SUPPORTING INFORMATION 3

Supporting information

Supporting information contains structures of all minima and transition states. It also contains rotational constants (GHZ) and scaled (0.96) vibrational frequencies (cm^{-1}).

n-C_4H_3+C_2H_2 : Minima

n-$C_4H_3.C_2H_2$ (cis)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.221728	1.856919	-0.000284
2	6	1.525738	0.685002	0.000063
3	6	1.938796	-0.680984	0.000555
4	6	1.119236	-1.719611	-0.000696
5	6	-2.280065	0.16085	0.000002
6	6	-3.438571	-0.172915	0.000185
7	1	0.942883	2.886385	-0.000554
8	1	3.022607	-0.8555	0.002043
9	1	1.229704	-2.796171	-0.000629
10	1	-4.462715	-0.470489	0.000337
11	1	-1.253655	0.46021	-0.000146

Vibrational frequencies

16.016448	222.727872	563.356128	778.307712	1999.000608	3352.399104
16.274304	337.198272	620.91648	792.963744	2132.082816	3386.531232
62.137824	516.170496	657.350016	984.037824	2932.288128	
66.289728	528.71712	767.308224	1229.700192	3142.024704	
85.685952	535.084032	768.52848	1587.218112	3282.651264	

Rotational constants (GHZ)

4.76068 1.47106 1.12380

n-$C_4H_3.C_2H_2$ (trans)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.213108	-0.797726	0.001838
2	6	-2.093467	-0.337663	-0.000234
3	6	-0.763503	0.185111	-0.002475
4	6	-0.492015	1.480878	-0.001833
5	6	2.85523	0.229597	0.003748
6	6	3.512995	-0.780678	-0.001288
7	1	-4.202975	-1.19414	0.003813
8	1	0.056701	-0.536618	-0.004681
9	1	-1.049439	2.409306	-0.000049
10	1	2.254567	1.112776	0.008018
11	1	4.104358	-1.668436	-0.005638

Vibrational frequencies

21.8472	212.185536	562.270368	844.299744	2000.413248	3355.135872
25.669536	352.069632	602.625312	857.157216	2128.081824	3390.371424
54.547488	494.853312	668.507136	969.258432	3002.372736	
62.3592	527.092608	752.162496	1241.180352	3133.230336	
81.517728	548.953824	753.511776	1572.035808	3291.049728	

Rotational constants (GHZ)
9.13873 1.06775 0.95605

lctt

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.415423	-2.237534	0
2	6	-1.280471	-1.03282	0
3	6	-1.166626	0.382099	0
4	6	0	1.06999	0
5	6	1.325438	0.458942	0
6	6	2.462111	1.135924	0
7	1	-1.526349	-3.297053	0
8	1	-2.100607	0.940245	0
9	1	-0.045143	2.155936	0
10	1	1.349409	-0.632226	0
11	1	2.772521	2.173498	0

Vibrational frequencies

125.55792	484.002336	756.576	1068.75504	1587.712608	3118.266048
133.875936	559.858848	821.71776	1195.276896	2121.58704	3349.789344
272.25792	617.893056	883.21872	1222.118304	3005.405856	
290.683872	659.844384	909.0384	1365.722112	3037.859136	
393.924768	673.84752	948.880608	1559.60016	3062.238624	

Rotational constants (GHZ)
10.24659 2.02978 1.69418

lctc

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.465265	-2.183006	0
2	6	-1.312964	-0.980199	0
3	6	-1.177865	0.433226	0
4	6	0	1.101072	0
5	6	1.31072	0.470203	0
6	6	2.460003	1.125693	0
7	1	-1.592777	-3.240544	0
8	1	-2.103092	1.005339	0
9	1	-0.021707	2.187192	0
10	1	1.317998	-0.626072	0
11	1	3.511798	0.872153	0

Vibrational frequencies

124.504128	479.854944	761.78928	1086.006624	1600.075584	3130.514592
156.470304	556.746432	777.996768	1192.456128	2120.620992	3350.630112
269.309664	616.316544	830.271648	1213.636032	2943.500064	
295.3296	652.124928	913.26768	1367.900448	3041.25264	
412.18368	684.900864	951.155424	1561.486464	3068.777568	

Rotational constants (GHZ)
9.82221 2.04590 1.69322

lcct

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.363764	0.086708	0
2	6	1.257093	0.584226	0
3	6	0	1.238361	0
4	6	-1.217068	0.645388	0
5	6	-1.539113	-0.786831	0
6	6	-0.704171	-1.813384	0
7	1	3.327917	-0.366362	0
8	1	0.03626	2.326024	0
9	1	-2.079373	1.308308	0
10	1	-2.609447	-1.006125	0
11	1	0.361615	-1.988656	0

Vibrational frequencies

88.67952	484.607712	741.81984	987.633408	1605.468864	3156.24576
146.319072	563.069184	835.396032	1211.162496	2114.385408	3349.395168
278.554464	608.976864	863.076768	1244.10048	2982.990144	
291.170112	658.641696	908.59104	1378.0992	3032.410464	
433.78272	703.059168	944.563776	1544.833248	3052.618656	

Rotational constants (GHZ)
6.62282 2.95280 2.04226

lccc

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.339528	0.072408	0
2	6	1.244492	0.59512	0
3	6	0	1.270662	0
4	6	-1.213279	0.669215	0
5	6	-1.476983	-0.767523	0
6	6	-0.576164	-1.73805	0
7	1	3.285496	-0.416981	0
8	1	0.041206	2.357768	0
9	1	-2.088189	1.31412	0
10	1	-2.53787	-1.046139	0
11	1	-0.606209	-2.819758	0

