 H X 0.39666547 0.08649225 -0.10767762 0.32875743 -0.06497659

Y 0.04322617 -0.02031956 0.08899882 0.04520322 -0.03536487

Z -0.12290197 0.09745154 0.00338310 -0.11629524 0.02923516

14 H X -0.39419450 0.12869519 0.03884604 0.33128801 -0.06387164

Y -0.04277134 -0.06260507 -0.06501516 0.04154636 -0.03859966

Z -0.12265493 -0.08173878 0.05030544 0.11706402 -0.02837431

15 H X -0.05266052 0.07020290 -0.08393803 0.29893288 -0.05820315

Y 0.01241662 -0.08693406 -0.09802370 -0.08200307 0.04300363

Z -0.02000878 -0.06353559 0.05275167 0.00003537 -0.01440542

16 H X 0.04795637 0.09902871 0.01894481 0.30104114 -0.05675365

Y -0.01112795 -0.02334726 0.13168023 -0.07680611 0.04752293

Z -0.02003138 0.08093529 0.01133490 0.00161324 0.01552871

FREQUENCY: 810.71 829.46 830.03 850.04 875.53

REDUCED MASS: 1.38048 1.44709 1.43960 6.61774 5.49895

IR INTENSITY: 0.00005 0.00026 0.00008 0.05914 0.00002

1 C X -0.00011279 -0.00023492 -0.00068277 0.11708962 0.00195283

Y 0.00000292 0.00016996 -0.00782876 -0.00117574 0.00024227

Z -0.00218320 0.00975948 0.00009284 0.00027635 -0.00135370

2 C X 0.00000640 -0.00015663 0.02142282 0.01581994 0.00049824

Y -0.00002782 0.00015851 -0.00529251 0.04465433 0.00129030

Z -0.00236805 -0.01124791 -0.00010422 0.00087029 -0.05704270

3 C X -0.00192791 0.01944608 -0.01092769 0.01643050 0.00013990

Y -0.00577937 0.00577369 0.00435640 -0.02336846 -0.05178125

Z 0.00060690 0.00468273 -0.00448868 -0.03838627 0.02770643

4 C X 0.00191311 -0.01920229 -0.01128304 0.01608548 0.00059473

Y 0.00583472 -0.00589038 0.00414733 -0.02565434 0.05083800

Z 0.00054683 0.00454747 0.00461533 0.03683957 0.02913225

5 C X 0.05954518 0.03748327 -0.07931774 -0.02626593 -0.03311857
Y 0.00783437 0.01106626 -0.01395293 0.05481937 0.09027522
Z -0.01153547 -0.01580789 0.02948988 -0.07477395 -0.04268288

6 C X -0.05950243 -0.03589345 -0.08000974 -0.02699317 0.03216743
Y -0.00795992 -0.01100430 -0.01416532 0.05686772 -0.08874172
Z -0.01166524 -0.01546337 -0.02982587 0.07481991 -0.04015310

7 C X -0.05739947 -0.05579535 0.06988118 -0.02522400 0.03297052
Y -0.00649894 -0.01207715 0.01490746 0.03762504 0.00872989
Z 0.01391938 0.02144818 -0.02191554 -0.08560896 0.09591125

8 C X 0.05742341 0.05451891 0.07094694 -0.02326182 -0.03394016
Y 0.00642462 0.01163392 0.01515016 0.03780951 -0.00753024
Z 0.01380424 0.02080291 0.02225902 0.08075195 0.09923975

9 C X 0.06762045 -0.08324149 0.00906562 -0.02439232 -0.02922062
Y -0.01976457 0.03165024 -0.00313922 -0.09454439 -0.08335310
Z -0.00133684 -0.00433075 0.00078447 -0.00865525 -0.05579875

10 C X -0.06758475 0.08305895 0.01059785 -0.02541622 0.02817557
Y 0.01994632 -0.03135829 -0.00386128 -0.09747082 0.07988775
Z -0.00134914 -0.00430711 -0.00079937 0.01117965 -0.05527840

11 H X -0.30835238 -0.19869592 0.41275201 -0.02498013 -0.05343090
Y -0.06423485 -0.03606686 0.09176213 0.05372198 0.05620012
Z 0.09596346 0.05115367 -0.09205360 -0.09317993 -0.10996840

12 H X 0.30841410 0.19076818 0.41648861 -0.02576046 0.05283701
Y 0.06411116 0.03397458 0.09242315 0.05456522 -0.05500276
Z 0.09581861 0.04936601 0.09299239 0.09581220 -0.10585603

13 H X 0.30074630 0.30228482 -0.35412692 -0.02973556 0.04754907
Y 0.05422094 0.01684638 -0.03928085 0.05535238 -0.06575541
Z -0.09995347 -0.08855841 0.11080325 -0.09278315 0.10180837

14 H X -0.30068857 -0.29547139 -0.35984572 -0.02944506 -0.04914744
Y -0.05431130 -0.01616793 -0.03947904 0.05376532 0.06812911
Z -0.10007074 -0.08667749 -0.11253409 0.08705457 0.10532329

15 H X -0.34948618 0.41794570 -0.05036437 -0.03638439 -0.07475675
Y 0.12606589 -0.13304083 0.01115499 -0.10365061 -0.11598891
Z 0.00824898 -0.03023683 0.01078324 0.00253486 0.01141118

16 H X 0.34960588 -0.41664333 -0.05843734 -0.03915784 0.07395121
Y -0.12588925 0.13298067 0.01349129 -0.10711461 0.11201594
Z 0.00825901 -0.02996893 -0.01142889 -0.00164927 0.01163489

FREQUENCY: 1087.85 1089.96 1100.55 1173.69 1175.47

REDUCED MASS: 2.19756 2.20400 1.38155 2.11358 2.16647

IR INTENSITY: 0.05430 0.05704 0.05694 0.02104 0.02543

1 C X -0.00148638 -0.00010911 0.02527021 0.00016466 -0.00122193
Y -0.07611378 -0.00229180 0.00176297 -0.02119621 0.09774525
Z 0.00150074 -0.07684985 -0.00041312 -0.09810778 -0.02129357

2 C X 0.05006387 0.00167672 -0.01716842 0.00473164 -0.02250878
Y -0.05283072 -0.00186626 0.03691314 -0.01475246 0.06572160
Z 0.00124421 -0.02030735 -0.00063670 0.07239864 0.01519281

3 C X -0.02232811 -0.04268954 -0.01842668 -0.02232951 0.00838581
Y -0.02524798 -0.01395397 -0.02006396 -0.05011169 -0.04904201

		Z	-0.01095900	-0.04171793	-0.02982297	-0.04471884	0.05426435
4	C	X	-0.02437516	0.04217375	-0.01754162	0.01755470	0.01714951
		Y	-0.02578423	0.01351533	-0.01991875	0.06698674	-0.02301133
		Z	0.01284021	-0.04214256	0.02883333	-0.01978020	-0.06830158
5	C	X	-0.03528897	0.00056255	0.00807525	-0.00654704	0.01917619
		Y	0.08847179	-0.03299956	-0.05316330	0.06409280	0.00151159
		Z	-0.04237096	-0.01204740	-0.00918593	0.00629587	0.05190821
6	C	X	-0.03485582	-0.00276345	0.00795728	-0.00173630	0.02005282
		Y	0.08514017	0.03880193	-0.05160000	-0.06074512	-0.02499833
		Z	0.04228448	-0.00950253	0.00898247	0.02771050	-0.04410214
7	C	X	0.01443314	0.03144970	0.00895256	0.01789247	-0.00968512
		Y	-0.02161955	0.01723391	0.03370391	-0.04653738	-0.03399909
		Z	0.02059988	0.09578976	0.04276933	0.01922423	-0.05868247
8	C	X	0.01590985	-0.03115984	0.00837197	-0.01257513	-0.01634994
		Y	-0.01992121	-0.01869281	0.03272817	0.05782262	-0.01159312
		Z	-0.02553917	0.09619195	-0.04061116	-0.00682762	0.06154463
9	C	X	0.01786537	0.02899750	0.00904346	0.01941591	-0.00403460
		Y	0.04623341	0.06598102	0.02187531	0.05147421	0.00122464
		Z	0.05728702	0.02833518	0.05708721	0.00812468	0.06428779
10	C	X	0.01920595	-0.02839380	0.00850937	-0.01623615	-0.01181714
		Y	0.04920241	-0.06451445	0.02075777	-0.04812226	-0.02050828
		Z	-0.05852676	0.02666454	-0.05658186	0.03339653	-0.05521401
11	H	X	-0.05052314	-0.05782188	-0.04238855	-0.02042226	0.05985300
		Y	0.11580151	-0.17671836	-0.18943751	0.08803500	0.14068652
		Z	0.01352890	-0.28167752	-0.26667849	0.05520986	0.33448820

12 H X -0.05237388 0.05594010 -0.04139686 -0.00586748 0.06217112
Y 0.10565397 0.18678438 -0.18429134 -0.14056547 0.09033084
Z -0.00094547 -0.28731843 0.25967351 0.18970814 -0.27819855

13 H X 0.07753614 0.01843315 -0.04299568 0.05577726 -0.02366770
Y -0.29137977 0.20726073 0.33554333 -0.35513939 -0.07720310
Z 0.02970695 0.08767762 0.03094819 0.04033734 -0.05648624

14 H X 0.07739998 -0.01350256 -0.04277343 -0.04234474 -0.04462450
Y -0.27527727 -0.22946848 0.32671977 0.36317028 0.07712327
Z -0.03406935 0.08742604 -0.02917448 0.01360163 0.06836923

15 H X -0.02415345 0.07928102 -0.04549780 0.06245603 -0.01021858
Y -0.10713370 0.12659386 -0.14787558 0.17878823 -0.10279656
Z 0.30034655 -0.07691653 0.32652789 -0.18598013 0.21953923

16 H X -0.02041053 -0.07953122 -0.04690144 -0.05300723 -0.03565752
Y -0.10140818 -0.12905613 -0.14981652 -0.12018576 -0.16865417
Z -0.29673206 -0.08478070 -0.32754260 -0.07808846 -0.27810182

FREQUENCY: 1266.47 1313.13 1316.82 1318.11 1440.02

REDUCED MASS: 1.48865 2.13084 1.95756 7.49533 1.81222

IR INTENSITY: 0.00035 0.50063 0.54389 0.10007 0.10138

1 C X -0.00050902 -0.01662761 0.00385482 0.04675916 -0.00051993
Y 0.00048370 -0.04096630 -0.00414777 -0.01438789 0.03821476
Z -0.00092020 0.00222157 -0.04380626 0.00425472 0.00310308

2 C X 0.00005332 0.02881671 -0.00171954 -0.03525469 0.01717737
Y -0.00092763 -0.04728471 0.00845536 0.10998110 -0.03329769

Z 0.09467630 0.00453943 -0.10578557 0.01121796 0.00292545

3 C X -0.00046982 0.00812387 -0.01695121 -0.04257274 -0.00936548
Y 0.08616707 -0.05585236 0.02889745 -0.08760139 0.01932743
Z -0.04921790 0.07590743 -0.03428730 -0.08334038 -0.03072003

4 C X 0.00126377 0.00656598 0.00933524 -0.04436502 -0.00681121
Y -0.08553716 -0.05180133 -0.05027109 -0.07938363 0.02378080
Z -0.05157938 -0.07178365 -0.02523973 0.08643150 0.02777102

5 C X 0.00263799 -0.01922386 0.00857538 0.00606308 -0.02468864
Y 0.00517770 0.03562286 -0.06922933 0.05416437 -0.00559050
Z 0.00242616 -0.02955322 -0.00672448 0.05675931 -0.09463691

6 C X -0.00258893 -0.01824596 -0.00929840 0.00773709 -0.02201494
Y -0.00621971 0.02851067 0.08197968 0.03890415 -0.01037431
Z 0.00309634 0.03010037 -0.01443572 -0.05413411 0.08813877

7 C X -0.00168594 -0.00523632 0.01849057 0.01054012 0.02568223
Y 0.00921028 -0.00971651 0.02941307 -0.08182992 -0.05875096
Z 0.00876011 -0.03233672 0.06583266 -0.01380415 0.05854073

8 C X 0.00152807 -0.00345768 -0.01683009 0.01377333 0.02337309
Y -0.00839210 -0.00605566 -0.04494965 -0.07458279 -0.04774203
Z 0.00882597 0.02550634 0.07075407 0.00103903 -0.05601443

9 C X 0.00300815 0.00933994 0.01091098 0.01666772 0.00094187
Y -0.00108363 0.02446112 0.01846018 0.04900702 0.00608740
Z -0.00818762 0.09549370 -0.00274794 -0.02870439 -0.04258737

10 C X -0.00320852 0.01040214 -0.00658908 0.01786289 -0.00347259
Y 0.00055376 0.02611100 -0.00639610 0.05029000 -0.00785007
Z -0.00972778 -0.09511846 -0.00647913 0.02990014 0.03640886

11 H X -0.05980396 -0.02763280 0.07822384 -0.01101258 0.04320721
Y -0.14018986 0.02799191 0.10712096 0.01410209 0.21091640
Z -0.28289233 -0.05745469 0.37011308 -0.03757982 0.33167650

12 H X 0.06047197 -0.02041021 -0.08199323 0.00535961 0.04173665
Y 0.14091082 0.03685465 -0.10043701 0.03545400 0.19033536
Z -0.28603129 0.02344552 0.37815131 -0.03797907 -0.30863894

13 H X 0.06260473 -0.05841987 0.05442199 -0.01791874 -0.02747087
Y -0.31684617 0.31155183 -0.16802192 0.09817129 0.34047107
Z 0.02717343 -0.05822610 0.08890194 -0.03121481 0.04054010

14 H X -0.06366880 -0.05173197 -0.06191959 -0.00834945 -0.02209817
Y 0.32233734 0.28709978 0.21029236 0.07090566 0.29870214
Z 0.02743894 0.04851234 0.09904649 0.01405826 -0.04127725

