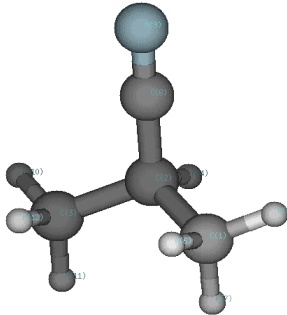
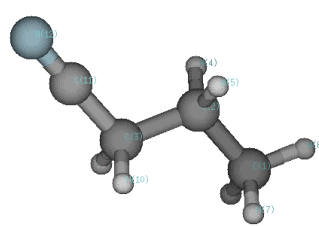


TABLE 1: CCSD(T)-F12/VTZ geometries and rotational constants, CCSD(T)-F12/AVTZ relative energies, and with MP2/VTZ anharmonic frequencies of iso- and n-isopropyl.

iso-PrCN ($C_s X^1A'$)				
	C	0.000000000	0.0019869814	-0.0002619615
	C	1.2680185437	0.1785275421	-0.8400710872
	C	-1.2680185437	0.1785275421	-0.8400710872
	H	0.000000000	0.7392640204	0.8063729169
	C	0.000000000	-1.3222354435	0.6418303426
	N	0.000000000	-2.3735331234	1.1289610857
	H	2.1641563088	0.0569423333	-0.2333323739
	H	1.2939854804	-0.5569886213	-1.6444782387
	H	1.2763159651	1.1750670285	-1.2817769921
	H	-2.1641563088	0.0569423333	-0.2333323739
	H	-1.2763159651	1.1750670285	-1.2817769921
	H	-1.2939854804	-0.5569886213	-1.6444782387
E(UMP2(full))/AVTZ	-211.041323			
E(CCSD(T))/AVTZ	-211.022850			
E(CCSD(T)-F12/AVTZ	-211.078641			
E_r (cm^{-1})	0.0			
ZPE (cm^{-1})	21957.2			
$E_r + \text{ZPE}$ (cm^{-1})	0.0			
Anharmonic frequencies (cm^{-1})	$\nu(a')$ = 3043.7, 3037.9, 2967.6, 2987.5, 2154.1, 1498.5, 1478.0, 1393.9, 1325.8, 1176.2, 1112.6, 929.6, 776.7, 537.5, 353.6, 281.7, 214.7			
	$\nu(a'')$ = 3043.0, 3035.2, 2994.4, 1462.2, 1453.1, 1373.6, 1296.5, 1121.8, 968.7, 931.8, 555.4, 229.1, 180.0			
anti-n-PrCN ($C_s X^1A'$)				
	C	1.4591486035	0.4800218209	0.0000000000
	C	0.0015307963	0.6366006245	0.0000000000
	C	-0.7238258334	-0.7132129912	0.0000000000
	C	-2.2353210659	-0.5224698232	0.0000000000
	H	-0.2802629668	1.2194096078	0.8791696296
	H	-0.2802629668	1.2194096078	-0.8791696296
	H	-0.4120731831	-1.2838609377	-0.8765022178
	H	-0.4120731831	-1.2838609377	0.8765022178
	H	-2.7498354307	-1.4828713429	0.0000000000
	H	-2.5590339214	0.0323742652	0.8824033386
	H	-2.5590339214	0.0323742652	-0.8824033386
	N	2.6072300730	0.3271858414	0.0000000000
E(UMP2(full))	-211.0389602			
E(CCSD(T))	-211.0214950			
E(CCSD(T)-F12/AVTZ	-211.077349			
E_r (cm^{-1})	283.5			
ZPE (cm^{-1})	22041.0			
$E_r + \text{ZPE}$ (cm^{-1})	367.2			
Harmonic frequencies (cm^{-1})	$\nu(a')$ =3117.1, 3098.1, 3086.4, 3074.5, 2203.2, 1522.2, 1507.5, 1483, 1420.5, 1389.4, 1304.8, 1128, 1978, 972.2, 890.4, 523.6, 343.4, 160.2			