Vibrational frequencies

118.927104	477.211488	734.672256	995.986944	1604.58576	3125.437344
122.246688	567.041184	820.617792	1199.1744	2114.373504	3352.011552
248.419488	604.03296	824.939616	1233.858432	2927.177088	
297.518496	635.905056	925.16832	1381.573152	3038.28336	
453.429792	697.449504	941.376576	1551.412992	3060.935136	

Rotational constants (GHZ)
6.38156 3.08159 2.07810

ltct

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.033404	-0.027677	-0.053861
2	6	-1.822356	-0.156055	0.018817
3	6	-0.418268	-0.348915	0.106813
4	6	0.493585	0.651249	-0.026593
5	6	1.963607	0.493077	0.039852
6	6	2.658919	-0.635043	-0.073240
7	1	-4.103422	0.104204	-0.117645
8	1	-0.076650	-1.365237	0.301848
9	1	0.132588	1.665408	-0.185522
10	1	2.519829	1.423576	0.178509
11	1	2.475154	-1.687771	-0.247922

Vibrational frequencies

61,19136	475,471008	805,34304	1032,1368	1614,552096	3131,222304
143,317344	544,346208	859,476672	1226,469792	2125,17312	3355,0632
175,335648	552,011424	874,74912	1271,931552	2991,56064	
254,840256	605,375616	950,115744	1294,504896	3032,770848	
440,020896	641,088768	967,203744	1557,163488	3055,303872	

Rotational constants (GHZ)
20.64276 1.61272 1.50023

C4Y-1

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.511375	-0.000389	-0.347655
2	6	1.384080	0.000669	0.087766
3	6	0.027455	0.000249	0.624500
4	6	-0.969800	1.021353	0.035112
5	6	-1.796675	-0.000584	-0.434267
6	6	-0.969135	-1.020988	0.034899
7	1	3.499424	-0.001659	-0.748190
8	1	0.053489	0.000261	1.723384
9	1	-0.964999	2.103286	-0.008397
10	1	-2.744634	-0.000643	-0.964006
11	1	-0.967076	-2.103107	-0.004924

Vibrational frequencies

149.875104	523.578336	881.321664	1088.764896	1405.448064	3131.627424
177.562656	570.21552	882.870048	1142.31168	2142.99792	3355.7472
358.297248	583.418592	909.486048	1163.38512	2916.260352	
466.206528	584.00784	941.20848	1284.94176	3087.532128	
479.12448	827.644512	991.905024	1288.360992	3121.010976	

Rotational constants (GHZ)
10.76365 2.59454 2.34276

FLV-1

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.165294	-0.095633	0
2	6	0	0.826997	0
3	6	1.201671	-0.035166	0
4	6	0.787501	-1.32374	0
5	6	-0.683933	-1.360515	0
6	6	-0.034943	2.151089	0
7	1	-0.795239	2.922947	0
8	1	2.21571	0.342267	0
9	1	1.423259	-2.202145	0
10	1	-1.275819	-2.26946	0
11	1	-2.197926	0.228199	0

Vibrational frequencies

200.035872	668.720544	871.834368	1074.382944	1565.268672	3128.617824
315.898752	710.705376	886.761216	1131.350592	1602.188832	3133.781184
496.830528	757.828224	900.729888	1267.546848	3092.546016	
605.904288	771.191232	973.891296	1342.988448	3104.832864	
651.139776	823.450368	1070.826624	1481.623584	3127.19376	

Rotational constants (GHZ)
8.33841 4.00588 2.70592

Phenyl

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.00000000	0.00000000	-1.40031705
2	6	0.00000000	-1.22655589	-0.77144436
3	6	0.00000000	-1.21379145	0.63308210
4	6	0.00000000	0.00000000	1.32475219
5	6	0.00000000	1.21379145	0.63308210
6	6	0.00000000	1.22655589	-0.77144436
7	1	0.00000000	-2.16357742	-1.32206191
8	1	0.00000000	-2.15400271	1.17993864
9	1	0.00000000	0.00000000	2.41136278
10	1	0.00000000	2.15400271	1.17993864
11	1	0.00000000	2.16357742	-1.32206191

Vibrational frequencies

386.934912	694.887456	947.714496	1139.717856	1531.130688	3070.650432
411.478464	784.290816	982.911936	1266.462048	1581.638112	3079.649376
577.308096	855.176928	1017.732864	1289.91216	3048.88368	
593.990592	918.604032	1039.996896	1418.925984	3055.161888	
645.450144	947.440032	1139.626368	1431.20688	3068.294784	

Rotational constants (GHZ)
6.26824 5.59969 2.95757

l-C_6H_4.H

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.547331	-2.060652	0
2	6	-1.355364	-0.864752	0
3	6	-1.188877	0.542668	0
4	6	0.000000	1.192245	0
5	6	1.274238	0.571986	0
6	6	2.385334	0.089084	0
7	1	-1.689563	-3.117401	0
8	1	-2.098224	1.140831	0
9	1	-0.010396	2.280569	0
10	1	3.038816	3.234799	0
11	1	3.351369	-0.362268	0

Vibrational frequencies

16.076832	222.727776	563.38848	778.220064	1999.00464	3352.42848
16.242912	337.148256	620.964576	792.965088	2132.059488	3386.568288
61.950336	516.130848	657.347712	983.979648	2932.237728	
66.216192	528.7488	767.29296	1229.656032	3142.093536	
85.722912	535.14624	768.371616	1587.235296	3282.728928	