15 H X -0.06369960 0.07744277 -0.01123575 0.03400882 -0.02256428
Y -0.18092247 0.24784964 -0.06257679 0.09703922 -0.06992238
Z 0.27015079 -0.22301598 0.12113280 -0.10065716 0.06702525

16 H X 0.06378279 0.07542483 0.02505149 0.03039006 -0.01651801
Y 0.18176520 0.23887584 0.10351663 0.08117503 -0.04292975
Z 0.27045297 0.20722566 0.15904581 0.07594976 -0.00993180

FREQUENCY: 1442.35 1521.40 1559.24 1577.33 1579.80

REDUCED MASS: 1.84541 2.89241 3.78717 7.82059 7.89896

IR INTENSITY: 0.10146 0.00536 0.00008 0.04271 0.04272

1 C X -0.00004358 0.01732372 -0.00000588 -0.00090188 -0.00000453
Y -0.00261784 0.00323720 0.00129460 0.13755978 0.16037381

Z 0.03761310 0.00189908 0.00741687 0.15940953 -0.13756412

2 C X -0.00144038 -0.01860847 -0.00009354 0.02129861 0.02423399
Y 0.00247528 0.06984590 -0.00061006 -0.08846875 -0.10089186
Z 0.04104714 -0.00003851 0.10363184 -0.00202354 0.00056137

3 C X -0.01420461 -0.01965895 -0.00097508 -0.03082495 0.00597112
Y -0.03169387 -0.03596491 0.08729130 -0.06700627 0.01718728
Z -0.01312932 -0.06598711 -0.05556138 -0.11059909 0.01873883

4 C X 0.01547228 -0.01901903 0.00079692 0.01129762 -0.03002295
Y 0.02808487 -0.03486327 -0.08780310 0.02874040 -0.06343012
Z -0.01765882 0.06357042 -0.05500051 -0.03716983 0.10836648

5 C X -0.01331288 0.00273115 -0.01829503 -0.00698326 0.00639309
Y 0.03414889 -0.06868107 0.00097448 0.01278150 0.02545188
Z -0.02580334 -0.04853361 -0.07342238 -0.00395236 0.03402560

6 C X 0.01720805 0.00293120 0.01867621 0.00710630 -0.00605827
Y -0.03315641 -0.06839695 -0.00057512 0.02417722 0.01590157
Z -0.04070868 0.04790722 -0.07499598 -0.03401095 -0.00010717

7 C X 0.01097662 0.00362505 0.01782771 0.00118934 0.01038457
Y -0.06448738 0.07561695 -0.06024280 0.02781808 -0.03593004
Z 0.00624782 0.03761297 0.03786879 0.01208720 0.00604469

8 C X -0.01488976 0.00367691 -0.01782904 0.01009591 0.00295668
Y 0.07343820 0.07462414 0.06011462 -0.04090938 0.02173277
Z 0.01525530 -0.03726427 0.03807029 -0.00383512 -0.01342433

9 C X 0.02773217 0.00265868 -0.01841770 -0.00171217 -0.01043240
Y 0.08814162 -0.00780258 -0.06607959 -0.00786305 -0.02129617
Z -0.03627329 0.08331200 0.03668237 0.03537790 0.01434719

10 C X -0.02756137 0.00261739 0.01833899 -0.01026223 -0.00338536
Y -0.08811290 -0.00764287 0.06594150 -0.02021945 -0.01158585
Z -0.04303999 -0.08264904 0.03642483 -0.00786201 -0.03820132

11 H X 0.00053051 0.04333363 0.00869639 -0.01633676 -0.02895795
Y 0.09814892 0.04959046 0.11279681 -0.02271290 -0.03946902
Z 0.08941734 0.21167807 0.14006163 -0.07626151 -0.08792477

12 H X -0.00726151 0.04310051 -0.00922264 -0.02686914 -0.01992176
Y -0.13082830 0.04925870 -0.11497381 -0.03567949 -0.02637021
Z 0.14075710 -0.21113644 0.14341029 0.07827510 0.08438532

13 H X -0.03251264 0.04336234 -0.00635581 0.02971285 -0.01348813
Y 0.22177698 -0.20230357 0.16907356 -0.11781933 0.03846398
Z -0.01249547 0.06551594 0.02852270 0.01891997 0.00497819

14 H X 0.03669732 0.04246122 0.00645097 -0.01867771 0.02744088
Y -0.27445234 -0.19908657 -0.17081315 0.06042740 -0.10956050
Z -0.00627718 -0.06494987 0.02867274 -0.00127619 -0.02005412

15 H X -0.03686710 0.04380458 0.00985153 0.03216391 0.00082091
Y -0.16488736 0.15645399 0.06937205 0.06999617 -0.01433444
Z 0.35586030 -0.14927065 -0.17592527 -0.08872743 -0.00026023

16 H X 0.04018136 0.04304995 -0.00970287 -0.00481243 0.03228151
Y 0.17460772 0.15421520 -0.06909921 -0.02696251 0.06867219
Z 0.36275425 0.14621743 -0.17547002 -0.01469591 0.08990576

FREQUENCY: 2058.12 2058.53 3350.48 3350.99 3368.24

REDUCED MASS: 10.66907 10.66776 1.09107 1.09130 1.09893

IR INTENSITY: 0.00319 0.00428 0.21202 0.17136 0.97264

1	C	X	-0.00000618	0.00005322	0.00005998	-0.00000025	-0.00000046
		Y	-0.03723834	0.02091598	0.00053523	-0.00000123	0.00000119
		Z	-0.02002459	-0.03657404	-0.00000797	0.00044210	-0.00091135
2	C	X	-0.00278085	0.00135690	-0.00101665	0.00000259	-0.00000019
		Y	0.03167786	-0.01757919	0.00045193	-0.00000114	-0.00000014
		Z	0.07128851	0.12760714	0.00002128	-0.00215234	-0.00411023
3	C	X	0.00264407	0.00148146	0.00060156	0.00067113	-0.00077093
		Y	0.08058373	-0.10018069	-0.00117679	-0.00116394	0.00158640
		Z	-0.01096322	0.07860584	0.00101142	0.00096370	-0.00093478
4	C	X	0.00011903	-0.00309759	0.00059896	-0.00067317	0.00076997
		Y	0.12757080	-0.01632872	-0.00117203	0.00116914	-0.00158189
		Z	0.07269028	0.03201483	-0.00100555	0.00096728	-0.00093051
5	C	X	-0.00186750	-0.01856138	0.01096280	0.01070177	0.01324399
		Y	-0.00413407	-0.05454039	-0.03195693	-0.03172913	-0.04204146
		Z	-0.01626164	-0.10853615	0.01541305	0.01534549	0.01757141
6	C	X	0.01493170	0.01145028	0.01092220	-0.01074125	-0.01321228
		Y	0.04427606	0.03201493	-0.03183191	0.03184228	0.04193642
		Z	-0.08422221	-0.07108635	-0.01535892	0.01540203	0.01753314
7	C	X	0.00245098	-0.01863815	-0.01324292	-0.01333970	0.01084175
		Y	-0.01976415	0.12190134	-0.00385161	-0.00355604	0.00521484
		Z	0.00481714	-0.00698061	-0.04370510	-0.04375073	0.03701960
8	C	X	0.01717874	0.00766493	-0.01319549	0.01338906	-0.01081106
		Y	-0.11427151	-0.04697506	-0.00384187	0.00357038	-0.00519938
		Z	-0.00847509	0.00046439	0.04355096	-0.04391374	0.03691346

9 C X -0.01520681 0.01104560 0.00000748 -0.00014532 -0.00023736
Y -0.05213584 0.04447145 0.00035854 -0.00006562 -0.00096511
Z 0.08106388 -0.06055717 0.00027889 -0.00028222 -0.00054148

10 C X -0.01736915 0.00718732 0.00000812 0.00014499 0.00023392
Y -0.06517832 0.02116618 0.00035886 0.00006343 0.00095549
Z -0.09403733 0.03734056 -0.00028037 -0.00028137 -0.00053720

11 H X -0.00521258 0.03031531 -0.12190780 -0.12059116 -0.14894754
Y 0.01079038 0.02956295 0.37523884 0.37058928 0.45877824
Z 0.01315030 0.04018636 -0.16969320 -0.16706521 -0.20110435

12 H X -0.02852139 -0.01134417 -0.12144008 0.12102178 0.14857723
Y -0.01977661 -0.02507952 0.37379857 -0.37191467 -0.45763619
Z 0.02735091 0.03224975 0.16904587 -0.16766532 -0.20060249

13 H X 0.00522860 0.03079022 0.14831518 0.14904237 -0.12051609
Y 0.01858830 -0.04990014 0.05132004 0.05175388 -0.04564582
Z 0.00288017 -0.00588449 0.49734847 0.49832654 -0.40314980

14 H X -0.02351153 -0.02056950 0.14778911 -0.14959528 0.12016805
Y 0.05223156 0.01015138 0.05113889 -0.05194556 0.04551403
Z -0.00652434 -0.00059862 -0.49559319 0.50018031 -0.40199091

15 H X 0.02908002 -0.01000515 -0.00097047 0.00076612 0.00403321
Y 0.01343676 -0.01479774 -0.00267913 0.00337768 0.00965185
Z -0.03230888 0.03710526 -0.00213533 0.00174227 0.00765402

16 H X 0.02372150 -0.01956308 -0.00097443 -0.00076052 -0.00399887
Y 0.01966246 -0.00361279 -0.00269414 -0.00336356 -0.00955934
Z 0.04853305 -0.00804642 0.00214408 0.00173119 0.00758491

FREQUENCY: 3369.27 3373.51 3391.00

REDUCED MASS: 1.09936 1.08822 1.09610

IR INTENSITY: 0.48374 0.19643 0.65194

1 C X -0.00061626 0.00000015 0.00046683

Y 0.00061196 0.00000026 0.00071931

Z -0.00000877 -0.00047017 0.00001274

2 C X -0.00134774 0.00000002 -0.00026861

Y 0.00039713 -0.00000001 -0.00018539

Z 0.00002865 -0.00009128 0.00000476

3 C X -0.00027923 -0.00081964 0.00084902

Y 0.00155962 -0.00168049 0.00235489

Z -0.00120235 0.00060019 -0.00108791

4 C X -0.00028152 0.00081952 0.00084926

Y 0.00156429 0.00168020 0.00235557

Z 0.00120720 0.00060057 0.00108665

5 C X 0.01318725 0.00035341 -0.00048545

Y -0.04205840 -0.00085972 0.00214571

Z 0.01676252 0.00058019 -0.00047267

6 C X 0.01322411 -0.00035319 -0.00048449

Y -0.04217132 0.00085892 0.00214354

Z -0.01681507 0.00057994 0.00047087

7 C X 0.01075127 0.00023161 -0.00062410

Y 0.00569644 0.00011612 -0.00081570

Z 0.03730256 0.00029872 -0.00208211

8	C	X	0.01077907	-0.00023147	-0.00062342
		Y	0.00570779	-0.00011598	-0.00081585
		Z	-0.03739659	0.00029821	0.00208023
9	C	X	-0.00090187	0.01703141	-0.01693417
		Y	-0.00253390	0.04549598	-0.04554648
		Z	-0.00114432	0.03154669	-0.03582930
10	C	X	-0.00090217	-0.01703163	-0.01693394
		Y	-0.00253578	-0.04549657	-0.04554588
		Z	0.00114491	0.03154723	0.03582902
11	H	X	-0.14730624	-0.00377437	0.00703520
		Y	0.45426918	0.01088526	-0.02032154
		Z	-0.20010102	-0.00452134	0.00857397
12	H	X	-0.14771184	0.00377141	0.00702774
		Y	0.45551592	-0.01087615	-0.02029876
		Z	0.20064885	-0.00451734	-0.00856432
13	H	X	-0.12163343	-0.00139870	0.00669842
		Y	-0.04633208	-0.00018053	0.00206240
		Z	-0.40458031	-0.00519258	0.02279297
14	H	X	-0.12193908	0.00139685	0.00669328
		Y	-0.04644745	0.00017976	0.00206039
		Z	0.40559959	-0.00518630	-0.02277637
15	H	X	0.00923002	-0.19085026	0.19029257
		Y	0.02551879	-0.52613071	0.51991322
		Z	0.01919376	-0.37772907	0.38063200
16	H	X	0.00923712	0.19085284	0.19029036

Y 0.02553485 0.52613779 0.51990697

Z -0.01920679 -0.37773423 -0.38062782

THERMOCHEMISTRY AT T= 298.15 K

USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.

P= 1.01325E+05 PASCAL.

ALL FREQUENCIES ARE SCALED BY 1.00000

THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)

835.91379 835.96511 1603.71396

THE ROTATIONAL SYMMETRY NUMBER IS 1.0

THE ROTATIONAL CONSTANTS ARE (IN GHZ)

2.15703 2.15689 1.12432

THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000)

0.128530 HARTREE/MOLECULE 28209.165392 CM**-1/MOLECULE

80.654132 KCAL/MOL 337.456889 KJ/MOL

	Q	LN Q
ELEC.	1.00000E+00	0.000000
TRANS.	5.56227E+07	17.834102
ROT.	3.78948E+05	12.845154
VIB.	5.42164E+00	1.690398
TOT.	1.14278E+14	32.369655

	E	H	G	CV	CP	S
	KJ/MOL	KJ/MOL	KJ/MOL	J/MOL-K	J/MOL-K	J/MOL-K
ELEC.	0.000	0.000	0.000	0.000	0.000	0.000
TRANS.	3.718	6.197	-44.210	12.472	20.786	169.066
ROT.	3.718	3.718	-31.842	12.472	12.472	119.271
VIB.	346.611	346.611	333.266	86.988	86.988	44.759
TOTAL	354.048	356.527	257.214	111.931	120.246	333.096

	E	H	G	CV	CP	S
	KCAL/MOL	KCAL/MOL	KCAL/MOL	CAL/MOL-K	CAL/MOL-K	CAL/MOL-K
ELEC.	0.000	0.000	0.000	0.000	0.000	0.000
TRANS.	0.889	1.481	-10.566	2.981	4.968	40.408
ROT.	0.889	0.889	-7.611	2.981	2.981	28.507
VIB.	82.842	82.842	79.653	20.791	20.791	10.698
TOTAL	84.620	85.212	61.476	26.752	28.739	79.612

.....END OF NORMAL COORDINATE ANALYSIS.....