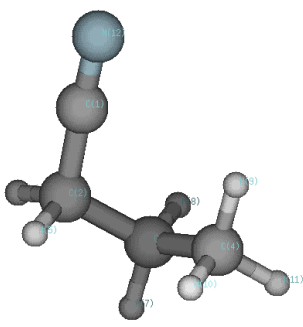
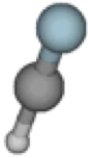
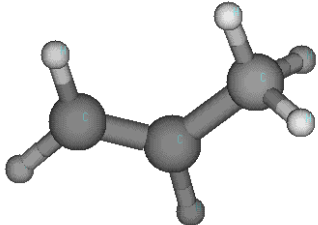
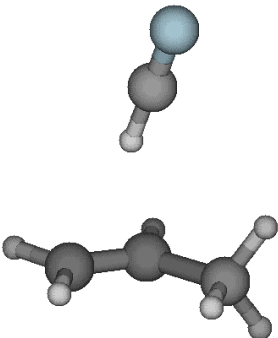
	$\omega(a'')$ =3165.5, 3147.7, 3130.3, 1517.2, 1338.7, 1269.5, 1135.2, 877.2, 749.6, 370.4, 247, 100	
<i>gauche-n-PrCN (C₁ X¹A)</i>		
	C 1.2888695482 0.0728024513 0.0407457108 C 0.1587440185 0.9814298537 0.2642489571 C -1.1272599089 0.4643135924 -0.3925136173 C -1.5690489416 -0.8809152546 0.1704828198 H 0.0185541701 1.0863840001 1.3420446516 H 0.4302523270 1.9619379736 -0.1288454680 H -1.9048732195 1.2138942637 -0.2344969068 H -0.9686695016 0.3879211974 -1.4697923987 H -2.4911251410 -1.2160681015 -0.3035127935 H -0.8062106729 -1.6423709296 0.0034826368 H -1.7476347905 -0.8124377940 1.2453182423 N 2.1623391122 -0.6631642527 -0.1512958342	
	E(MP2)	-211.039468
	E(CCSD(T))	-211.021806
	E(CCSD(T)-F12/AVTZ)	-211.077679
	E_r (cm ⁻¹)	211.1
	ZPE (cm ⁻¹)	22090.7
	$E_r + ZPE$ (cm ⁻¹)	344.6
	Anharmonic frequencies (cm ⁻¹)	$\nu(a')$ = 3036.5, 3029.3, 3008.5, 3001.6, 2994.4, 3008.1, 2955.7, 2158.8, 1504, 1492.9, 1476.4, 1456.6, 1391.2, 1344.1, 1332.1, 1265.8, 1235.9, 1112, 1083.8, 1060.1, 927.2, 874.9, 848.8, 768.9, 552, 368.9, 351.1, 259.6, 172.8, 109.2

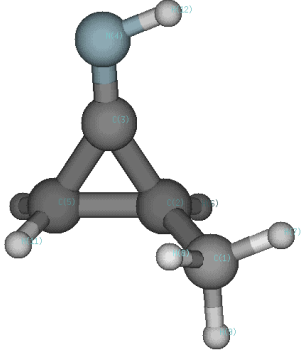
TABLE II: Geometries, energies, harmonic frequencies computed with UMP2(full)/AVTZ

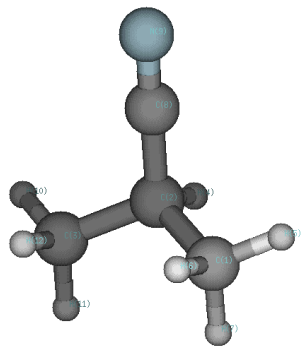
HCN		
	H	0.000000 0.000000 -1.564138
	C	0.000000 0.000000 -0.505556
	N	0.000000 0.000000 0.656782
E(UMP2)	-93.292044	
E(UCCSD(T))	-93.281103	
Rotational constants (MHz)	Be= 44008.3219	
Harmonic frequencies (cm ⁻¹)	$\omega(\pi)=703$	$\omega(\sigma)=2048, 3493$
ZPE (cm ⁻¹)	3474.94	