Rotational constants (GHZ)
4.75991 1.47286 1.12481

n-C_4H_3+C_2H_2 : Transition states

TS(n-C_4H_3.C_2H_2 (cis)→lctt)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.940251	-1.680128	0.000000
2	6	-1.603023	-0.516886	0.000000
3	6	-1.244880	0.865231	0.000000
4	6	0.000000	1.327078	0.000000
5	6	1.771090	-0.325103	0.000000
6	6	2.880444	0.175418	0.000000
7	1	-2.232502	-2.705583	0.000000

8	1	-2.082734	1.573649	0.000000
9	1	0.390258	2.337417	0.000000
10	1	0.964536	-1.027840	0.000000
11	1	3.780158	0.748701	0.000000

Vibrational frequencies

*i*272.123904	250.657056	571.682496	815.832672	1909.9872	3353.939808
60.62832	343.904832	617.187744	826.481568	2128.868448	3367.662336
85.785792	549.203328	676.83408	994.187808	2936.19456	
90.499488	549.995136	753.33936	1226.909472	3123.869472	
201.5112	556.902336	768.323712	1574.63952	3274.668384	

Rotational constants (GHZ)

6.5998759 1.9002788 1.4754560

TS(n-C_4H_3.C_2H_2 (cis)→lcct)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.025044	2.110233	0.000000
2	6	0.000000	1.465397	0.000000
3	6	1.258326	0.795030	0.000000
4	6	1.458815	-0.517348	0.000000
5	6	-0.367207	-2.148553	0.000000
6	6	-1.440138	-1.575174	0.000000
7	1	-1.937258	2.661999	0.000000
8	1	2.134232	1.456602	0.000000
9	1	2.392359	-1.071915	0.000000
10	1	0.374473	-2.915975	0.000000
11	1	-2.272321	-0.908226	0.000000

Vibrational frequencies

i 263.600928	265.778016	562.289568	819.6216	1918.932192	3354.9072
25.991904	340.730016	607.781184	826.765536	2129.791296	3381.817248
88.059744	552.493344	671.113728	1010.465856	2930.77536	
105.139584	554.986656	737.104704	1234.37616	3087.578784	
176.904672	558.714624	739.67856	1582.559424	3300.555744	

Rotational constants (GHZ)
4.9521050 2.5773782 1.6951293

TS(n-C_4H_3.C_2H_2 (trans)→ltct)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.234496	-0.142566	-0.055992
2	6	-2.029265	-0.162479	0.061531
3	6	-0.609177	-0.203566	0.212269
4	6	0.204966	0.741153	-0.243533
5	6	2.550691	0.402053	0.246678
6	6	2.922068	-0.668778	-0.197867
7	1	-4.294472	-0.114450	-0.166683
8	1	-0.191230	-1.064217	0.737973
9	1	0.024940	1.655865	-0.799038
10	1	2.547158	1.348739	0.740610
11	1	3.084886	-1.620840	-0.651381

Vibrational frequencies

*i*277.317984	242.27712	562.233984	868.101792	1910.2584	3355.333824
39.769056	363.123744	597.576864	879.85392	2124.972384	3374.258688
58.582848	502.921152	690.372768	979.895328	3008.24496	
81.756864	549.380352	724.473696	1242.470784	3099.237792	
179.459328	556.894752	740.79744	1566.62736	3294.681696	

Rotational constants (GHZ)
17.9922404 1.2636870 1.2074749

TS(lctt→lctc)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.464346	-2.203487	0.000000
2	6	-1.307178	-1.001381	0.000000
3	6	-1.174330	0.412427	0.000000
4	6	0.000000	1.086177	0.000000
5	6	1.319994	0.456192	0.000000
6	6	2.463504	1.102154	0.000000
7	1	-1.592602	-3.260980	0.000000
8	1	-2.101828	0.981306	0.000000
9	1	-0.026519	2.172220	0.000000
10	1	1.308233	-0.641353	0.000000
11	1	3.386855	1.636318	0.000000

Vibrational frequencies

*i*719.430336	419.849856	686.632032	1045.655424	1586.041056	3315.545856
126.61968	493.591104	745.665984	1185.104832	2120.878656	3350.212416
140.710464	558.860544	832.6584	1228.02672	2920.293408	
272.376	585.561312	891.524256	1362.569088	3038.05728	
301.110144	615.67344	949.132992	1563.878496	3067.683744	

Rotational constants (GHZ)
10.10024 2.02247 1.68505

TS(lctt→lcct)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.332628	-0.872888	0.049752
2	6	-1.504779	0.005683	-0.047224
3	6	-0.577727	1.077227	-0.174570
4	6	0.744634	0.991514	0.057767
5	6	1.459977	-0.243623	0.496561
6	6	2.046098	-1.070887	-0.340181
7	1	-3.044170	-1.660523	0.139808
8	1	-0.992068	2.036560	-0.481468
9	1	1.347073	1.889526	-0.070717
10	1	1.497003	-0.438653	1.571997
11	1	2.178713	-1.149065	-1.412252

Vibrational frequencies

i 131.375808	543.0744	733.635936	999.312288	1611.091584	3119.51328
123.661152	574.61856	818.351232	1191.110112	2131.963968	3350.651136
210.43632	580.41024	845.4408	1202.345664	2975.415168	
311.84208	614.259072	906.048288	1352.83584	3022.696608	
352.415328	712.86096	940.467744	1595.090208	3041.168352	

Rotational constants (GHZ)
7.12424 2.43276 1.94711

TS(Ictc→Iccc)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.301271	-0.949651	0.051821
2	6	-1.514127	-0.034001	-0.040066
3	6	-0.638345	1.081816	-0.154859
4	6	0.692267	1.046394	0.033936
5	6	1.470748	-0.164532	0.413148
6	6	2.059311	-0.979855	-0.431942
7	1	-2.976746	-1.769217	0.133681
8	1	-1.103679	2.031958	-0.412730
9	1	1.249182	1.976148	-0.071965
10	1	1.563025	-0.359396	1.491598
11	1	2.656712	-1.880529	-0.372807