Acepentalene GS minimum 1¹A'

CAS(10/10)/cc-pVDZ

Cs

C	6.0	0.8262180243	0.0188712069	0.0000000000
C	6.0	0.3342899419	1.2731946704	0.0000000000
C	6.0	0.4866882706	-0.7073903596	-1.2079447458
C	6.0	0.4866882706	-0.7073903596	1.2079447458
C	6.0	-0.0762920311	1.5369356912	-1.4235383816
C	6.0	-0.0762920311	1.5369356912	1.4235383816
C	6.0	0.0533913414	0.3784589971	-2.1466882698
C	6.0	0.0533913414	0.3784589971	2.1466882698
C	6.0	0.0502315386	-1.9280260570	-0.7604003098
C	6.0	0.0502315386	-1.9280260570	0.7604003098
H	1.0	-0.3970176144	2.4851291800	-1.8302751771
H	1.0	-0.3970176144	2.4851291800	1.8302751771
H	1.0	-0.1380576737	0.2804883186	-3.2046693469
H	1.0	-0.1380576737	0.2804883186	3.2046693469
H	1.0	-0.4591978145	-2.6920532304	-1.3314779513
H	1.0	-0.4591978145	-2.6920532304	1.3314779513

FREQUENCY: 206.60 291.84 292.01 466.89

REDUCED MASS: 3.83075 3.71830 3.98807 2.84597

IR INTENSITY: 0.19370 0.00097 0.05774 0.01645

1	C	X	0.14322191	0.00574501	0.05456391	0.00003145
		Y	0.00411662	-0.00078144	-0.00768824	-0.00009733
		Z	-0.00029817	0.01117065	-0.00119777	0.01067638
2	C	X	0.02108337	0.01435970	0.13540692	-0.00009922
		Y	-0.03203554	0.00295237	0.02753974	-0.00015224
		Z	-0.00039582	0.00612704	-0.00073880	-0.01008938
3	C	X	0.08907249	0.08933238	-0.02900951	0.04106117
		Y	0.00262683	-0.00243740	0.00193554	0.00470724
		Z	-0.00146306	-0.00670125	0.00961023	0.00051960
4	C	X	0.08927276	-0.09354288	-0.00955718	-0.04112872
		Y	0.00249705	0.00275392	0.00131117	-0.00480371
		Z	0.00069054	-0.00852406	-0.00811790	0.00066605
5	C	X	-0.05903250	-0.09802444	0.03807956	-0.06755407
		Y	-0.04587697	-0.04547085	0.02419618	-0.03381335
		Z	0.02927030	0.03288792	0.03448428	0.00723331
6	C	X	-0.05853818	0.10389618	0.01676061	0.06751860
		Y	-0.04586630	0.04958579	0.01409276	0.03390076
		Z	-0.02992784	0.02505283	-0.04076414	0.00683104
7	C	X	-0.00202409	-0.01383108	-0.12097209	0.07195347
		Y	-0.02389435	-0.02732667	-0.00102038	-0.00500550
		Z	0.01504936	0.01739943	0.05096709	-0.01202234
8	C	X	-0.00142770	-0.01185739	-0.12103662	-0.07187062
		Y	-0.02391546	0.02649896	-0.00675373	0.00532916
		Z	-0.01574116	0.00640289	-0.05361666	-0.01207034

9 C X -0.05974511 0.09521919 0.03111737 -0.10931206
Y 0.06041888 -0.01750789 -0.02108908 0.06697311
Z 0.00979324 -0.04039338 0.00442669 0.00326969

10 C X -0.05960862 -0.08649293 0.05045547 0.10935440
Y 0.06033295 0.01260989 -0.02434420 -0.06710917
Z -0.01072983 -0.04043620 0.00391846 0.00331254

11 H X -0.16119206 -0.23162232 0.02263081 -0.14992606
Y -0.06640617 -0.08201581 0.02828880 -0.05775020
Z 0.06345358 0.05420037 0.05587867 0.01695773

12 H X -0.16038375 0.23144605 -0.02632393 0.14997963
Y -0.06636610 0.08620433 0.01042168 0.05799065
Z -0.06392999 0.04147904 -0.06610162 0.01627389

13 H X -0.05264676 -0.07290550 -0.27305614 0.11788983
Y -0.04235229 -0.04033068 -0.02016920 -0.00863948
Z 0.02615471 0.02951125 0.08070225 -0.01990337

14 H X -0.05163732 0.01408792 -0.28203426 -0.11750994
Y -0.04227579 0.03520917 -0.02815427 0.00938564
Z -0.02677578 0.01203207 -0.08521248 -0.01986126

15 H X -0.18898885 0.16263546 0.01719171 -0.27815750
Y 0.14758361 -0.02830094 -0.01891128 0.16777003
Z 0.00752478 -0.08692875 0.01422953 0.01719346

16 H X -0.18868769 -0.15520431 0.05105671 0.27821448
Y 0.14738798 0.02351427 -0.02454367 -0.16799741
Z -0.00846833 -0.08801896 0.00407320 0.01713490

FREQUENCY: 513.17 544.57 625.30 646.06 696.72

REDUCED MASS: 3.79391 3.07127 3.18064 5.70892 1.89707

IR INTENSITY: 0.19625 0.01357 0.42491 0.36062 0.00389

1 C X 0.01123934 0.00020380 -0.05999684 -0.00016679 0.00036539

Y -0.07597714 0.00013770 0.01067734 -0.00004222 0.00081676

Z 0.00031448 0.04546993 -0.00043165 -0.06443446 0.02603050

2 C X -0.01038014 -0.00016007 0.14636432 -0.00086405 0.00012002

Y -0.08739746 -0.00002779 0.09887797 -0.00030012 0.00109596

Z -0.00021483 -0.00168341 0.00021308 -0.01564651 -0.04131508

3 C X -0.00848587 0.07269739 -0.02896777 0.11806467 -0.01045012

Y -0.02121044 0.02637374 -0.00377817 -0.05222686 0.05203000

Z -0.02744131 0.01890628 0.01659633 -0.07022103 0.03956877

4 C X -0.00872742 -0.07284638 -0.03016325 -0.11734375 0.00967349

Y -0.02162844 -0.02647752 -0.00303653 0.05247779 -0.05207960

Z 0.02806170 0.01925209 -0.01743967 -0.07106868 0.03760937

5 C X -0.02822128 0.07686861 -0.05200668 0.02387516 0.00941476

Y 0.02611950 -0.00703756 -0.02040431 0.04695351 0.05606538

Z 0.11156319 -0.02487594 0.01201552 0.01431393 -0.05606248

6 C X -0.02836480 -0.07674204 -0.05258476 -0.02320680 -0.01040635

Y 0.02534037 0.00707957 -0.02035748 -0.04680313 -0.05622145

Z -0.11112988 -0.02454516 -0.01164177 0.01397683 -0.05687415

7 C X 0.02737307 -0.07451576 0.08938261 -0.03906385 0.04264168

Y 0.09420243 -0.05823990 0.00468109 0.03963202 0.04657027

Z 0.02024980 0.04363181 -0.00747693 -0.00334829 -0.03143911

8 C X 0.02770145 0.07429507 0.08976283 0.03839749 -0.04197866
Y 0.09360297 0.05821249 0.00480923 -0.04013743 -0.04750981
Z -0.01950489 0.04400133 0.00760318 -0.00466666 -0.03379656

9 C X 0.00582827 -0.00997816 -0.02642278 0.00124390 0.01719371
Y -0.03453331 0.05179129 -0.01701236 -0.00003654 0.03857174
Z -0.01461982 -0.05454014 -0.00798694 0.08736519 0.05024052

10 C X 0.00520984 0.01008852 -0.02621003 -0.00121006 -0.01745997
Y -0.03464880 -0.05185740 -0.01693562 0.00042229 -0.03928613
Z 0.01495421 -0.05454503 0.00844608 0.08711614 0.04983005

11 H X -0.05107106 0.05561819 -0.29115137 -0.01090133 -0.32039649
Y 0.06209676 -0.02106106 -0.09415206 0.04682095 -0.01421345
Z 0.21384387 -0.03799794 0.02848879 0.03814996 0.03929904

12 H X -0.05131697 -0.05478622 -0.29157133 0.01383028 0.32435532
Y 0.06112433 0.02128607 -0.09401346 -0.04626755 0.01435780
Z -0.21300835 -0.03749147 -0.02822228 0.03854790 0.04167405

13 H X 0.07670872 -0.20148284 -0.09579277 -0.05274608 -0.33237658
Y 0.19344155 -0.13836583 -0.04557514 0.11964447 -0.10535080
Z 0.00328098 0.07441946 0.03156801 -0.01044253 0.05034570

14 H X 0.07721354 0.20174394 -0.09510777 0.05380564 0.33887974
Y 0.19299344 0.13856569 -0.04632793 -0.12032342 0.10472411
Z -0.00247241 0.07492554 -0.03148258 -0.01152531 0.04900502

15 H X 0.01097453 -0.13970274 0.10515634 -0.08206073 0.09971049
Y -0.05476460 0.17582621 -0.08177472 0.00722442 0.00931227
Z 0.00599080 -0.10714446 -0.03738338 0.14909534 0.01641778

16 H X 0.00994364 0.13952721 0.10663857 0.08139314 -0.09970907

Y -0.05492375 -0.17588069 -0.08206044 -0.00602985 -0.00928820

Z -0.00608788 -0.10737068 0.03846125 0.14925803 0.01714807

FREQUENCY: 700.38 719.75 739.28 768.64 810.02

REDUCED MASS: 2.43556 2.52563 3.43695 2.87626 1.71189

IR INTENSITY: 0.68765 0.09520 0.32080 1.53222 0.30565

1 C X 0.04506436 0.00053962 0.06077534 0.09787404 0.12489880

Y 0.04548319 -0.00028577 -0.01710244 0.01858798 0.00869616

Z -0.00003224 -0.03171711 0.00007140 -0.00001889 0.00004587

2 C X 0.01298160 0.00055917 0.10298677 -0.07426108 -0.01930346

Y 0.06246740 -0.00021997 -0.00366004 -0.03964119 -0.05226121

Z 0.00022906 0.05943618 -0.00024450 0.00001824 0.00002060

3 C X -0.02873295 -0.02140386 -0.07068900 -0.09774883 -0.05112907

Y -0.00252332 -0.05862612 0.02486456 0.02703158 0.03116198

Z 0.07830708 -0.04499557 -0.04167793 0.05331497 0.01886901

4 C X -0.02863068 0.02092215 -0.07153051 -0.09773722 -0.05127336

Y -0.00202529 0.05870976 0.02449609 0.02724535 0.03135937

Z -0.07831837 -0.04500706 0.04130526 -0.05344013 -0.01913471

5 C X -0.05379468 0.07109850 -0.05043427 0.02924374 -0.00527383

Y 0.00169014 -0.04685469 -0.04746931 0.01126589 -0.01954525

Z 0.03558263 0.05488266 -0.01602981 -0.01110727 -0.00157371

6 C X -0.05304215 -0.07224480 -0.04968830 0.02912444 -0.00533780

Y 0.00277812 0.04686030 -0.04820239 0.01134969 -0.01947843

Z -0.03451219 0.05485189 0.01493114 0.01129710 0.00162612

7	C	X	0.01141600	0.05062484	-0.02417078	0.05916462	0.00825853
		Y	-0.02665000	-0.01874622	0.00781096	0.00141104	-0.00058250
		Z	0.09746904	-0.00110920	-0.09606546	0.00692850	-0.02352674
8	C	X	0.01248932	-0.05117609	-0.02326666	0.05911162	0.00839354
		Y	-0.02551777	0.01909136	0.00718693	0.00143506	-0.00064239
		Z	-0.09628282	-0.00089705	0.09499655	-0.00685200	0.02332386
9	C	X	-0.00349298	-0.04562241	0.04797646	0.04682783	-0.04679560
		Y	-0.03377113	-0.04836213	0.01092727	-0.02908940	0.03383436
		Z	0.01301414	-0.03789940	-0.01619391	-0.01466044	0.03167800
10	C	X	-0.00346642	0.04610476	0.04759034	0.04694629	-0.04655178
		Y	-0.03323391	0.04805894	0.01030799	-0.02889152	0.03390229
		Z	-0.01433227	-0.03773875	0.01736573	0.01452528	-0.03166198
11	H	X	0.22611929	-0.19859343	0.12454351	-0.17260465	0.08722770
		Y	0.04341476	-0.11574612	0.01487957	-0.03611420	0.02012746
		Z	-0.08791337	0.11210579	-0.01355255	0.04106607	0.01819410
12	H	X	0.21724992	0.20226742	0.12337273	-0.17246531	0.08725114
		Y	0.04242835	0.11725617	0.01349358	-0.03597026	0.02015280
		Z	0.08626414	0.11244354	0.01231452	-0.04079542	-0.01798075
13	H	X	0.34573335	-0.29376052	0.19731692	-0.18226042	-0.04742406
		Y	0.01051007	-0.01371656	0.08303647	-0.10342367	-0.03136307
		Z	0.03583759	0.06182129	-0.14667176	0.06203678	-0.01092776
14	H	X	0.33579475	0.29927920	0.19526866	-0.18203469	-0.04741019
		Y	0.00870048	0.01547089	0.08192897	-0.10362815	-0.03188987
		Z	-0.03689212	0.06329863	0.14495398	-0.06192777	0.01064647
15	H	X	-0.03917034	-0.01676422	-0.14456824	-0.21705683	0.44951503