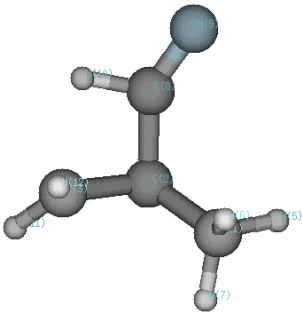
CH ₃ CHCH ₂		
	C	-1.223715 -0.162121 0.000000
	C	0.129623 0.457776 0.000000
	C	1.272075 -0.222427 0.000000
	H	0.172667 1.538408 0.000000
	H	-1.793300 0.144853 -0.875611
	H	-1.153817 -1.247138 0.000000
	H	-1.793300 0.144853 0.875611
	H	2.224600 0.281685 0.000000
	H	1.275250 -1.302026 0.000000
E(UMP2)	-117.688965	
E(UCCSD(T))	-117.689998	
Rotational constants (MHz)	Ae=47022.6123	Be=9430.6045 Ce=8251.6137
Harmonic frequencies (cm ⁻¹)	$\omega(a')=3192,3173,3137,3070,1716,1522,1466,1420,1326,1202,952,945,595$	$\omega(a'')=3262,3154,1509,1087,1039,946,424,215$
ZPE (cm ⁻¹)	17681.75	

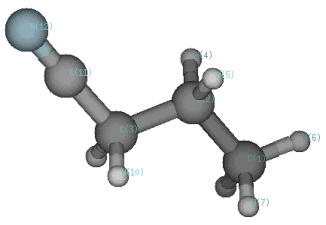
vdw vdw1(R1) Reactant_mep2		
	C	-1.4291019443 -1.1080097576 -0.0051514954
	C	-0.9239945715 0.285921886 -0.1366120076
	C	-0.1428514220 0.8929512883 0.7546130116
	C	1.9991009535 -1.2724980305 -1.0346377967
	N	2.7740793166 -1.9794607247 -1.5365611999
	H	0.1653092551 0.3871323282 1.6587907385
	H	0.1950453263 1.9061382643 0.6067844127
	H	-1.2160780359 0.8317070606 -1.0246353141
	H	1.2907082796 -0.6247294357 -0.5785412593
	H	-1.1003850234 -1.7245339955 -0.8415400046
	H	-1.0804911642 -1.5653556848 0.9176780650
	H	-2.5173829697 -1.1262651985 -0.0079901502
E(UMP2)	-210.98949916447	
E(UCCSD(T))	-210.97653577	
Rotational constants (MHz)	Ae=8171.4105	Be=1867.0950 Ce=1608.0291
Anharmonic frequencies (cm ⁻¹)	$\nu(a')=3453, 3264, 3185, 3170, 3155, 3135, 3069, 2045, 1710, 1521, 1504, 1466, 1424, 1327, 1203, 1088, 1041, 956,$	

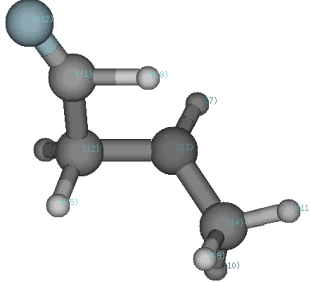
	950, 944, 836, 791, 605, 424, 221, 149, 133, 117, 73, 49
ZPE (cm ⁻¹)	21512.46

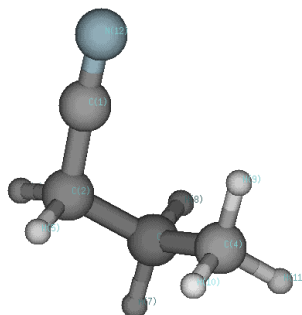
vdw2(R2) TRIANGLE				
	C	1.1599143339	-0.9211959848	0.0961131985
	C	2.4052068596	-0.126190072	-0.1677073080
	C	2.2979374014	1.2485023681	-0.6444506123
	N	1.9999114464	2.4629504337	-0.4712997906
	C	2.7366014847	0.2741410214	-1.6306443193
	H	3.2678498507	-0.3660943555	0.4388600020
	H	0.8145949373	-0.7840283857	1.1185530553
	H	0.3633033403	-0.5972259373	-0.5708614887
	H	1.3321905708	-1.9826792679	-0.0686417795
	H	3.7745794397	0.2647097673	-1.9252628660
	H	2.0337883726	-0.0423598208	-2.3870915548
	H	1.7089609625	2.6097482333	0.4954994635
E(UMP2)	-210.97418637765			
E(UCCSD(T))	-210.95780708			
Rotational constants (MHz)	Ae=9482.9666	Be=4213.6512	Ce=3314.9341	
Anharmonic frequencies (cm ⁻¹)	ν(a')=3459, 3248, 3177, 3160, 3152, 3148, 3072, 1853, 1530, 1512 1455, 1426, 1363, 1273, 1187, 1151, 1133, 1087, 1032, 1023, 987, 898, 833, 757, 726, 493, 395, 323, 215, 171			
ZPE (cm ⁻¹)	22626.74			