Vibrational frequencies

i 158.544096	543.0672	720.247008	1010.945664	1634.591616	3126.978144
120.653664	551.56368	769.941024	1200.22752	2134.036416	3356.269152
216.380256	572.174016	812.478336	1211.265312	2898.343296	
309.319872	605.7	912.151488	1367.319936	3027.546528	
359.047872	716.270208	941.835168	1602.097536	3045.440064	

Rotational constants (GHZ)
7.01797 2.44120 1.90948

TS(Icct→Iccc)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.332628	-0.872888	0.049752
2	6	-1.504779	0.005683	-0.047224
3	6	-0.577727	1.077227	-0.174570
4	6	0.744634	0.991514	0.057767
5	6	1.459977	-0.243623	0.496561
6	6	2.046098	-1.070887	-0.340181
7	1	-3.044170	-1.660523	0.139808
8	1	-0.992068	2.036560	-0.481468
9	1	1.347073	1.889526	-0.070717
10	1	1.497003	-0.438653	1.571997
11	1	2.178713	-1.149065	-1.412252

Vibrational frequencies

i 699.91536	463.851744	710.212032	984.035424	1605.317184	3322.40784
109.2096	494.97552	757.852608	1198.916928	2114.384544	3350.700576
131.380704	567.260832	809.05488	1240.14384	2892.870816	
258.95568	590.000928	867.201696	1373.835168	3034.490112	
298.698528	600.855264	941.776608	1546.244352	3054.904512	

Rotational constants (GHZ)
7.12424 2.43276 1.94711

TS(Ictc→I-C_6H_4 + H)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.376827	-0.968488	-0.062997
2	6	1.575887	-0.059906	-0.029616
3	6	0.710904	1.062468	-0.011577
4	6	-0.640757	1.032862	0.027962
5	6	-1.479453	-0.123815	0.052814
6	6	-2.451736	-0.843214	-0.142597
7	1	3.051577	-1.793870	-0.084896
8	1	1.192254	2.038268	-0.044195
9	1	-1.170274	1.983626	0.020236
10	1	-0.437954	-1.211197	1.296282
11	1	-3.185633	-1.616267	-0.191365

Vibrational frequencies

*i*716.8968	372.130176	589.928064	854.65584	1592.90592	3341.54304
75.436416	424.347552	600.492768	923.04432	2020.87008	3355.157376
175.241664	470.583648	614.534496	1003.195392	2127.073248	
238.50432	557.287968	706.887936	1214.54976	3041.452032	
275.969376	581.597088	742.811136	1375.178688	3057.699648	

Rotational constants (GHZ)

7.90421 2.18166 1.73381

TS(Iccc→I-C_6H_4 + H)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.288074	0.910314	0.000000
2	6	1.504269	-0.013254	0.000000
3	6	0.634573	-1.131158	0.000000
4	6	-0.719819	-1.080143	0.000000
5	6	-1.474380	0.132243	0.000000
6	6	-1.787014	1.315858	0.000000
7	1	2.959711	1.738511	0.000001
8	1	1.105164	-2.112791	0.000000
9	1	-1.273067	-2.013559	0.000000
10	1	-3.235086	-0.701297	0.000004
11	1	-2.230942	2.285971	0.000000

Vibrational frequencies

*i*659.140896	369.447648	587.158368	868.534176	1572.845856	3344.725728
51.856512	455.448096	601.829184	931.827168	2028.856128	3355.104864
112.13376	484.780128	603.333312	1003.471008	2129.804448	
233.395584	552.014016	720.257664	1210.308288	3046.79904	
271.61952	569.092224	747.26832	1374.98496	3085.262784	

Rotational constants (GHZ)

6.51119 2.62323 1.86989

TS(Iccc→C4Y-1)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.394174	0.327956	-0.313835
2	6	-1.326807	-0.127140	0.037048
3	6	-0.141838	-0.774788	0.501046
4	6	1.060736	-0.930956	-0.256969
5	6	1.585936	0.371224	-0.468075
6	6	1.021045	1.097577	0.528720
7	1	-3.309709	0.758709	-0.648451
8	1	-0.350783	-1.517548	1.279498
9	1	1.586829	-1.877645	-0.363535
10	1	2.286547	0.702687	-1.234379
11	1	0.957727	2.150559	0.799257

Vibrational frequencies

*i*638.275584	487.75584	740.736192	1028.397312	1439.031936	3063.183744
160.790784	505.119936	841.921632	1115.600736	2110.90272	3356.789856
184.318752	605.021856	847.526496	1200.726912	2962.619808	
366.052512	612.165312	886.289568	1363.776	3028.532352	
424.218336	711.452736	928.265568	1373.91792	3054.222336	

Rotational constants (GHZ)
8.12978 2.78315 2.37195

TS(Iccc→FLV-1)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.692572	2.155090	0.000000
2	6	0.000000	1.134725	0.000000
3	6	1.184784	0.333973	0.000000
4	6	1.081784	-1.013145	0.000000
5	6	-0.259888	-1.597459	0.000000
6	6	-1.292581	-0.766015	0.000000
7	1	-1.493455	2.860575	0.000000
8	1	2.141708	0.847128	0.000000
9	1	1.962988	-1.647856	0.000000
10	1	-0.369549	-2.685300	0.000000
11	1	-2.370853	-0.857558	0.000000