Y 0.02071621 -0.10769507 0.08502595 0.12895268 -0.24239004
Z -0.02524460 0.01615905 0.05374529 0.00807291 -0.03562967
16 H X -0.03718679 0.01450135 -0.14513044 -0.21687410 0.44895065
Y 0.01991447 0.10881358 0.08457319 0.12926893 -0.24163540
Z 0.02387554 0.01580317 -0.05252372 -0.00799400 0.03584774

FREQUENCY: 826.16 851.05 875.15 879.53 882.85
REDUCED MASS: 1.59947 6.82677 2.30130 1.26331 1.76355
IR INTENSITY: 0.00049 0.15562 0.05143 0.00652 0.01604

1 C X -0.00041710 0.11020689 0.00095769 -0.02877582 -0.00060288
Y -0.00009457 0.01910121 0.00022741 -0.01075740 -0.00027655
Z -0.00805789 0.00023555 -0.00588704 -0.00000810 -0.00679493
2 C X 0.00009084 -0.00228889 0.00005145 0.00213227 -0.00000543
Y -0.00019952 0.04148756 0.00052093 -0.00650331 -0.00045624
Z -0.01582404 0.00063586 -0.03628255 0.00002869 0.03708734
3 C X -0.03191756 0.03434746 0.02647228 0.01346053 -0.00682666
Y -0.01454623 -0.05896268 -0.04444768 -0.00174921 0.03270809
Z 0.01474293 -0.01285124 0.01241974 -0.00649699 -0.02055266
4 C X 0.03141187 0.03467961 -0.02588221 0.01362695 0.00661171
Y 0.01525659 -0.05956813 0.04343998 -0.00195212 -0.03211238
Z 0.01468607 0.01198037 0.01282379 0.00655310 -0.02084814
5 C X -0.00311843 -0.03875991 -0.06895437 -0.06494984 -0.03053674
Y 0.02447408 0.07628096 0.05965684 -0.01553666 -0.06726678
Z -0.00699022 -0.07411947 -0.02583943 0.01821591 0.03984403

6	C	X	0.00344363	-0.03924828	0.06790309	-0.06549958	0.03058134
		Y	-0.02543419	0.07726669	-0.05867023	-0.01540279	0.06674407
		Z	-0.00767558	0.07389132	-0.02463683	-0.01815712	0.03913552
7	C	X	0.02165931	-0.00765926	0.05373030	0.05625670	0.03080346
		Y	0.01063202	0.04392751	0.01554795	0.01776201	0.00726739
		Z	0.01303552	-0.03635522	0.07146162	-0.00591964	-0.06955300
8	C	X	-0.02163894	-0.00672206	-0.05360753	0.05665901	-0.03047360
		Y	-0.01107963	0.04362823	-0.01472274	0.01792441	-0.00753691
		Z	0.01302985	0.03345544	0.07254124	0.00584264	-0.07019217
9	C	X	0.09076309	-0.03317394	-0.04423964	0.00993120	0.04288592
		Y	-0.07219327	-0.09727840	-0.04388411	0.00345293	0.03679301
		Z	-0.01683696	-0.00804235	-0.03489788	-0.00074999	0.03546013
10	C	X	-0.09042686	-0.03516090	0.04372100	0.00982949	-0.04253672
		Y	0.07326394	-0.09736088	0.04220284	0.00324862	-0.03582669
		Z	-0.01693646	0.00912182	-0.03472326	0.00083044	0.03538856
11	H	X	-0.08469824	-0.02878313	0.24263272	0.43578999	0.37890612
		Y	0.00131013	0.06809704	0.10782898	0.10563603	0.04897744
		Z	0.00266365	-0.11581164	-0.16529847	-0.09742429	-0.01236049
12	H	X	0.08542398	-0.02709361	-0.24027469	0.43863515	-0.37711600
		Y	-0.00203690	0.06898376	-0.10628946	0.10650632	-0.04883690
		Z	0.00161405	0.11743908	-0.16240762	0.09849327	-0.01337114
13	H	X	-0.00742706	-0.04110655	-0.23051514	-0.39216312	-0.31942991
		Y	-0.01104337	0.04625117	-0.11119049	-0.08142075	-0.01129942
		Z	0.02070790	-0.03597079	0.13666961	0.08535138	-0.00568469
14	H	X	0.00773066	-0.04205020	0.22729242	-0.39478035	0.31854512

Y 0.01065340 0.04379754 0.11179172 -0.08201393 0.01017943
Z 0.02071270 0.03240468 0.13722259 -0.08604515 -0.00668556
15 H X -0.47796144 -0.04028963 0.02094849 -0.06292820 -0.05986676
Y 0.22997897 -0.09148062 -0.10526426 0.03869631 0.11196710
Z 0.07979451 -0.01551473 -0.01057913 0.01627925 0.02541945
16 H X 0.47880344 -0.03388680 -0.02208779 -0.06326507 0.06022208
Y -0.22928180 -0.09596109 0.10382200 0.03844083 -0.11089837
Z 0.07958455 0.01808605 -0.01051744 -0.01647028 0.02542539

FREQUENCY: 973.21 1067.79 1089.37 1139.62 1164.19
REDUCED MASS: 2.23841 3.17509 4.36103 2.07082 1.16509
IR INTENSITY: 0.03472 0.04029 0.08209 0.04159 0.02698

1 C X 0.00719119 0.02576354 -0.00074197 -0.03672708 0.00023441
Y 0.00066785 0.12517841 -0.00284847 0.03361711 -0.00030725
Z -0.00015708 0.00346841 0.13220066 0.00049553 -0.04264159
2 C X -0.00572851 -0.06655724 0.00143566 0.00915353 0.00001940
Y -0.00846145 0.10474898 -0.00236590 -0.00103781 -0.00005216
Z 0.00002533 -0.00129430 -0.00780737 -0.00018232 -0.01688900
3 C X 0.01196807 0.00136364 0.04603304 0.03585039 -0.00196413
Y 0.02534486 -0.02107390 -0.02364061 0.00652965 0.00379661
Z 0.00635826 -0.00998575 0.06765616 0.09738775 -0.01739026
4 C X 0.01204581 -0.00062303 -0.04679656 0.03521106 0.00183004
Y 0.02523870 -0.01973319 0.02434358 0.00672529 -0.00375775
Z -0.00633728 0.01286630 0.06937517 -0.09610700 -0.01722393

5 C X 0.00186027 0.04584075 -0.00714389 0.00119318 -0.00410313
Y -0.01083607 -0.07516684 -0.00350640 0.00858758 0.04065576
Z 0.00231208 0.06601321 -0.01000371 0.01972694 0.03173433

6 C X 0.00184993 0.04572740 0.00506900 0.00125518 0.00408614
Y -0.01088355 -0.07400465 0.00716260 0.00838333 -0.04096046
Z -0.00232824 -0.06531245 -0.00726569 -0.01951992 0.03218194

7 C X -0.01109192 -0.00543418 -0.03599191 -0.01915690 0.00751302
Y -0.00670803 -0.00081050 0.03299469 -0.00258328 -0.03967901
Z -0.00134120 -0.03776404 -0.09319381 -0.08695270 -0.02000700

8 C X -0.01116724 -0.00372709 0.03682271 -0.01876833 -0.00753384
Y -0.00661003 -0.00265961 -0.03358989 -0.00266147 0.04008402
Z 0.00155444 0.03333217 -0.09661701 0.08559948 -0.02043393

9 C X -0.01708148 -0.01384422 -0.03815237 -0.00911654 0.00093293
Y -0.01059128 -0.03602745 -0.06505875 -0.03651578 0.00226854
Z -0.15294243 -0.00042028 -0.03641863 0.04158550 0.00224591

10 C X -0.01715128 -0.01203903 0.03899171 -0.00860010 -0.00089589
Y -0.01074895 -0.03285580 0.06764137 -0.03570650 -0.00216145
Z 0.15300197 -0.00133159 -0.03540198 -0.04204490 0.00236072

11 H X 0.04583513 0.04997554 0.04616576 0.05261277 0.04801882
Y 0.00410741 -0.09925166 0.09683707 0.17795502 0.21216991
Z 0.00326444 0.02093380 0.17603335 0.36730397 0.38250678

12 H X 0.04600888 0.04660741 -0.04876402 0.05156516 -0.04866076
Y 0.00422675 -0.10352369 -0.09319468 0.17488362 -0.21457348
Z -0.00352067 -0.01004664 0.17907960 -0.36140156 0.38724827

13 H X 0.01086816 -0.12155407 -0.04757581 0.02277561 0.10583818

Y -0.02801440 0.31288829 0.06292368 -0.17399993 -0.46198517
Z -0.00342186 -0.04736705 -0.10239168 -0.08668313 -0.00076984
14 H X 0.01062434 -0.11794090 0.05389838 0.02256303 -0.10667448
Y -0.02762378 0.30627682 -0.07994900 -0.17130916 0.46610525
Z 0.00364721 0.04248769 -0.10652185 0.08534747 -0.00106319
15 H X 0.09758981 -0.02713885 -0.06542753 -0.01850245 0.00503538
Y 0.10242439 -0.02802906 -0.10861628 0.07124619 -0.01102887
Z -0.41887535 -0.00211136 0.04422004 -0.09104136 0.01541921
16 H X 0.09736745 -0.02407838 0.06728791 -0.01793308 -0.00494201
Y 0.10214906 -0.02266503 0.10920781 0.07236560 0.01074864
Z 0.41864786 0.00431451 0.04342821 0.09101917 0.01505974

FREQUENCY: 1211.80 1237.58 1310.71 1371.09 1421.37

REDUCED MASS: 1.87052 2.33841 1.71201 2.03512 1.51479

IR INTENSITY: 0.32116 0.00094 0.00761 0.09732 0.13430

1 C X -0.02854841 -0.00008870 -0.00006560 -0.01876806 -0.00247744
Y -0.05229746 0.00124708 -0.00051375 -0.00076333 0.00798177
Z 0.00048521 0.03736407 0.03347062 -0.00053279 0.00012889
2 C X 0.03200434 -0.00056530 0.00025515 0.01117468 0.01196437
Y -0.06529844 0.00047127 -0.00020173 -0.03421509 -0.00629370
Z 0.00173987 0.19517345 -0.10623463 0.00006275 -0.00004377
3 C X 0.01434368 0.01344945 0.00632177 0.04022421 -0.00765267
Y 0.00383181 0.02885693 0.08101304 0.07992522 -0.01421439
Z 0.09709727 -0.03877459 -0.02984971 0.06664446 0.00605301

4	C	X	0.01355023	-0.01373654	-0.00633887	0.03959565	-0.00741551
		Y	0.00380322	-0.02914710	-0.08127162	0.07898676	-0.01446321
		Z	-0.09582352	-0.03755730	-0.03025038	-0.06521136	-0.00650864
5	C	X	-0.00416026	-0.01462333	0.01145058	0.00692587	-0.02094175
		Y	-0.02585313	0.03398542	-0.04035771	-0.03684315	0.00628120
		Z	-0.04085466	-0.02989708	0.01228236	-0.01086088	-0.07869955
6	C	X	-0.00385914	0.01518035	-0.01167699	0.00678030	-0.02056400
		Y	-0.02622361	-0.03448766	0.04077058	-0.03647567	0.00629914
		Z	0.03986798	-0.03123594	0.01258845	0.01098124	0.07702051
7	C	X	-0.01255697	-0.01197207	0.00428794	-0.01543710	0.02286483
		Y	0.04537154	-0.00109509	0.00980140	0.03463801	-0.06481103
		Z	-0.00433366	-0.03172386	0.04148883	-0.00301971	0.03965660
8	C	X	-0.01199925	0.01237594	-0.00443035	-0.01522186	0.02231384
		Y	0.04493260	0.00010484	-0.00940293	0.03427610	-0.06336989
		Z	0.00298038	-0.03224674	0.04181889	0.00271070	-0.03864039
9	C	X	0.00684691	-0.00153952	0.00895028	-0.01971055	0.00589866
		Y	0.00253326	-0.00917921	0.00970403	-0.02947440	0.02903380
		Z	0.04938897	-0.00840829	-0.03165752	-0.07575657	-0.03546806
10	C	X	0.00733002	0.00145984	-0.00880417	-0.01945538	0.00562759
		Y	0.00333158	0.00921873	-0.00958280	-0.02908127	0.02847757
		Z	-0.04976579	-0.00786484	-0.03243769	0.07526393	0.03525630
11	H	X	-0.03729833	-0.04694148	0.02544511	0.01109209	0.02659677
		Y	-0.11083595	-0.06034017	-0.03155334	-0.06109413	0.21163323
		Z	-0.20747190	-0.24705925	0.04480287	-0.05606303	0.35024014
12	H	X	-0.03656017	0.04834045	-0.02613703	0.01095045	0.02600534

Y -0.10987026 0.06235469 0.03074575 -0.06027937 0.20728478
Z 0.20327487 -0.25381707 0.04776955 0.05523911 -0.34261578
13 H X -0.07847985 0.05942564 0.01018294 0.00797186 -0.07806779
Y 0.35556608 -0.23596227 0.00820861 -0.00144458 0.36750124
Z -0.02122724 -0.02763295 0.04983426 -0.00061720 0.02085293
14 H X -0.07820457 -0.05972227 -0.00977961 0.00803536 -0.07652197
Y 0.35515994 0.23592755 -0.00971304 -0.00163177 0.35998001
Z 0.01964618 -0.02819563 0.05012271 0.00029247 -0.02016892
15 H X 0.04031666 -0.06557360 -0.08397320 -0.11246970 -0.00658625
Y 0.15695588 -0.12367394 -0.27150369 -0.29350979 -0.05612474
Z -0.17656408 0.20045259 0.42884797 0.34464186 0.09308433
16 H X 0.04132929 0.06516313 0.08485136 -0.11156778 -0.00628817
Y 0.15812734 0.12204233 0.27423838 -0.29102754 -0.05494814
Z 0.17713970 0.19857484 0.43207640 -0.34174911 -0.09036901