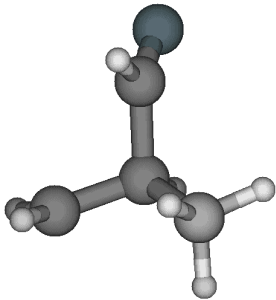
iso-PrCN (iso-propyl) iso-C₃H₇CN Product_mep1= iso-C₃H₇CN				
	C	1.1101925805	-0.8413177279	-0.0240084307
	C	2.2718836034	0.0528841166	-0.4341479007
	C	1.9773481302	1.5190155388	-0.1495574353
	H	2.4506796995	-0.0696252684	-1.5023771344
	H	1.3226970709	-1.8851406816	-0.2362103904
	H	0.916178969	-0.7388014105	1.0408923605
	H	0.2166377867	-0.5469609999	-0.5688201595
	C	3.4860773155	-0.3567348195	0.2508392782
	N	4.4500300869	-0.6807486398	0.8223536079
	H	2.8062152529	2.1529389517	-0.4510132715
	H	1.0869780506	1.8220199163	-0.6948403140
	H	1.7997384539	1.6661980243	0.9129667900
E(UMP2)	-211.04132280246			
E(UCCSD(T))	-211.02285003			
Rotational constants (MHz)	Ae=8106.4049	Be=4004.3570	Ce=2943.4345	
Harmonic frequencies (cm ⁻¹)	ν(a')=3172, 3172, 3166, 3163, 3091, 3084, 3083, 2215, 1534, 1528, 1512, 1510, 1433, 1410, 1364, 1331, 1211, 1156, 1137, 994, 963, 942, 792, 559, 541, 357, 283, 217, 210, 183			
ZPE (cm ⁻¹)	22663.83			

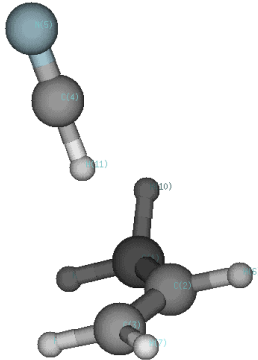
(ts-mep1)ts-iso-propyl(mep1)				
	C	1.0717580333	-0.7996756625	-0.1592190675
	C	2.3062607374	0.0750730598	-0.0723502289
	C	2.9890230179	0.2225636788	-1.4201534410
	H	2.9570069343	-0.2469740322	0.7386615221
	H	0.5305133075	-0.7985069731	0.7817542761
	H	0.4088549364	-0.4339687848	-0.9409419836
	H	1.3638796535	-1.8186993716	-0.4026440196
	C	1.9015017161	1.4924376733	0.0186247718
	N	1.6307088846	2.4559671832	0.6452149568
	H	2.0283680242	1.6420337747	-1.2407677720
	H	3.9473802131	0.7148134984	-1.4457193321
H	2.7595835415	-0.4647860439	-2.2193936822	
E(UMP2)	-210.84724864158			
E(UCCSD(T))	-210.86042357			
Rotational constants (MHz)	Ae=18810.5446	Be=2521.7722	Ce=2393.4955	
Anharmonic frequencies (cm ⁻¹)	v(a')=-2010, 3292, 3186, 3180, 3159, 3110, 3080, 2313, 1677, 1522, 1522, 1476, 1422, 1342, 1299, 1188, 1134, 1064, 977, 942, 919, 863, 811, 609, 500, 445, 348, 276, 255, 163			
ZPE (cm ⁻¹)	21044.32			