Vibrational frequencies

*i*427.027296	505.0536	731.462112	982.882752	1602.538272	3133.531584
167.5176	507.39456	828.399552	1138.294368	1954.495392	3334.250016
235.775712	590.946528	836.946816	1206.588768	2981.364864	
325.422144	629.016672	921.499776	1358.246112	3073.240416	
483.264576	707.873664	922.577664	1526.157312	3091.492416	

Rotational constants (GHZ)
7.02299 3.50252 2.33700

TS(Iccc→Phenyl)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.696780	-1.770069	0.000000
2	6	-1.217876	-0.659639	0.000000
3	6	-1.205835	0.752717	0.000000
4	6	0.000000	1.383389	0.000000
5	6	1.290770	0.709044	0.000000
6	6	1.498907	-0.610317	0.000000
7	1	-0.483325	-2.815553	0.000000
8	1	-2.134286	1.316520	0.000000
9	1	0.014072	2.471184	0.000000
10	1	2.162621	1.373588	0.000000
11	1	2.425803	-1.176494	0.000000

Vibrational frequencies

*i*316.779648	462.76128	728.73792	1011.699168	1576.93392	3082.38576
223.790112	541.923168	846.93168	1172.768832	2011.836288	3339.05136
297.52848	634.829472	861.83856	1241.43792	2942.50032	
341.512896	672.536736	933.180576	1382.364864	3052.54464	
439.58544	725.183424	965.424672	1502.061984	3072.944928	

Rotational constants (GHZ)
5.57685 4.39147 2.45684

i-C_4H_3+C_2H_2 : Minima

i-C_4H_3.C_2H_2

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.439312	1.940120	0.000004
2	6	1.121753	0.822193	-0.000006
3	6	1.735083	-0.348369	-0.000006
4	6	2.285076	-1.458062	0.000007
5	6	-2.058384	-0.812069	-0.000004
6	6	-3.179892	-0.369520	0.000003
7	1	-0.652931	1.941208	0.000008
8	1	0.925049	2.917570	0.000004
9	1	2.906330	-2.325002	0.000017
10	1	-1.059763	-1.190451	-0.000029
11	1	-4.176373	0.010919	0.000019

Vibrational frequencies

24.250272	145.477344	541.398048	858.061056	1949.922816	3338.792736
42.768768	237.82464	560.944032	875.124192	2000.073696	3393.768672
49.51632	240.370944	595.9488	958.586304	2975.203968	
88.036512	425.575104	755.079168	1400.624064	3037.220544	
121.067424	534.753024	757.66224	1739.68512	3295.935744	

Rotational constants (GHZ)
4.63869 1.59462 1.18668

bcc

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.485663	-0.593321	-0.044414
2	6	1.358611	-0.153946	-0.012574
3	6	0.005529	0.317055	0.030588
4	6	-0.267600	1.637425	0.016880
5	6	-1.047487	-0.732135	0.097956
6	6	-2.336009	-0.558219	-0.117481
7	1	3.486590	-0.959562	-0.076194
8	1	-1.292129	1.992010	0.068945
9	1	0.523731	2.376092	-0.045442
10	1	-0.684004	-1.736933	0.342516
11	1	-3.226433	-1.172757	-0.115554

Vibrational frequencies

46.805088	510.335904	699.166368	958.791648	1612.634592	3143.354016
157.915872	534.246528	712.822848	1185.585696	2133.955584	3354.80448
264.770304	553.64304	799.645728	1258.151424	2947.161696	
276.030336	603.57888	868.945536	1389.734112	3055.895136	
457.503552	668.41728	888.81072	1579.544064	3140.919168	

Rotational constants (GHZ)
7.95056 2.50907 1.91388

bct

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.484358	-0.511837	0.119890
2	6	-1.346239	-0.109737	0.031531
3	6	0.019736	0.304591	-0.084027
4	6	0.360981	1.607736	-0.055485
5	6	1.020862	-0.795325	-0.248066
6	6	2.253418	-0.773119	0.215121
7	1	-3.494151	-0.844450	0.202228
8	1	1.393213	1.916714	-0.185343
9	1	-0.384237	2.382948	0.086594
10	1	0.657305	-1.681551	-0.771253
11	1	2.881473	-0.107515	0.793994

Vibrational frequencies

79.279968	527.892768	706.346688	933.783072	1611.886368	3140.764704
162.021024	540.969888	743.13072	1187.2848	2131.223424	3354.58464
262.704	567.54768	863.984832	1244.487552	3010.90992	
277.79904	602.320512	885.199104	1390.669344	3055.426176	
414.966144	688.400352	888.429216	1577.42784	3131.702976	

Rotational constants (GHZ)
7.6590243 2.5652819 1.9650062

btt

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.889784	-1.276575	0.000000
2	6	1.034406	-0.421485	0.000000
3	6	0.000000	0.571092	0.000000
4	6	0.300685	1.886442	0.000000
5	6	-1.410236	0.111284	0.000000
6	6	-1.813221	-1.144318	0.000000
7	1	2.656169	-2.018095	0.000000
8	1	-0.483155	2.638290	0.000000
9	1	1.328065	2.233541	0.000000
10	1	-2.150176	0.914331	0.000000
11	1	-1.359410	-2.126712	0.000000

Vibrational frequencies

138.110592	521.57136	702.269088	941.393376	1601.781984	3142.420992
149.302944	566.809632	731.357952	1211.512896	2138.299872	3354.887328
269.079264	573.482976	860.3736	1258.245984	3003.757152	
287.22624	605.277984	869.417856	1393.174464	3051.910656	
432.117984	693.600576	884.89488	1577.946048	3138.411936	