FREQUENCY: 1443.53 1520.97 1558.35 1579.85 1623.42

REDUCED MASS: 1.98618 6.53372 5.05872 4.72823 6.12766

IR INTENSITY: 0.04687 0.09942 0.06677 0.00027 0.02339

1 C X 0.00020172 -0.00064883 0.01277495 0.00010684 -0.00849217
Y -0.00033777 0.00072615 -0.05442487 -0.00003212 -0.01563315
Z -0.04358988 0.19485084 0.00112873 -0.04876448 0.00045125
2 C X 0.00006728 0.00056113 -0.01479605 -0.00014203 0.01358573
Y 0.00027487 -0.00113816 0.02756801 0.00017583 -0.03671691
Z -0.08152174 -0.04791434 0.00011902 0.06006690 -0.00008592

3 C X 0.01524192 -0.03489883 -0.00523202 0.01623755 0.01565182
Y 0.00440121 -0.05608552 -0.06838235 0.03643641 0.11354830
Z 0.03744657 -0.10354495 0.06745708 -0.00594175 -0.03735276

4 C X -0.01555445 0.03533721 -0.00487894 -0.01629709 0.01582890
Y -0.00504528 0.05687638 -0.06777278 -0.03638283 0.11404944
Z 0.03755376 -0.10442535 -0.06846508 -0.00562658 0.03714789

5 C X 0.02376847 -0.00128337 -0.00563998 0.00348597 -0.00934890
Y -0.02247098 -0.01473717 0.07538787 -0.09277227 0.06298752
Z 0.07994818 -0.00624455 0.06744370 -0.08911587 0.04211678

6 C X -0.02432524 0.00122909 -0.00554912 -0.00340012 -0.00933033
Y 0.02304220 0.01372197 0.07532330 0.09294479 0.06290516
Z 0.08157435 -0.00498150 -0.06763049 -0.08964059 -0.04205500

7 C X -0.02416713 -0.00304433 -0.00013558 -0.01044959 0.01799641
Y 0.07983998 0.03953841 -0.06154442 0.09183082 -0.10034326
Z -0.02889263 0.02080288 -0.06053093 0.05252246 -0.01928741

8 C X 0.02463887 0.00291638 -0.00014066 0.01047961 0.01801277
Y -0.08143167 -0.03832475 -0.06163042 -0.09208510 -0.10039418
Z -0.02940754 0.02002730 0.06062573 0.05268055 0.01924789

9 C X -0.01296758 0.01341087 0.01611036 -0.01801764 -0.01900998
Y -0.02634939 0.01662173 0.06737054 -0.04875883 -0.06569144
Z 0.00344029 0.02129016 -0.05073703 0.02292862 0.03459180

10 C X 0.01317906 -0.01357253 0.01594587 0.01799640 -0.01917577
Y 0.02712350 -0.01701904 0.06710550 0.04865267 -0.06607351
Z 0.00396790 0.02152101 0.05087282 0.02277542 -0.03469660

11 H X -0.00868171 -0.00145894 -0.02737041 0.03562807 -0.02360456

Y -0.19467206 -0.02117116 -0.01822491 0.02485508 0.00954490
Z -0.27512080 -0.00771999 -0.16810925 0.19579281 -0.10185006
12 H X 0.00899526 0.00155809 -0.02727472 -0.03562667 -0.02355131
Y 0.19917309 0.02111768 -0.01838286 -0.02519223 0.00958923
Z -0.28150146 -0.00891341 0.16811031 0.19639286 0.10162704
13 H X 0.06819334 0.03560344 -0.03701166 0.04420784 -0.04069557
Y -0.31511529 -0.13538458 0.07118999 -0.09379712 0.15659244
Z -0.00993980 0.03419673 -0.08339704 0.07670703 -0.03945542
14 H X -0.06979438 -0.03505727 -0.03714536 -0.04427494 -0.04072398
Y 0.32226705 0.13484061 0.07175149 0.09368998 0.15684376
Z -0.01004676 0.03321596 0.08352953 0.07690286 0.03941619
15 H X 0.00710646 0.02999113 0.01390317 -0.00570439 -0.02927167
Y 0.01812358 0.08719480 -0.05311034 0.03305199 0.00004845
Z -0.07821198 -0.09037485 0.12852723 -0.10903887 -0.06267624
16 H X -0.00681899 -0.03070330 0.01368457 0.00576918 -0.02936496
Y -0.01833559 -0.08835372 -0.05377663 -0.03282022 0.00001583
Z -0.07908945 -0.09150845 -0.12897075 -0.10864371 0.06319165

FREQUENCY: 1656.65 1718.17 3343.58 3344.22 3355.87

REDUCED MASS: 5.44923 9.93457 1.08996 1.09073 1.09117

IR INTENSITY: 0.01474 0.00979 0.00261 0.22413 0.26834

1 C X -0.00012854 -0.04010453 -0.00000005 0.00002872 0.00000019
Y 0.00022294 0.20386427 0.00000060 0.00054361 0.00000035
Z 0.03854364 -0.00115106 0.00029450 0.00000004 -0.00077415

2 C X 0.00017039 0.06916799 -0.00000018 -0.00064288 -0.00000005
Y -0.00034977 -0.16592758 0.00000019 0.00055965 0.00000000
Z -0.02855838 -0.00027888 -0.00183270 0.00002149 0.00039518

3 C X 0.01674386 -0.00811873 0.00022727 0.00023049 -0.00093457
Y 0.11435700 -0.04272853 -0.00051988 -0.00054062 -0.00284484
Z -0.05396815 -0.00500512 0.00062749 0.00087931 0.00145744

4 C X -0.01667886 -0.00827023 -0.00022676 0.00023085 0.00093444
Y -0.11416423 -0.04276457 0.00051890 -0.00054159 0.00284444
Z -0.05407217 0.00579659 0.00062563 -0.00088071 0.00145784

5 C X -0.00153052 -0.00839944 0.01375385 0.01345721 -0.00055650
Y 0.02667073 0.02684670 -0.03983843 -0.03876267 0.00162550
Z 0.02608740 0.01149103 0.01735985 0.01680813 -0.00077420

6 C X 0.00144605 -0.00848620 -0.01372758 0.01348345 0.00055631
Y -0.02643775 0.02698156 0.03976193 -0.03883746 -0.00162470
Z 0.02608942 -0.01136453 0.01732780 -0.01684278 -0.00077427

7 C X 0.01145404 0.00292380 -0.00697407 -0.00728683 -0.00001617
Y -0.05720906 -0.00697876 -0.00230142 -0.00249366 0.00010732
Z -0.00362468 -0.00062581 -0.03604110 -0.03771906 -0.00015065

8 C X -0.01140891 0.00294077 0.00695983 -0.00730117 0.00001565
Y 0.05697034 -0.00711584 0.00229650 -0.00249878 -0.00010768
Z -0.00358681 0.00063720 -0.03596739 0.03779392 -0.00014776

9 C X -0.03996916 0.00035577 0.00058406 0.00039263 0.02756892
Y -0.10425877 0.00759059 0.00097014 0.00059826 0.04330824
Z 0.04921205 -0.01290111 0.00056051 0.00047422 0.02870076

10 C X 0.03993122 0.00032644 -0.00058340 0.00039434 -0.02756894

Y 0.10416784 0.00742968 -0.00096914 0.00060102 -0.04330828
Z 0.04924014 0.01270545 0.00055977 -0.00047591 0.02870075
11 H X -0.00848371 -0.02131447 -0.15643405 -0.15192305 0.00607524
Y -0.00408833 -0.01666501 0.45914732 0.44523393 -0.01729663
Z -0.05055641 -0.09001403 -0.19800840 -0.19282363 0.00758168
12 H X 0.00832640 -0.02142177 0.15613291 -0.15221803 -0.00607260
Y 0.00414996 -0.01650675 -0.45826502 0.44609971 0.01728902
Z -0.05006286 0.09018946 -0.19762644 0.19319775 0.00757857
13 H X -0.01865015 0.01072753 0.07594574 0.07904500 -0.00002174
Y 0.07068398 -0.00647537 0.03783690 0.03889517 0.00069145
Z -0.01184685 -0.00596692 0.41743810 0.43324533 -0.00049668
14 H X 0.01857529 0.01070211 -0.07579131 0.07920263 0.00002744
Y -0.07021015 -0.00645360 -0.03776094 0.03897443 -0.00068846
Z -0.01173533 0.00600858 0.41659206 -0.43411288 -0.00052799
15 H X -0.00866432 -0.00536580 -0.00735508 -0.00471741 -0.31543478
Y 0.04450212 -0.00939429 -0.01093691 -0.00700929 -0.48125024
Z -0.21101949 0.01770627 -0.00868257 -0.00528761 -0.35107414
16 H X 0.00854007 -0.00533212 0.00734689 -0.00473789 0.31543497
Y -0.04466512 -0.00899703 0.01092492 -0.00704048 0.48125059
Z -0.21113268 -0.01699682 -0.00867343 0.00531191 -0.35107428

FREQUENCY: 3365.21 3365.28 3369.22

REDUCED MASS: 1.10359 1.10313 1.09489

IR INTENSITY: 1.01094 0.67847 0.37459

1	C	X	-0.00000134	0.00060513	0.00042933
		Y	-0.00000025	-0.00030313	0.00042361
		Z	0.00100737	0.00001567	0.00000668
2	C	X	-0.00000271	0.00103983	0.00015106
		Y	0.00000163	-0.00048278	-0.00027401
		Z	0.00274323	0.00000224	0.00000109
3	C	X	0.00065984	0.00011396	0.00106001
		Y	-0.00117612	-0.00207240	0.00276230
		Z	0.00093461	0.00138046	-0.00154158
4	C	X	-0.00066013	0.00011183	0.00106010
		Y	0.00118407	-0.00206777	0.00276257
		Z	0.00093889	-0.00137847	0.00154095
5	C	X	-0.01149520	-0.01185970	-0.00285098
		Y	0.03599832	0.03655819	0.00881360
		Z	-0.01183789	-0.01197950	-0.00290487
6	C	X	0.01154126	-0.01181706	-0.00284992
		Y	-0.03613864	0.03642468	0.00881044
		Z	-0.01188586	0.01193590	0.00290375
7	C	X	-0.00801373	-0.00743274	-0.00209063
		Y	-0.00745951	-0.00716084	-0.00192415
		Z	-0.04729056	-0.04444847	-0.01215967
8	C	X	0.00804083	-0.00740276	-0.00208989
		Y	0.00748613	-0.00713304	-0.00192349
		Z	-0.04745303	0.04427196	0.01215552
9	C	X	-0.00063028	0.00700371	-0.02653125

		Y	-0.00074797	0.01106192	-0.04128169
		Z	-0.00065059	0.00791678	-0.03078545
10	C	X	0.00060660	0.00700716	-0.02653086
		Y	0.00071054	0.01106654	-0.04128106
		Z	-0.00062394	-0.00792025	0.03078509
11	H	X	0.12605149	0.12819591	0.03156226
		Y	-0.37067649	-0.37592627	-0.09190360
		Z	0.15564801	0.15897028	0.03862396
12	H	X	-0.12654276	0.12772956	0.03155160
		Y	0.37211722	-0.37455445	-0.09187207
		Z	0.15625783	-0.15839488	-0.03861095
13	H	X	0.09181748	0.08683663	0.02405204
		Y	0.04985538	0.04770746	0.01219048
		Z	0.50883799	0.47843697	0.13228571
14	H	X	-0.09213408	0.08649429	0.02404428
		Y	-0.05002966	0.04752138	0.01218619
		Z	0.51058180	-0.47653919	-0.13224245
15	H	X	0.00566959	-0.07975614	0.30459870
		Y	0.00962316	-0.12061072	0.46061238
		Z	0.00607142	-0.09093475	0.34490400
16	H	X	-0.00539976	-0.07978997	0.30459445
		Y	-0.00921549	-0.12066610	0.46060568
		Z	0.00576351	0.09097116	-0.34489940

THERMOCHEMISTRY AT T= 298.15 K

USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.

P= 1.01325E+05 PASCAL.

ALL FREQUENCIES ARE SCALED BY 1.00000

THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)

784.21609 894.59977 1597.69849

THE ROTATIONAL SYMMETRY NUMBER IS 1.0

THE ROTATIONAL CONSTANTS ARE (IN GHZ)

2.29922 2.01553 1.12855

THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000)

0.126591 HARTREE/MOLECULE 27783.492809 CM**-1/MOLECULE

79.437072 KCAL/MOL 332.364709 KJ/MOL

	Q	LN Q
ELEC.	1.00000E+00	0.000000
TRANS.	5.56227E+07	17.834102
ROT.	3.78984E+05	12.845250
VIB.	5.39397E+00	1.685281
TOT.	1.13706E+14	32.364633

E	H	G	CV	CP	S
KJ/MOL	KJ/MOL	KJ/MOL	J/MOL-K	J/MOL-K	J/MOL-K

ELEC.	0.000	0.000	0.000	0.000	0.000	0.000
TRANS.	3.718	6.197	-44.210	12.472	20.786	169.066
ROT.	3.718	3.718	-31.843	12.472	12.472	119.272
VIB.	341.483	341.483	328.187	86.850	86.850	44.597
TOTAL	348.920	351.399	252.135	111.794	120.108	332.935

	E	H	G	CV	CP	S
	KCAL/MOL	KCAL/MOL	KCAL/MOL	CAL/MOL-K	CAL/MOL-K	CAL/MOL-K
ELEC.	0.000	0.000	0.000	0.000	0.000	0.000
TRANS.	0.889	1.481	-10.566	2.981	4.968	40.408
ROT.	0.889	0.889	-7.611	2.981	2.981	28.507
VIB.	81.617	81.617	78.439	20.758	20.758	10.659
TOTAL	83.394	83.986	60.262	26.719	28.707	79.573
.....END OF NORMAL COORDINATE ANALYSIS.....						