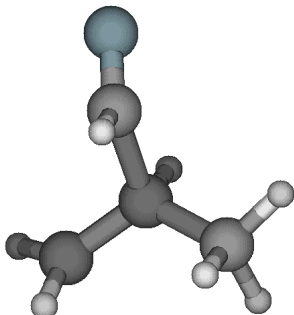
a-C₃H₇CN (a-propyl) Product mep1 =a-propyl				
	C	2.3297991089	-0.2710784448	0.0159859615
	C	0.8455885073	-0.5723991144	-0.0346888252
	C	0.0287963336	0.7131312427	-0.0514667394
	H	0.549427409	-1.1685361273	0.8262527302
	H	0.6063994187	-1.1551485156	-0.9221015593
	H	2.9139569605	-1.1871002919	0.0280348663
	H	2.6370309868	0.3119303551	-0.8499776882
	H	2.5797046569	0.2985078737	0.9089038881
	H	0.2468492122	1.3035823885	0.8371222571
	H	0.3040156998	1.3170624311	-0.9147664653
	C	-1.3966070787	0.4584474903	-0.1000407316
	N	-2.5378382148	0.2233427125	-0.1387936940
	E(UMP2)	-211.03896021651		
	E(UCCSD(T))	-211.02149496		
Rotational constants (MHz)	Ae=24072.3384	Be=2297.4797	Ce=2181.5253	
Harmonic frequencies (cm ⁻¹)	v(a')=3163, 3155, 3139, 3122, 3097, 3086, 3077, 2225, 1528, 1528, 1515, 1485, 1428, 1398, 1346, 1309, 1280, 1141, 1133, 1085, 986, 896, 879, 736, 526, 377, 349, 242, 162, 93			
ZPE (cm ⁻¹)	22752.05			

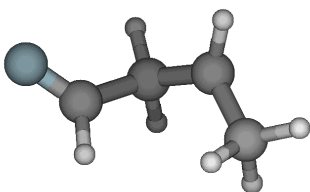
(ts-a-propyl(MEP1)) ts-mep1				
	C	1.9119700543	-0.2680571495	0.1230199209
	C	0.5254022961	-0.3347439089	-0.3968497235
	C	-0.3418328220	0.9094211208	-0.4669369419
	H	-0.8598495983	-0.6838245373	0.5694507181
	H	0.2994698240	-1.0770330978	-1.1477416221
	H	2.3364585396	-1.2574532592	0.2625428815
	H	2.5546174255	0.2746555732	-0.5776644977
	H	1.9493450425	0.2640595081	1.0711811582
	H	0.0118899506	1.6577811517	0.2392614790
	H	-0.4639486280	1.3696994572	-1.4448485502
	C	-1.5503399750	0.2831269881	0.1015689632
	N	-2.7218961092	0.2269231534	0.2280982147
	E(UMP2)	-210.84808359124		
E(UCCSD(T))	-210.86282892			
Rotational constants (MHz)	Ae=18810.5446	Be=2521.7722	Ce=2393.4955	
Anharmonic frequencies (cm ⁻¹)	ν(a')=-2028, 3215, 3171, 3160, 3119, 3100, 3033, 2324, 1672, 1511, 1506, 1482, 1430, 1396, 1276, 1232, 1164, 1138, 1047, 968, 956, 885, 859, 653, 548, 476, 347, 224, 177, 94			
ZPE (cm ⁻¹)	21087.78			