Rotational constants (GHZ)
4.8557518 3.6795891 2.0933167

btc

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.234356	1.887916	0.000000
2	6	0.000000	0.558799	0.000000
3	6	-1.377485	0.028226	0.000000
4	6	-1.711050	-1.248290	0.000000
5	6	1.083841	-0.380028	0.000000
6	6	1.993731	-1.176309	0.000000
7	1	-0.585950	2.599936	0.000000
8	1	1.242942	2.285738	0.000000
9	1	2.796579	-1.877984	0.000000
10	1	-2.165125	0.791783	0.000000
11	1	-2.628798	-1.821356	0.000000

Vibrational frequencies

144.08784	508.599744	711.0072	953.29056	1609.599648	3141.146304
154.223712	564.853824	718.437408	1218.496512	2140.760352	3356.092608
268.140384	582.757728	816.171648	1267.511232	2937.699456	
281.394624	602.384832	829.410624	1392.495648	3051.871296	
443.015424	685.503648	880.574592	1580.809344	3139.537824	

Rotational constants (GHZ)
4.9153413 3.5561827 2.0633656

C4Y-2

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.689893	0.003945	-0.000216
2	6	-1.468432	-0.029891	-0.000094
3	6	-0.087346	-0.047870	0.000231
4	6	0.934161	-1.045303	0.000051
5	6	1.957666	-0.124052	-0.000125
6	6	0.989241	1.059799	0.000046
7	1	1.004001	1.696210	0.893216
8	1	1.003697	1.696133	-0.893181
9	1	3.038851	-0.191787	-0.000258
10	1	0.896604	-2.130113	0.000098
11	1	-3.755529	0.029790	0.000768

Vibrational frequencies

152.222496	513.58272	871.656192	1054.385472	1463.272992	3123.383328
174.403008	579.377472	919.7688	1166.018784	2006.539968	3350.247168
379.150176	584.299296	977.299968	1236.299136	2934.346944	
382.37856	622.280736	1020.401088	1326.95184	2976.335424	
485.294976	854.848608	1045.958688	1417.358976	3092.413824	

Rotational constants (GHZ)
13.02135 2.41911 2.06693

C4

Structure

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.679531	1.889515	0.000000
2	6	0	0.000000	0.743576	0.000000
3	6	0	-0.377392	-0.731505	0.000000
4	6	0	-1.496248	-1.412798	0.000000
5	6	0	1.416103	0.312744	0.000000
6	6	0	1.095502	-1.007462	0.000000
7	1	0	1.665822	-1.929464	0.000000
8	1	0	2.353860	0.856917	0.000000
9	1	0	-1.765085	1.897278	0.000000
10	1	0	-0.172511	2.850388	0.000000
11	1	0	-1.832696	-2.439538	0.000000

Vibrational frequencies

210.024192	674.64432	815.971008	1041.592128	1638.400896	3128.047968
234.291744	680.815584	856.8432	1130.05968	1694.764512	3157.608384
286.19616	702.448896	886.008192	1246.88928	3044.495232	
391.88592	730.724736	891.095808	1405.36176	3101.663136	
608.676096	775.420704	965.513568	1494.883872	3123.728544	

Rotational constants (GHZ)
5.8273144 4.3461774 2.4894641

FLV-2

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.114091	-0.194208	0.000000
2	6	0.585287	-1.441303	0.000000
3	6	-0.900453	-1.361263	0.000000
4	6	-1.204860	-0.054915	0.000000
5	6	0.000000	0.783243	0.000000
6	6	0.079395	2.123422	0.000000
7	1	-0.810760	2.745351	0.000000
8	1	2.162352	0.080103	0.000000
9	1	1.138093	-2.375473	0.000000
10	1	1.039347	2.632668	0.000000
11	1	-1.569789	-2.212509	0.000000

Vibrational frequencies

192.539712	696.725472	884.276256	1160.811168	1560.732576	3121.569312
324.588576	742.545984	919.215744	1230.230688	1647.451584	3126.9552
390.710688	745.717056	924.38064	1293.048096	3045.519264	
603.2544	783.196032	945.479328	1404.81168	3086.432256	
647.40672	876.56976	1068.046656	1474.668096	3113.0976	

Rotational constants (GHZ)
9.0349655 3.7485774 2.6493647

b-C_6H_4.H

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.426386	-0.741431	0.000112
2	6	-1.344620	-0.201699	0.000035
3	6	-0.046887	0.411608	-0.000058
4	6	0.103296	1.754014	-0.000104
5	6	1.084389	-0.471937	-0.000070
6	6	2.022221	-1.235241	-0.000078
7	1	-3.383833	-1.210995	0.000181
8	1	1.090697	2.202657	-0.000156
9	1	-0.760072	2.410247	-0.000078
10	1	3.848796	1.410812	0.001124
11	1	2.852335	-1.904607	-0.000088

Vibrational frequencies

6.48432	238.320576	567.12144	731.504736	1585.179168	3354.902112
47.65008	345.978048	605.112864	892.93632	2136.343776	3355.918464
101.673024	468.56928	607.41456	922.641984	2143.155936	
132.32784	561.342528	658.4352	1235.880576	3059.918688	
226.299456	561.479616	708.958752	1381.5768	3150.451392	

Rotational constants (GHZ)
5.97488 2.62981 1.82607

i-C_4H_3+C_2H_2 : Transition states

TS(i-C_4H_3.C_2H_2→bct)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.481298	-0.767964	-0.000024
2	6	-1.488214	-0.053340	-0.000011
3	6	-0.273502	0.575839	0.000008
4	6	0.260474	1.785266	0.000015
5	6	1.285330	-1.071401	0.000053
6	6	2.451357	-0.690195	-0.000044
7	1	-3.396480	-1.314774	-0.000037
8	1	1.338530	1.924911	0.000032
9	1	-0.356902	2.684370	0.000004
10	1	0.524292	-1.824673	0.000154
11	1	3.365678	-0.139064	-0.000142