Acepentalene GS Transition State 1¹A"

CAS(10/10)/cc-pVDZ

Cs

C	6.0	0.7921027344	-0.0210894412	0.0000000000
C	6.0	0.4532772677	1.4001955984	0.0000000000
C	6.0	0.4135721183	-0.6752325306	-1.1632201856
C	6.0	0.4135721183	-0.6752325306	1.1632201856
C	6.0	0.0480368061	1.6478578079	-1.3493916412
C	6.0	0.0480368061	1.6478578079	1.3493916412
C	6.0	-0.0097998451	0.3901735699	-2.0433251067
C	6.0	-0.0097998451	0.3901735699	2.0433251067
C	6.0	-0.0132318327	-2.0323972853	-0.6868225697
C	6.0	-0.0132318327	-2.0323972853	0.6868225697
H	1.0	-0.2870219511	2.5833443235	-1.7717013103
H	1.0	-0.2870219511	2.5833443235	1.7717013103
H	1.0	-0.4165937889	0.2799104241	-3.0384386427
H	1.0	-0.4165937889	0.2799104241	3.0384386427
H	1.0	-0.2576515076	-2.8836339096	-1.3049053968
H	1.0	-0.2576515076	-2.8836339096	1.3049053968

FREQUENCY: i2670.60

REDUCED MASS: 9.28034

IR INTENSITY: 5.32955

1 C X 0.00003439

Y 0.00000613

Z 0.07641039

2 C X -0.00002626

Y 0.00000206

Z -0.08807588

3 C X -0.02824413

Y -0.00047463

Z -0.09234315

4 C X 0.02823630

Y 0.00042005

Z -0.09229241

5 C X 0.02565174

Y 0.03776369

Z 0.09525998

6 C X -0.02565012

Y -0.03779223

Z 0.09521167

7 C X 0.02337766

Y -0.11210248

Z 0.00535842

8 C X -0.02339239

		Y 0.11216097
		Z 0.00535913
9	C	X 0.00214809
		Y -0.00315511
		Z -0.01050232
10	C	X -0.00214435
		Y 0.00316859
		Z -0.01049048
11	H	X -0.07312023
		Y -0.01093039
		Z 0.04956253
12	H	X 0.07320892
		Y 0.01092268
		Z 0.04956127
13	H	X -0.06007062
		Y -0.02767126
		Z 0.02911186
14	H	X 0.06010024
		Y 0.02770867
		Z 0.02912862
15	H	X 0.00932196
		Y -0.00944847
		Z -0.00023567
16	H	X -0.00933238
		Y 0.00945378

Z -0.00023786

FREQUENCY: 211.06 290.82 292.23

REDUCED MASS: 3.75995 4.67898 3.71420

IR INTENSITY: 0.20075 0.01124 0.00359

- 1 C

X 0.15466124 -0.00001916 0.01552297

Y -0.00472826 0.00002414 0.00928379

Z -0.00020933 0.00548045 0.00006005
- 2 C

X 0.08699355 0.00005607 -0.09389794

Y -0.00284113 -0.00000714 -0.01374649

Z -0.00030510 0.00313952 0.00002652
- 3 C

X 0.07124828 0.10426238 0.06054326

Y 0.00121242 -0.00842502 -0.00133574

Z 0.00893099 -0.00967790 -0.00712362
- 4 C

X 0.07147963 -0.10439537 0.06049520

Y 0.00101153 0.00845333 -0.00142032

Z -0.00951518 -0.00963049 0.00718735
- 5 C

X -0.04045294 -0.11041994 -0.05901064

Y -0.02406991 -0.03592996 -0.02783836

Z 0.03301641 0.02237229 -0.01445841
- 6 C

X -0.04007447 0.11044823 -0.05893936

Y -0.02414441 0.03590251 -0.02790619

Z -0.03353373 0.02242799 0.01458692

7	C	X	-0.05415453	-0.01211031	0.10768409
		Y	-0.01660055	-0.01784198	-0.01375014
		Z	0.05122503	0.01373839	-0.04889106
8	C	X	-0.05362775	0.01206274	0.10769969
		Y	-0.01674106	0.01783294	-0.01385160
		Z	-0.05171842	0.01382354	0.04899253
9	C	X	-0.03868579	0.09288944	-0.06510343
		Y	0.04148841	-0.01575147	0.04329287
		Z	0.00242397	-0.03331621	-0.00013947
10	C	X	-0.03854624	-0.09281364	-0.06514366
		Y	0.04133706	0.01572445	0.04323912
		Z	-0.00333024	-0.03330822	0.00006522
11	H	X	-0.14703139	-0.17627344	-0.09938772
		Y	-0.04184536	-0.05375097	-0.04564894
		Z	0.07907427	0.03572147	-0.02125521
12	H	X	-0.14652587	0.17634555	-0.09927337
		Y	-0.04195636	0.05374866	-0.04573333
		Z	-0.07940860	0.03576831	0.02145744
13	H	X	-0.17679459	-0.01240019	0.21312726
		Y	-0.04884628	-0.04307006	-0.02796066
		Z	0.10580418	0.01665716	-0.09128088
14	H	X	-0.17597390	0.01248815	0.21314388
		Y	-0.04891957	0.04310010	-0.02806214
		Z	-0.10617547	0.01680338	0.09138499
15	H	X	-0.13996137	0.17493419	-0.17124509

Y 0.07623335 -0.02906397 0.07197892
Z -0.00639081 -0.04702215 0.00099667

16 H X -0.13966928 -0.17477598 -0.17130994
Y 0.07593766 0.02899653 0.07187374
Z 0.00533481 -0.04703370 -0.00115347

FREQUENCY: 464.75 527.59 551.50 632.60 652.56
REDUCED MASS: 3.18874 3.69578 3.01647 5.47515 4.86888
IR INTENSITY: 0.00009 0.11528 0.01894 0.25280 0.24126

1 C X -0.00006521 -0.00045676 0.00273834 -0.00033599 0.03490430
Y -0.00005807 0.00017675 -0.06509616 -0.00016911 0.03966966
Z -0.01505605 -0.07944877 -0.00021905 -0.02846204 -0.00086007

2 C X -0.00018050 -0.00122607 0.06410239 -0.00060871 0.14325638
Y 0.00002787 0.00052334 -0.05709412 -0.00012613 0.09816255
Z -0.00524767 -0.00354057 -0.00032887 0.00609799 0.00105242

3 C X -0.01734015 -0.00391481 -0.02471897 0.13924762 -0.08344262
Y -0.00565993 -0.02590976 -0.01248913 -0.03322349 0.01784606
Z -0.00316341 -0.06127641 -0.02442439 -0.05780940 0.05458816

4 C X 0.01759701 0.00548121 -0.02452223 -0.13840211 -0.08382566
Y 0.00556243 0.02558875 -0.01263868 0.03286218 0.01951879
Z -0.00330272 -0.06232012 0.02411253 -0.05788455 -0.05727848

5 C X -0.10039720 0.01058515 -0.04901841 0.02655126 -0.05544138
Y -0.01359351 0.05677704 0.02041358 0.00641670 -0.04026286
Z 0.03405397 0.02454053 0.09662577 0.00196397 -0.02397111

6 C X 0.10047495 -0.00959207 -0.04897254 -0.02618863 -0.05556156
Y 0.01376639 -0.05604875 0.01908703 -0.00564139 -0.03855554
Z 0.03393175 0.02516449 -0.09624387 0.00144608 0.02403014

7 C X 0.09617625 -0.00206654 0.04447098 -0.01570679 0.04365074
Y 0.01586804 0.05969702 0.08602222 0.01095623 -0.03638081
Z -0.05028322 -0.02940096 -0.00092871 0.02597135 -0.02340274

8 C X -0.09612598 0.00193673 0.04440997 0.01593308 0.04447031
Y -0.01583515 -0.06066213 0.08481933 -0.01062205 -0.03594579
Z -0.05058238 -0.03096077 0.00075855 0.02507948 0.02189888

9 C X -0.07791104 0.05647775 -0.00493959 -0.09939464 -0.01226232
Y 0.01432842 -0.07078163 -0.04166658 0.02245438 0.00065068
Z 0.02996081 0.09361247 -0.00466795 0.02917108 0.00249179

10 C X 0.07782147 -0.05689095 -0.00590825 0.09920545 -0.01126189
Y -0.01438673 0.07084730 -0.04097992 -0.02294348 0.00207367
Z 0.02993952 0.09343772 0.00592425 0.02914879 -0.00257303

11 H X -0.17715879 0.00151583 -0.17025938 -0.00352192 -0.06818058
Y -0.02767224 0.06976641 0.03637558 -0.00165909 -0.07307076
Z 0.06289827 0.05662810 0.22895844 0.00672572 -0.08861376

12 H X 0.17723631 0.00012770 -0.16955450 0.00256619 -0.07184626
Y 0.02779727 -0.06965948 0.03483707 0.00220578 -0.07194265
Z 0.06285313 0.05903514 -0.22761758 0.00562922 0.08705999

13 H X 0.22948013 0.01346429 0.10806489 -0.15897210 0.09787327
Y 0.03798556 0.13877201 0.16623048 0.01829964 -0.07123333
Z -0.10806477 -0.04615109 -0.03552714 0.08338743 -0.04242091

14 H X -0.22990959 -0.01698582 0.10776192 0.15770178 0.09722780

Y -0.03803550 -0.14121549 0.16427992 -0.01792143 -0.07327148
Z -0.10857504 -0.04929065 0.03516228 0.08186612 0.03997730
15 H X -0.14529482 0.12039669 0.08168701 -0.13666700 0.17488973
Y 0.02170826 -0.15251170 -0.08029714 0.01093375 -0.03358579
Z 0.04544431 0.18362516 0.01370308 0.05726882 -0.02260665
16 H X 0.14517890 -0.12205521 0.07982971 0.13554271 0.17562759
Y -0.02170683 0.15339917 -0.07876460 -0.01109348 -0.03039244
Z 0.04548375 0.18403364 -0.01160219 0.05732580 0.02486648

FREQUENCY: 705.12 724.18 728.57 746.81 779.90
REDUCED MASS: 1.64853 1.78080 2.06152 2.22981 5.18229
IR INTENSITY: 0.33608 0.00941 0.75278 1.11801 0.06232

1 C X 0.03877305 0.00120386 -0.01236326 0.01417593 0.16753774
Y -0.02437460 0.00061321 -0.03113827 0.01678426 -0.01140037
Z 0.00006152 0.02641301 -0.00006820 -0.00019271 0.00024656
2 C X -0.04116726 0.00025858 0.08046794 -0.02321512 -0.10835845
Y -0.07491957 0.00183675 -0.04247473 0.05801324 -0.07042439
Z -0.00027629 -0.06717159 0.00010253 0.00026480 -0.00068250
3 C X 0.00139260 0.00418201 0.01644228 0.06448948 -0.08683807
Y 0.01854733 0.04807686 0.01400941 -0.03546215 0.02171021
Z -0.02787928 0.04031147 -0.04694806 0.02011773 0.06214177
4 C X 0.00106989 -0.00440974 0.01587672 0.06439078 -0.08761198
Y 0.01833195 -0.04889185 0.01441627 -0.03459360 0.02129984
Z 0.02762387 0.03794726 0.04513507 -0.01971156 -0.06240340

5	C	X	0.02693117	0.02022889	-0.05221198	-0.03747332	0.00635375
		Y	-0.02888022	0.06654779	-0.05268509	0.03655083	0.00312257
		Z	-0.00745208	-0.05306587	0.00496941	0.00481308	0.01969992
6	C	X	0.02688296	-0.02251467	-0.05207370	-0.03608403	0.00791933
		Y	-0.02948407	-0.06628916	-0.05275194	0.03755685	0.00202057
		Z	0.00701727	-0.05300467	-0.00540496	-0.00254493	-0.01930838
7	C	X	-0.00841825	0.03643695	-0.07051777	-0.01452974	-0.00012908
		Y	-0.00305022	0.02754380	0.01474434	0.01090030	0.00298719
		Z	-0.04118439	-0.01510757	-0.04935059	0.08497655	0.03145624
8	C	X	-0.00844088	-0.03615689	-0.06983993	-0.01358721	0.00059515
		Y	-0.00346443	-0.02781675	0.01415653	0.01200091	0.00302811
		Z	0.04077413	-0.01783030	0.04787454	-0.08249312	-0.03103185
9	C	X	-0.05014418	0.02027451	0.02820965	-0.06864599	0.02786609
		Y	0.07725149	0.03751271	0.04572866	-0.04675928	0.00627142
		Z	-0.00019888	0.03596991	-0.00097970	0.00174055	0.00025264
10	C	X	-0.05008410	-0.02187434	0.02876982	-0.06834020	0.02801099
		Y	0.07719591	-0.03893837	0.04653860	-0.04656076	0.00585614
		Z	0.00067150	0.03584179	0.00155627	-0.00293683	0.00024567
11	H	X	-0.01627556	-0.40630015	0.35268471	0.23836904	0.15500914
		Y	-0.01761685	-0.01843690	0.06159589	0.07150496	0.04993092
		Z	0.05397856	0.09383396	-0.06170118	-0.13922864	0.00942516
12	H	X	-0.01407638	0.41748424	0.35214893	0.22064798	0.14409525
		Y	-0.01788972	0.02003506	0.06110118	0.06863785	0.04579353
		Z	-0.05341253	0.10163275	0.06157125	0.13510662	-0.01225422
13	H	X	-0.12053209	-0.23952173	0.21267064	0.21781902	0.16817935

Y -0.01609857 -0.06918680 0.06754876 0.02453474 -0.00174509
Z 0.00613832 0.10853999 -0.17284570 -0.01053544 -0.03529450
14 H X -0.11889953 0.24886300 0.21341394 0.20656502 0.16348012
Y -0.01624358 0.06867735 0.06562138 0.02399061 -0.00143955
Z -0.00585945 0.10946398 0.17117682 0.00791298 0.03351277
15 H X 0.50458342 0.02475536 -0.06744284 0.24557330 -0.04939882
Y -0.10860270 0.06655227 0.05193934 -0.12752153 0.05346504
Z 0.03556151 -0.00624865 0.02821473 -0.01468722 -0.03249900
16 H X 0.50447005 -0.01779168 -0.06766677 0.24671983 -0.04926825
Y -0.10842045 -0.06940599 0.05434475 -0.12788663 0.05302088
Z -0.03483711 -0.00493369 -0.02576196 0.01306323 0.03294458