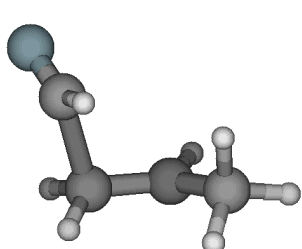
(g-propyl) g-C₃H₇CN				
	C	1.2453158476	0.0298336670	0.0635063051
	C	0.1567311228	0.9657065395	0.2677932569
	C	-1.1316199969	0.4859031106	-0.3918180098
	C	-1.5963938194	-0.8476459507	0.1576364745
	H	0.0037794813	1.0840132956	1.3395419399
	H	0.4532366437	1.9346723126	-0.1283302582
	H	-1.8913224146	1.2485980327	-0.2309974119
	H	-0.9710137554	0.4125696760	1.4658584038
	H	-0.8460074577	-1.6169636960	-0.0104934647
	H	-1.7774030852	-0.7820629535	1.2289673441
	H	-2.5186267273	-1.1657441734	-0.3207149345
	N	2.0986171611	-0.7436718605	-0.1185288375
	E(UMP2)	-211.03946801837		
E(UCCSD(T))	-211.02180638			
Rotational constants (MHz)	Ae=10092.6647	Be=3365.0542	Ce=2763.5906	
Anharmonic frequencies (cm ⁻¹)	ν(a')=3163, 3155, 3141, 3129, 3093, 3089, 3078, 2223, 1530, 1525, 1511, 1484, 1432, 1383, 1369, 1301, 1274, 1139, 1114, 1086, 949, 890, 867, 770, 557, 372, 355, 258, 173, 105			
ZPE (cm ⁻¹)	22764.34			

(Reactant mep1) Product mep2=reactant-mep1				
	C	-0.8700865842	-1.4747950221	0.0518583304
	C	0.2648767145	-0.4658096727	0.0776314024
	C	1.1429175113	-0.5414758276	-1.1018793513
	H	0.8422611382	-0.5634816801	0.9923516702
	H	-1.5248231958	-1.3419632827	0.9092351091
	H	-1.4612594331	-1.3588527601	-0.8552195733
	H	-0.4703030413	-2.4848536679	0.0683710889
	C	-0.3352889637	0.9447118747	0.0901867067
	N	-0.0581211845	1.7898936517	0.9148005647
	H	-1.0439129056	1.1547254118	-0.7128663688
	H	2.1596132894	-0.1977294809	-1.0467935629
H	0.7153066548	-0.7144535442	-2.0752310162	
E(UMP2)	-210.88905056837			
E(UCCSD(T))	-210.89363658			
Rotational constants (MHz)	Ae=8158.1220	Be=4133.8646	Ce=3098.9744	
Anharmonic frequencies (cm ⁻¹)	v(a')=3306, 3208, 3171, 3157, 3129, 3078, 3069, 2165, 1526, 1522, 1496, 1419, 1371, 1301, 1237, 1192, 1143, 1073, 957, 941, 925, 823, 602, 489, 360, 336, 306, 235, 222, 110			
ZPE (cm ⁻¹)	21942.85			

Reactant mep2				
	C	-0.8584422146	-1.3089403880	0.1433777874
	C	0.5221338386	-0.7823039851	-0.0357092928
	C	-1.0341326454	2.2724079442	0.1340039259
	N	-1.7101561114	3.1597141472	0.4626284416
	C	1.0027278585	-0.2976535735	-1.1790194482
	H	1.1688857643	-0.7962834108	0.8322191936
	H	-1.3948103046	-0.7499641714	0.9098847953
	H	-1.4230860145	-1.2504841705	-0.7840225898
	H	-0.8364385329	-2.3478046301	0.4673931235
	H	-0.4154008463	1.4613614248	-0.1640092115
	H	2.0127873331	0.0727264893	-1.2509403399
H	0.3934168752	-0.2728476761	-2.0714723850	
E(UMP2)	-210.98949916447			
E(UCCSD(T))	-210.97653577			
Rotational constants (MHz)	Ae=8170.8441	Be=1866.1846	Ce=1607.3617	
Anharmonic frequencies (cm ⁻¹)	v(a')=3453, 3264, 3185, 3170, 3155, 3135, 3069, 2045, 1710, 1521, 1504, 1466, 1424, 1327, 1203, 1088, 1041, 956, 950, 944, 836, 790, 605, 425, 221, 149, 133, 117, 73, 49			
ZPE (cm ⁻¹)	21512.46			