Vibrational frequencies

*i*437.2488	281.612064	557.731872	866.8536	1843.837056	3348.61824
10.533504	376.661376	584.770848	868.906752	2010.9144	3350.682528
114.494496	461.986656	617.3304	998.435808	3003.130272	
196.225824	498.632736	743.551776	1394.015328	3084.7464	
221.68656	537.04752	793.081056	1675.50864	3259.397088	

Rotational constants (GHZ)

5.9625935 2.3024884 1.6610607

TS(bct→btt)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.266955	-0.769566	-0.011300
2	6	1.209498	-0.181370	0.026613
3	6	-0.059803	0.473197	0.086183
4	6	-1.246574	-0.376234	0.487209
5	6	-1.860974	-1.196163	-0.333546
6	6	-0.199430	1.783470	-0.177535
7	1	3.204421	-1.276274	-0.047253
8	1	-1.172293	2.262765	-0.125003
9	1	0.651902	2.399674	-0.450152
10	1	-1.581381	-0.276557	1.522329
11	1	-1.760683	-1.509606	-1.365666

Vibrational frequencies

*i*121.426176	517.65888	712.5936	934.79808	1610.469888	3131.945376
160.142784	556.670112	738.114048	1200.597984	2128.710336	3355.17024
219.040032	589.395744	840.43344	1221.670176	2998.900992	
326.868384	607.209696	875.003232	1388.268576	3047.560608	
333.46416	667.963968	897.864864	1596.486336	3128.960352	

Rotational constants (GHZ)

5.5408127 3.0279959 2.1064009

TS(bct→bcc)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.506079	-0.538688	-0.031022
2	6	1.368525	-0.126045	-0.009129
3	6	0.002440	0.304050	0.019176
4	6	-1.023612	-0.789015	0.061603
5	6	-2.317999	-0.649036	-0.055905
6	6	-0.311383	1.614344	0.013279
7	1	3.516511	-0.878581	-0.052203
8	1	-1.348176	1.935158	0.045673
9	1	0.456227	2.379227	-0.023299
10	1	-0.594085	-1.788944	0.202702
11	1	-3.374772	-0.540519	-0.160888

Vibrational frequencies

*i*692.56992	478.664544	604.102176	915.952224	1614.012672	3317.43504
25.57152	528.961728	699.388032	1185.607104	2131.8072	3354.68256
158.493408	534.028032	788.514624	1251.36288	2923.792128	
265.9032	563.895552	797.283648	1387.622112	3053.196	
283.229568	589.16592	886.578624	1571.318016	3140.876352	

Rotational constants (GHZ)
8.0866147 2.4949014 1.9091658

TS(bcc→btc)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.243425	-0.897940	-0.022524
2	6	1.221059	-0.250771	0.011975
3	6	-0.007754	0.478497	0.069177
4	6	-1.246851	-0.305672	0.417164
5	6	-1.921453	-1.053041	-0.424932
6	6	-0.056572	1.804340	-0.141614
7	1	3.149467	-1.458717	-0.059820
8	1	-0.997857	2.343158	-0.091161
9	1	0.838253	2.373933	-0.372380
10	1	-1.575884	-0.232705	1.462436
11	1	-2.805100	-1.678149	-0.394547

Vibrational frequencies

*i*141.553056	512.646624	713.771232	947.73792	1625.67408	3133.296288
157.983072	555.634656	717.77232	1206.84	2130.179136	3355.1784
223.848096	589.948608	786.184416	1224.641568	2922.646656	
321.30384	616.314528	852.516288	1390.361472	3048.940704	
343.365888	638.622144	899.149728	1600.19712	3131.090784	

Rotational constants (GHZ)
5.6212427 2.9655268 2.0516714

TS(btt→btc)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.247849	1.894536	0.000000
2	6	0.000000	0.568611	0.000000
3	6	-1.395598	0.056448	0.000000
4	6	-1.754427	-1.201627	0.000000
5	6	1.069439	-0.385148	0.000000
6	6	1.961657	-1.201473	0.000000
7	1	-0.566735	2.613328	0.000000
8	1	1.259760	2.284140	0.000000
9	1	2.754119	-1.914861	0.000000
10	1	-2.154072	0.851569	0.000000
11	1	-2.066591	-2.222270	0.000000

Vibrational frequencies

*i*736.7267	464.0642	642.4238	967.0554	1667.3976	3458.5300
147.6121	557.6982	728.4116	1253.0956	2228.5753	3495.5795
151.0133	594.6115	764.6573	1313.7589	3028.5642	
281.1135	616.8514	849.4231	1450.6596	3177.4607	
298.2123	618.1456	919.0659	1650.2563	3268.3966	

Rotational constants (GHZ)
4.84122 3.60916 2.06769

TS(bcc→b-C_6H_4+H)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.229847	-0.961511	0.000045
2	6	-1.223166	-0.292260	0.000011
3	6	-0.019174	0.490064	-0.000010
4	6	-0.063744	1.838184	-0.000070
5	6	1.206972	-0.276372	0.000010
6	6	1.982971	-1.218861	-0.000071
7	1	-3.120084	-1.548584	0.000068
8	1	0.847419	2.425867	-0.000084
9	1	-1.015804	2.356973	-0.000103
10	1	2.574675	1.207420	0.000748
11	1	2.789725	-1.917146	-0.000119