FREQUENCY: 807.60 832.82 833.44 843.67 871.87
REDUCED MASS: 1.78999 1.67887 1.47817 5.08750 1.63972
IR INTENSITY: 0.04098 0.04808 0.04089 0.15202 0.01641

1 C X -0.00154514 -0.01107407 -0.04315509 0.12586172 -0.00004900
Y 0.00010869 0.00305772 0.01041244 -0.01349322 -0.00000315
Z 0.02051312 -0.01869711 0.00619523 0.00082566 -0.01051399
2 C X 0.00132986 0.00122960 0.00702962 -0.00471127 -0.00028528
Y 0.00080900 -0.00086219 -0.00203990 0.03420866 -0.00040125
Z -0.05795472 0.06044037 -0.01948749 -0.00067315 0.03286458
3 C X 0.01931062 -0.03194581 0.01667713 0.00777306 0.00879983
Y 0.05082234 -0.02091128 0.00904762 -0.00666255 0.01517243
Z 0.00378980 0.00089947 0.01015433 -0.04229819 -0.02090428

4	C	X	-0.01917670	0.03602637	-0.00539417	0.00623076	-0.00869626
		Y	-0.05087259	0.02173032	-0.00580512	-0.00852887	-0.01509748
		Z	0.00449004	-0.00446492	-0.00939423	0.04095106	-0.02117249
5	C	X	-0.07879296	0.00935173	0.06328871	0.01348190	0.02419343
		Y	0.05254659	-0.06325671	0.00888327	0.03706226	-0.04940939
		Z	-0.00020825	0.02079264	-0.01037939	-0.08561223	0.02415138
6	C	X	0.07796295	0.02965902	0.05751651	0.01332843	-0.02460536
		Y	-0.05358659	0.05840531	-0.03046202	0.03551846	0.04963889
		Z	-0.00026664	0.02490574	-0.00450366	0.08449245	0.02352859
7	C	X	0.02126289	0.05662574	-0.08604901	-0.05317403	-0.01810021
		Y	-0.00248373	0.00646378	-0.03035562	0.03611397	-0.00253535
		Z	-0.02539988	-0.01744861	0.05503607	-0.08498590	-0.04700780
8	C	X	-0.01978228	-0.09772483	-0.03663030	-0.04985433	0.01860856
		Y	0.00217958	-0.02155110	-0.02127504	0.03633819	0.00254181
		Z	-0.02385839	-0.04531970	-0.03649923	0.08303161	-0.04763213
9	C	X	0.01706296	-0.00588084	0.00522786	-0.01781866	0.09125433
		Y	0.05181347	-0.02602657	0.04735653	-0.07582785	0.02375370
		Z	0.04559316	-0.02218309	0.01173533	-0.00431209	0.03301184
10	C	X	-0.01668574	0.00679530	0.00060756	-0.01808926	-0.09132212
		Y	-0.05120100	0.04560505	0.02309153	-0.07797559	-0.02371585
		Z	0.04560230	-0.02435413	0.00439864	0.00647408	0.03300543
11	H	X	0.42167499	-0.02525091	-0.33185511	-0.16044791	-0.00011070
		Y	0.17653124	-0.08428835	-0.07826835	-0.00162658	-0.04162903
		Z	-0.12668990	0.00727352	0.11098425	-0.04672126	0.06338119
12	H	X	-0.42117322	-0.17482132	-0.28771178	-0.15955355	0.00352035

Y -0.17775219 0.02454467 -0.11492759 -0.00411572 0.04300187
Z -0.12535191 -0.05790123 -0.09554576 0.04822823 0.06322574
13 H X -0.13181558 -0.31627110 0.54024811 0.05237087 -0.04343694
Y -0.09670614 0.02817955 0.00943324 0.06888541 0.04875233
Z 0.04641841 0.13372166 -0.20461544 -0.13766254 -0.04346803
14 H X 0.12160086 0.57607726 0.25767267 0.04091309 0.04212454
Y 0.09556911 -0.01489486 0.02470393 0.06904353 -0.04929582
Z 0.04310600 0.23145141 0.08751003 0.12951522 -0.04493659
15 H X 0.00966952 0.04482790 0.02178287 -0.03013004 -0.47502614
Y 0.08495036 -0.06181899 0.05427755 -0.08847808 0.22225543
Z 0.00276247 0.00790933 -0.00201959 0.01167836 -0.01519346
16 H X -0.01096944 -0.02386481 0.04365351 -0.03114847 0.47533152
Y -0.08417668 0.07799011 0.00734562 -0.09096977 -0.22219438
Z 0.00227034 0.00769901 -0.00272871 -0.01031696 -0.01501554

FREQUENCY: 883.88 1069.99 1080.55 1109.85 1151.41

REDUCED MASS: 2.68826 1.63886 2.60947 2.74094 1.79150

IR INTENSITY: 0.01933 0.05934 0.01738 0.00879 0.04709

1 C X -0.00060547 0.00916017 -0.00028614 -0.01088937 0.03140796
Y 0.00025918 -0.02265378 0.00139475 0.11316530 0.07503838
Z 0.00922408 0.00043064 0.09508432 -0.00005356 0.00086424
2 C X -0.00049959 -0.02446839 -0.00042872 -0.02831989 -0.03914223
Y -0.00055189 0.02270015 0.00007724 0.01803451 0.08887085
Z 0.04697274 -0.00027654 0.01886494 -0.00013420 -0.00050796

3 C X 0.00318617 -0.01645899 0.03820525 0.03330516 -0.01032167
Y 0.04747906 -0.01554413 0.04028979 0.03716452 0.00054000
Z -0.02106419 -0.01810405 0.04050366 0.05019170 -0.02869921

4 C X -0.00288802 -0.01665691 -0.03793911 0.03352597 -0.01016213
Y -0.04748946 -0.01571113 -0.04017594 0.03731927 -0.00013624
Z -0.02163043 0.01835847 0.04102033 -0.05058945 0.02782547

5 C X 0.03190514 0.00879361 0.00587782 0.03011387 0.02215226
Y -0.06963770 -0.08097393 0.01279232 -0.07835487 -0.02762867
Z 0.02727945 -0.02775260 0.00527484 0.04573487 0.07001854

6 C X -0.03244875 0.00854159 -0.00559584 0.03017943 0.02235178
Y 0.06992496 -0.08005709 -0.01274636 -0.07810762 -0.02672825
Z 0.02581279 0.02822674 0.00388082 -0.04583126 -0.07040963

7 C X -0.03673273 0.01537549 -0.03625579 -0.02212180 -0.00423748
Y -0.00687668 0.06712979 -0.00752291 0.01420120 -0.03980772
Z -0.07773912 0.05615199 -0.09056391 -0.04418641 -0.01967780

8 C X 0.03794239 0.01561258 0.03677733 -0.02229866 -0.00431161
Y 0.00657526 0.06668056 0.00665594 0.01396835 -0.04067076
Z -0.07957608 -0.05658333 -0.09141123 0.04472706 0.02042924

9 C X -0.02209298 0.01279200 -0.02961045 -0.02601762 -0.00213460
Y 0.08766042 0.01973963 -0.08210080 -0.06012243 -0.00250916
Z 0.04677971 0.00242070 -0.03270899 -0.02399620 0.05259329

10 C X 0.02191459 0.01296804 0.02911417 -0.02617805 -0.00223811
Y -0.08736908 0.02027089 0.08138163 -0.06050490 -0.00255738
Z 0.04675410 -0.00265954 -0.03257045 0.02419508 -0.05237071

11 H X -0.00611631 -0.06140985 0.04421708 0.06044410 0.06170362

Y -0.05235122 -0.23219282 0.13650952 -0.03254391 -0.00429746
Z 0.09989162 -0.29066736 0.24178885 0.13913720 0.09854244
12 H X 0.01141981 -0.06224879 -0.04222684 0.06070013 0.06206678
Y 0.05421035 -0.23207581 -0.13540296 -0.03130157 -0.00101043
Z 0.09947782 0.29265100 0.23938328 -0.14120678 -0.10384124
13 H X -0.01092263 -0.06195180 -0.03040279 -0.05390780 -0.00295382
Y 0.04550409 0.36733517 -0.16529242 0.18173081 0.09425277
Z -0.09590982 0.06107094 -0.08215371 -0.05115904 -0.03624595
14 H X 0.00856215 -0.06114850 0.02963511 -0.05395623 -0.00278784
Y -0.04680134 0.36489728 0.16432695 0.17940725 0.08680890
Z -0.09942703 -0.06149112 -0.08359909 0.05156873 0.03646980
15 H X 0.36428519 -0.01913652 -0.09894885 0.04347901 -0.08003116
Y 0.01971891 -0.00621886 -0.16924973 0.09997684 -0.23940755
Z -0.01324583 0.05350132 0.11026098 -0.28185530 0.41569246
16 H X -0.36338651 -0.01863410 0.09932742 0.04308471 -0.07967053
Y -0.01943337 -0.00507420 0.16834199 0.09930143 -0.23851204
Z -0.01285981 -0.05279316 0.11065459 0.28158077 -0.41398969

FREQUENCY: 1189.43 1230.28 1247.30 1313.31 1319.69

REDUCED MASS: 1.95784 3.47392 1.66961 3.05452 2.54774

IR INTENSITY: 0.09361 0.01445 0.00923 0.09340 0.35509

1 C X -0.00017988 0.04009295 0.00147928 0.01076061 -0.00117560
Y -0.00009947 -0.02968006 -0.00045602 -0.00039521 0.00174396
Z 0.11290730 0.00070487 -0.05809331 0.00889393 0.07822080

2 C X 0.00007397 -0.03108178 -0.00126236 -0.01024558 0.00115899
Y -0.00011238 0.11251445 0.00302570 0.00425884 -0.00180362
Z -0.02365285 -0.00403888 0.13411220 0.01339477 0.12111290

3 C X 0.00456642 -0.03124699 -0.01491627 -0.01140018 0.00865993
Y 0.09832576 -0.06764239 0.05437509 0.10106905 -0.07452916
Z -0.03954307 -0.08256104 -0.05774665 -0.09582992 0.02135003

4 C X -0.00505397 -0.03183262 0.01298568 -0.01257409 -0.00630356
Y -0.09922438 -0.06256916 -0.05740827 0.11671330 0.04990242
Z -0.03763236 0.08610830 -0.05162573 0.09753198 0.00160505

5 C X -0.00954964 0.00726050 0.00267172 0.01131243 -0.01421681
Y -0.03583996 0.03025525 0.02273770 -0.02135025 0.08565043
Z -0.02354312 0.05958847 -0.00186778 0.03326454 -0.00859982

6 C X 0.00927348 0.00710639 -0.00226227 0.01449247 0.01083122
Y 0.03717801 0.03170561 -0.02114423 -0.03966439 -0.07794524
Z -0.02348748 -0.05869695 -0.00595593 -0.03538019 -0.00049229

7 C X -0.00270486 0.00337446 0.01050870 0.00663245 -0.02104235
Y 0.03152604 -0.06390429 -0.01245240 0.00356566 -0.02996303
Z 0.02471906 -0.01056464 0.01493940 0.03021638 -0.07050626

8 C X 0.00340161 0.00385913 -0.01001519 0.01095518 0.02004935
Y -0.03224479 -0.06458908 0.00818232 0.00974927 0.02711788
Z 0.02342612 0.00964150 0.01468081 -0.04479084 -0.06415858

9 C X -0.00400078 0.00996159 0.00508613 -0.01360050 -0.00155308
Y -0.02325807 0.03192608 0.00464856 -0.04783623 0.00281471
Z 0.00087950 -0.04493443 0.00466669 -0.04809181 0.01078791

10 C X 0.00401042 0.01012234 -0.00468238 -0.01322457 0.00429249

Y 0.02351864 0.03169884 -0.00321523 -0.04797860 0.00756615
Z 0.00273510 0.04458970 0.00733683 0.04959481 0.00032267
11 H X -0.03271230 0.01792652 -0.07410327 -0.01453025 -0.08592893
Y -0.16970773 0.00096814 -0.06860983 -0.12739811 -0.05845738
Z -0.29209426 -0.02161228 -0.15135132 -0.16587130 -0.30836203
12 H X 0.03207615 0.01250116 0.07623030 0.00418169 0.08806613
Y 0.17011908 -0.00530072 0.06768420 -0.11419047 0.08715599
Z -0.28993005 0.03597898 -0.14811726 0.09836461 -0.33767281
13 H X 0.01343109 -0.00405168 0.07169941 0.06417103 -0.06122432
Y 0.23204447 0.13506159 -0.46998744 -0.27538004 0.17147254
Z 0.00109437 -0.03424852 0.04284362 0.04470204 -0.09151420
14 H X -0.01316205 0.00037700 -0.07206510 0.07604170 0.04486702
Y -0.23563875 0.11058137 0.48224218 -0.30668753 -0.10010744
Z -0.00074443 0.03214673 0.04423396 -0.06346750 -0.08144953
15 H X -0.06545490 0.05971835 -0.02400749 -0.02273202 0.02282781
Y -0.14430466 0.16865836 -0.05494146 -0.05534187 0.08894658
Z 0.18895495 -0.25617174 0.09705295 -0.05556002 -0.11417918
16 H X 0.06769952 0.05698557 0.02696454 -0.02802361 -0.01670271
Y 0.14998540 0.16270142 0.06304258 -0.07561835 -0.07408925
Z 0.19946806 0.24690488 0.11025621 0.02740001 -0.12174688