ts_mep2				
	C	-0.8863636228	-1.4297772176	0.0490186485
	C	0.3221676206	-0.5281088481	0.0570240674
	C	-0.4095407446	1.0842378521	0.0815918322
	N	-0.0441463034	1.8310549543	0.9137088301
	C	1.1309509979	-0.4691677485	-1.0905784377
	H	0.8556432325	-0.5205537051	0.9958380504
	H	-1.5605719262	-1.1889419848	0.8663657101
	H	-1.4286127172	-1.3378736778	-0.8902823240
	H	-0.5706674894	-2.4649469866	0.1543183283
	H	-1.1390246793	1.0855910958	-0.7120998402
	H	2.1319050058	-0.0800508365	-1.0406395430
	H	0.7045066260	-0.6363938972	-2.0664893220
E(UMP2)	-210.88144453047			
E(UCCSD(T))	-210.89660685			
Rotational constants (MHz)	Ae=7955.8619	Be=4028.8099	Ce=3056.9173	
Anharmonic frequencies (cm ⁻¹)	ν(a')=-999, 3300, 3222, 3204, 3203, 3168, 3155, 3078, 2172, 1534, 1521, 1512, 1432, 1410, 1259, 1203, 1147, 1082, 1018, 947, 918, 874, 771, 480, 438, 372, 317, 254, 224, 114			
ZPE (cm ⁻¹)	21672.24			

Reactant_mep1 (Product_mep2 =reactant_mep1)				
	C	1.1134948109	-0.2691748351	-0.0748088760
	C	0.0656105708	0.6055951989	0.6270804275
	C	-1.2449172809	0.3828811014	-0.0053904417
	C	-1.9514865246	-0.9045209688	0.1839747062
	H	0.0574047254	0.2998194802	1.6728920410
	H	0.3923211063	1.6369065433	0.5607683136
	H	-1.5165011803	1.0101474551	-0.8362719736
	H	0.9392827837	-1.344334226	-0.0283056287
	H	-1.4894449975	-1.7091069929	-0.3989215336
	H	-1.9285647805	-1.2163451992	1.2272019078
	H	-2.9887254223	-0.8415107259	-0.1319510690
	N	2.0676461888	0.1796731690	-0.6691478735
E(UMP2)	-210.89053210217			
E(UCCSD(T))	-210.89746555			
Rotational constants (MHz)	Ae=13509.2483	Be=2866.2445	Ce=2644.9309	
Harmonic frequencies (cm ⁻¹)	ν(a')=3249, 3177, 3161, 3104, 3092, 3077, 3020, 2149, 1511, 1506, 1491, 1435, 1399, 1300, 1258, 1215, 1184, 1090, 1018, 961, 913, 894, 831, 519, 448, 399, 279, 148, 110, 81			
ZPE (cm ⁻¹)	22015.50			

ts_mep2				
	C	-1.8953564417	-0.9118654051	0.1800444074
	C	-1.1896349950	0.3738987884	-0.0196586145
	C	1.1882300952	-0.4064265687	-0.1760282133
	N	2.1047839718	0.1152290572	-0.6933557341
	C	0.0245558629	0.640137172	0.6325150052
	H	-1.4649021984	0.9840438279	-0.8632736769
	H	-1.4497460990	-1.6980809078	-0.4421913259
	H	-1.8336150665	-1.2447515053	1.2136691551
	H	-2.9423255655	-0.8465371496	-0.1012619330
	H	0.8317470347	-1.4175830272	-0.0495132510
	H	0.4500492158	1.6233229440	0.5121818326
	H	0.1328731857	0.2508817743	1.6389123482
E(UMP2)	-210.88371470769			
E(UCCSD(T))	-210.90149729			
Rotational constants (MHz)	Ae=12665.1794	Be=2895.2286	Ce=2625.6959	
Anharmonic frequencies (cm ⁻¹)	ν(a')=-1004, 3255, 3237, 3198, 3167, 3145, 3114, 3009, 2185, 1538, 1512, 1501, 1444, 1409, 1255, 1214, 1150, 1097, 1034, 1000, 947, 924, 830, 656, 433, 410, 288, 157, 111, 110			
ZPE (cm ⁻¹)	21672.68			