FREQUENCY: 1436.20 1448.35 1453.45 1481.56 1531.72

REDUCED MASS: 2.31653 1.98953 2.39189 2.66857 3.28610

IR INTENSITY: 0.06712 0.01778 0.07222 0.04061 0.05036

1	C	X	0.00001225	0.00712560	-0.00017248	0.00040680	0.00008430
		Y	0.00268220	-0.01393816	0.00405241	0.05101387	-0.00215277
		Z	0.07760550	0.00170500	0.10323331	-0.00656043	-0.10393210
2	C	X	0.00071975	-0.02155902	0.00174015	0.03509417	-0.00061474
		Y	-0.00237455	0.08125662	-0.00557039	-0.08759670	0.00160055
		Z	0.06645628	0.00060808	0.04787968	-0.00475265	0.08542125
3	C	X	-0.02402997	-0.01691595	-0.01822756	-0.00477096	0.01174114
		Y	-0.06136925	-0.01743456	0.00608790	0.06544988	0.08177723
		Z	-0.04000042	-0.03846443	-0.07964971	-0.03469973	0.01591395
4	C	X	0.02342433	-0.01629102	0.01817752	-0.00694896	-0.01137858
		Y	0.06150903	-0.01768996	-0.00389771	0.06207975	-0.08088756
		Z	-0.03790709	0.03551983	-0.07824980	0.04170036	0.01527316
5	C	X	-0.02203732	-0.00663131	-0.02027071	-0.02435971	-0.01232382
		Y	0.00785128	-0.06931509	-0.02016152	0.03333773	0.02498508
		Z	-0.06571067	-0.08464994	-0.06914995	-0.04641546	-0.03872617
6	C	X	0.02071247	-0.00614390	0.01863453	-0.02644009	0.01265105
		Y	-0.00657439	-0.06826976	0.02549665	0.03310725	-0.02581407
		Z	-0.06261380	0.08275490	-0.06874719	0.05299065	-0.03928592
7	C	X	0.01270745	0.01674367	0.01230459	0.02317714	0.01908714
		Y	-0.01074910	0.03609891	0.01607927	-0.09705037	-0.10833704
		Z	0.01840060	0.04991487	0.03188899	0.04015123	0.02068966
8	C	X	-0.01127783	0.01644418	-0.01106533	0.02389455	-0.01940136
		Y	0.00747942	0.03476235	-0.02312004	-0.09562722	0.10881706
		Z	0.01571560	-0.04890831	0.03049985	-0.04149405	0.02112659
9	C	X	0.02972175	0.00579713	-0.01366233	-0.00795959	-0.00895605

Y 0.08735370 0.00709507 -0.05877185 -0.01869949 -0.02192029
Z -0.03055857 -0.02996027 0.05009190 -0.02923146 0.00294381
10 C X -0.02995673 0.00649838 0.01294656 -0.00759386 0.00903179
Y -0.08768481 0.00994346 0.05757705 -0.01884754 0.02200578
Z -0.02987297 0.03217010 0.04990455 0.02726606 0.00287628
11 H X 0.01797760 0.08035332 0.02279717 0.00005107 -0.00730833
Y 0.14703021 0.18782775 0.10437866 0.09919340 0.10753780
Z 0.19611763 0.42460918 0.17036529 0.06206806 0.11646443
12 H X -0.01694242 0.07961289 -0.02572344 0.00058041 0.00831983
Y -0.14007876 0.18552011 -0.10390562 0.10890318 -0.10769294
Z 0.18944672 -0.41988250 0.18228867 -0.07423391 0.11468131
13 H X -0.00609833 0.02065245 0.02596260 -0.01631744 -0.02833586
Y 0.07450853 -0.06319597 -0.01864284 0.37561081 0.30684432
Z 0.01860576 0.07057443 0.03599403 0.00922877 -0.00297736
14 H X 0.00499875 0.01933141 -0.02825977 -0.01513938 0.02834394
Y -0.05852908 -0.05894841 0.04520229 0.37255536 -0.30754148
Z 0.01673215 -0.06916272 0.03699257 -0.01105663 -0.00255351
15 H X -0.03977004 -0.00920971 0.05500129 -0.01522704 -0.01230776
Y -0.14369564 -0.00643562 0.18367356 -0.05696415 -0.01394056
Z 0.32404409 -0.01033967 -0.31601381 0.01465283 -0.00963542
16 H X 0.03973888 -0.01181018 -0.05484375 -0.01326248 0.01229424
Y 0.14282504 -0.01502468 -0.18519719 -0.05053452 0.01407358
Z 0.32435133 -0.00475733 -0.31599264 -0.00700325 -0.00970693

FREQUENCY: 1586.67 1615.00 3343.86 3344.26 3363.75

REDUCED MASS: 4.50808 8.35200 1.09152 1.09240 1.09821

IR INTENSITY: 0.04077 0.00900 0.39026 0.08542 0.64478

1 C X -0.00846188 0.01788289 -0.00000012 -0.00020228 -0.00000121
Y -0.02102374 0.20618262 0.00000018 -0.00080420 -0.00000274
Z 0.00095717 -0.00398849 0.00037675 0.00001938 0.00128052

2 C X -0.00285168 0.02946831 0.00000023 0.00021454 -0.00000354
Y 0.01275176 -0.09511476 -0.00000015 -0.00038276 0.00000242
Z 0.00063288 -0.00133616 -0.00072144 0.00000867 0.00344043

3 C X 0.01303371 -0.02754714 0.00059227 -0.00036465 0.00036742
Y -0.01262718 -0.08981746 -0.00119233 0.00131612 -0.00142944
Z 0.05816417 -0.04725437 0.00128066 -0.00098564 -0.00007727

4 C X 0.01321518 -0.02815389 -0.00059229 -0.00036454 -0.00036645
Y -0.01219209 -0.09181901 0.00119260 0.00131700 0.00143155
Z -0.05876180 0.04915152 0.00128051 0.00098500 -0.00007891

5 C X 0.00366676 -0.00344569 0.00868411 -0.00883942 -0.01582740
Y 0.00680988 0.00244819 -0.02331436 0.02334915 0.04710286
Z 0.01303529 -0.00474720 0.01158655 -0.01229062 -0.01927466

6 C X 0.00384922 -0.00395050 -0.00868322 -0.00884123 0.01586312
Y 0.00675747 0.00227506 0.02331196 0.02335628 -0.04720462
Z -0.01357219 0.00620672 0.01158561 0.01229178 -0.01932074

7 C X -0.01011364 0.00397432 -0.01963275 0.01955736 -0.01038788
Y 0.00046116 0.03327384 -0.00422194 0.00476948 -0.00558690
Z -0.01857857 0.01061669 -0.04822905 0.04834227 -0.02695395

8 C X -0.01010109 0.00371111 0.01963096 0.01955869 0.01041364

		Y	0.00024119	0.03509541	0.00422108	0.00476791	0.00559937
		Z	0.01852938	-0.01026676	-0.04822443	-0.04834494	-0.02702007
9	C	X	0.00601123	0.00350308	0.00028700	-0.00026286	0.00101606
		Y	0.02741393	0.01160246	0.00113307	-0.00090252	0.00359086
		Z	-0.17245721	-0.02798222	0.00076294	-0.00067926	0.00243418
10	C	X	0.00596384	0.00368808	-0.00028701	-0.00026286	-0.00101574
		Y	0.02736300	0.01184576	-0.00113315	-0.00090247	-0.00358930
		Z	0.17257020	0.02763802	0.00076287	0.00067949	0.00243271
11	H	X	-0.00550703	-0.01293629	-0.09903030	0.10018820	0.18209692
		Y	-0.01560637	-0.02378451	0.27630679	-0.27751217	-0.51207340
		Z	-0.03145050	-0.04883113	-0.12807287	0.12914836	0.22995580
12	H	X	-0.00541632	-0.01295239	0.09901887	0.10021624	-0.18249081
		Y	-0.01616916	-0.02291757	-0.27627668	-0.27759176	0.51318432
		Z	0.03179647	0.04865880	-0.12805897	-0.12918510	0.23045707
13	H	X	-0.01433202	0.02328064	0.22372275	-0.22358195	0.11840712
		Y	0.02030946	-0.12384854	0.05956615	-0.05910887	0.03503466
		Z	-0.02297995	0.01890041	0.54602553	-0.54478134	0.29029325
14	H	X	-0.01436929	0.02364106	-0.22370147	-0.22359199	-0.11870159
		Y	0.02073132	-0.12705642	-0.05956050	-0.05911126	-0.03512090
		Z	0.02296104	-0.01876255	0.54597377	0.54480445	0.29100039
15	H	X	-0.06526277	-0.00760502	-0.00400588	0.00285562	-0.01212396
		Y	-0.21290861	-0.00920055	-0.01399137	0.00915690	-0.04132016
		Z	0.15311752	0.00216367	-0.01104504	0.00715719	-0.03025718
16	H	X	-0.06535446	-0.00724507	0.00400577	0.00285595	0.01211951
		Y	-0.21324908	-0.00802550	0.01399110	0.00915751	0.04130365

Z -0.15340587 -0.00121891 -0.01104483 -0.00715791 -0.03024682

FREQUENCY: 3364.95 3367.46 3389.05

REDUCED MASS: 1.09826 1.08749 1.09974

IR INTENSITY: 0.42582 0.18888 0.72384

1 C X -0.00055863 -0.00000001 0.00054171

Y 0.00088883 0.00000039 0.00078659

Z -0.00003036 -0.00000383 0.00001101

2 C X -0.00128096 0.00000020 -0.00011612

Y 0.00015861 -0.00000023 -0.00002429

Z -0.00001502 -0.00048984 0.00000797

3 C X -0.00041880 -0.00062823 0.00075744

Y 0.00141323 -0.00103460 0.00188407

Z -0.00079612 -0.00032830 -0.00070051

4 C X -0.00041816 0.00062802 0.00075758

Y 0.00140862 0.00103491 0.00188462

Z 0.00079721 -0.00032797 0.00069976

5 C X 0.01615315 0.00105166 0.00001937

Y -0.04691926 -0.00276894 0.00003753

Z 0.02016318 0.00147582 0.00002382

6 C X 0.01611711 -0.00105044 0.00002064

Y -0.04681507 0.00276521 0.00003460

Z -0.02011758 0.00147451 -0.00002595

7 C X 0.01070000 0.00148131 -0.00060723

		Y	0.00456966	0.00019050	-0.00025268
		Z	0.02728840	0.00352843	-0.00119076
8	C	X	0.01067616	-0.00148060	-0.00060647
		Y	0.00455963	-0.00019045	-0.00025268
		Z	-0.02722745	0.00352672	0.00118881
9	C	X	-0.00012633	0.01371105	-0.01364784
		Y	-0.00068903	0.04553473	-0.04576804
		Z	-0.00046794	0.03230360	-0.03890892
10	C	X	-0.00012305	-0.01371114	-0.01364781
		Y	-0.00067768	-0.04553514	-0.04576789
		Z	0.00045976	0.03230390	0.03890894
11	H	X	-0.18334137	-0.01166992	0.00095149
		Y	0.51249938	0.03289265	-0.00134865
		Z	-0.23138091	-0.01431634	0.00011173
12	H	X	-0.18293727	0.01165470	0.00094101
		Y	0.51136505	-0.03285138	-0.00131891
		Z	0.23087247	-0.01429772	-0.00009861
13	H	X	-0.12117600	-0.01544390	0.00570284
		Y	-0.03601958	-0.00388402	0.00107499
		Z	-0.29439133	-0.03725240	0.01324875
14	H	X	-0.12091213	0.01543633	0.00569625
		Y	-0.03594139	0.00388168	0.00107300
		Z	0.29374664	-0.03723327	-0.01323280
15	H	X	0.00144591	-0.15248914	0.15199007
		Y	0.00610766	-0.53245789	0.52781509

Z 0.00507337 -0.38289926 0.38594036
16 H X 0.00140697 0.15249013 0.15198986
Y 0.00597497 0.53246171 0.52781396
Z -0.00497638 -0.38290207 -0.38593968

THERMOCHEMISTRY AT T= 298.15 K

USING IDEAL GAS, RIGID ROTOR, HARMONIC NORMAL MODE APPROXIMATIONS.

P= 1.01325E+05 PASCAL.

ALL FREQUENCIES ARE SCALED BY 1.00000

THE MOMENTS OF INERTIA ARE (IN AMU*BOHR**2)

808.66445 868.55619 1603.07778

THE ROTATIONAL SYMMETRY NUMBER IS 1.0

THE ROTATIONAL CONSTANTS ARE (IN GHZ)

2.22971 2.07596 1.12477

1 IMAGINARY FREQUENCY VIBRATION(S) IS(ARE) EXCLUDED

FROM THE FOLLOWING THERMOCHEMICAL ANALYSIS.

THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000)

0.122609 HARTREE/MOLECULE 26909.540066 CM**-1/MOLECULE

76.938313 KCAL/MOL 321.909902 KJ/MOL

Q LN Q

ELEC. 1.00000E+00 0.000000

TRANS. 5.56227E+07 17.834102
ROT. 3.79841E+05 12.847508
VIB. 5.22827E+00 1.654081
TOT. 1.10462E+14 32.335691

	E	H	G	CV	CP	S
	KJ/MOL	KJ/MOL	KJ/MOL	J/MOL-K	J/MOL-K	J/MOL-K
ELEC.	0.000	0.000	0.000	0.000	0.000	0.000
TRANS.	3.718	6.197	-44.210	12.472	20.786	169.066
ROT.	3.718	3.718	-31.848	12.472	12.472	119.291
VIB.	330.893	330.893	317.810	85.841	85.841	43.881
TOTAL	338.329	340.808	241.752	110.784	119.099	332.238

	E	H	G	CV	CP	S
	KCAL/MOL	KCAL/MOL	KCAL/MOL	CAL/MOL-K	CAL/MOL-K	CAL/MOL-K
ELEC.	0.000	0.000	0.000	0.000	0.000	0.000
TRANS.	0.889	1.481	-10.566	2.981	4.968	40.408
ROT.	0.889	0.889	-7.612	2.981	2.981	28.511
VIB.	79.085	79.085	75.958	20.517	20.517	10.488
TOTAL	80.863	81.455	57.780	26.478	28.465	79.407

.....END OF NORMAL COORDINATE ANALYSIS.....