Vibrational frequencies

*i*603.232608	349.442016	583.920576	733.374432	1591.349664	3344.887008
57.227616	454.914528	606.334368	903.874944	2046.656064	3354.532992
149.651616	521.508096	624.061344	913.311936	2140.390944	
236.39184	561.889344	655.166976	1221.453504	3060.49488	
303.215232	566.197824	711.427104	1377.70512	3152.081088	

Rotational constants (GHZ)
5.4190307 3.0000750 1.9310244

TS(btc→b-C_6H_4+H)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.161061	1.820648	0.040298
2	6	0.094733	0.471888	-0.029570
3	6	-1.159331	-0.210255	-0.145794
4	6	-2.213793	-0.806921	-0.201473
5	6	1.274855	-0.344414	0.004806
6	6	2.254643	-1.051944	0.030754
7	1	-0.739694	2.423836	0.013145
8	1	1.116290	2.326618	0.126848
9	1	3.122813	-1.670773	0.055540
10	1	-2.844663	-1.030772	2.000179
11	1	-3.127752	-1.322919	-0.389840

Vibrational frequencies

*i*283.567584	250.737888	603.85488	732.72048	1577.352768	3353.049984
49.837248	356.219136	608.103168	890.98272	2107.994688	3354.547968
133.011552	469.0704	622.932096	923.437824	2141.821056	
170.758848	561.976032	660.702912	1236.638208	3061.799904	
238.787424	565.935648	703.578816	1380.319872	3152.556288	

Rotational constants (GHZ)
5.7891106 2.6539866 1.8852626

TS(bcc→C4Y-2)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.034393	-0.361168	-0.388989
2	6	0.984927	-0.928058	0.231818
3	6	-0.025868	0.109303	0.198885
4	6	0.682906	1.327172	0.081189
5	6	-1.409787	-0.062088	0.004437
6	6	-2.604972	-0.221042	-0.146297
7	1	1.471269	1.557739	0.785866
8	1	0.257549	2.183573	-0.443759
9	1	3.065263	-0.639559	-0.598747
10	1	0.889462	-1.927245	0.654641
11	1	-3.653143	-0.359222	-0.284258

Vibrational frequencies

*i*661.823424	497.910624	717.522144	989.346816	1485.736032	3128.348064
156.227136	519.146688	810.412416	1123.143936	2075.79744	3352.306272
174.709632	594.293088	859.415616	1278.37008	3019.687104	
387.366336	603.780384	876.059712	1323.928992	3037.408608	
481.934016	658.270848	891.515424	1459.816896	3070.44192	

Rotational constants (GHZ)
10.0467095 2.4887522 2.0758653

TS(btc→C4)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.597313	1.883876	0.000000
2	6	0.000000	0.683678	0.000000
3	6	1.409733	0.285310	0.000000
4	6	1.369028	-1.046627	0.000000
5	6	-0.652551	-0.634084	0.000000
6	6	-1.607445	-1.425574	0.000000
7	1	-0.013389	2.799309	0.000000
8	1	-1.677996	1.975905	0.000000
9	1	-2.176397	-2.329878	0.000000
10	1	2.271376	0.951373	0.000000
11	1	2.067695	-1.876186	0.000000

Vibrational frequencies

*i*624.734016	493.241856	714.093024	930.318336	1634.085504	3136.33392
188.469984	568.924896	754.03008	1148.696064	1895.177376	3318.49536
229.631712	591.163488	824.29824	1241.542944	3043.597344	
269.511264	624.147744	855.03216	1398.94512	3052.509024	
367.197024	689.9616	867.263136	1545.660288	3111.078144	

Rotational constants (GHZ)
5.0302662 4.3324290 2.3276707

TS(btc→FLV-2)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.019445	2.086867	0.000000
2	6	0.000000	0.743842	0.000000
3	6	1.173247	-0.101755	0.000000
4	6	1.372710	-1.326566	0.000000
5	6	-1.196169	-0.133242	0.000000
6	6	-1.000812	-1.444238	0.000000
7	1	-0.957662	2.633898	0.000000
8	1	0.896405	2.667960	0.000000
9	1	1.907793	-2.252704	0.000000
10	1	-2.187727	0.323065	0.000000
11	1	-1.635995	-2.321661	0.000000

Vibrational frequencies

*i*448.866912	523.647264	719.879616	936.647616	1635.949056	3135.6864
199.234272	589.550496	760.437984	1172.182272	1884.186048	3307.817184
299.73216	606.541152	840.24192	1232.83104	3012.73728	
332.719392	691.101312	864.165024	1399.446048	3052.710912	
505.344192	698.595936	888.043872	1563.236544	3123.970176	

Rotational constants (GHZ)
6.2770679 3.8616047 2.3908016

Hydrogen shifts

TS(FLV-1→FLV-2)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.481021	-1.445832	0.000000
2	6	0.983203	-1.188697	0.000000
3	6	1.288616	0.147085	0.000000
4	6	0.000000	0.811072	0.000000
5	6	-1.034836	-0.210850	0.000000
6	6	-0.819452	1.875756	0.000000
7	1	-0.783352	2.964122	0.000000
8	1	-1.884083	0.927994	0.000000
9	1	-0.942336	-2.424634	0.000000
10	1	1.716744	-1.991428	0.000000
11	1	2.273965	0.592738	0.000000

Vibrational frequencies

*i*2301.119424	680.774112	867.402528	1058.972064	1511.6832	3129.658176
78.384672	689.085216	893.022912	1146.507552	1577.773056	3135.537216
457.599744	717.299232	903.080736	1240.230816	1770.206112	
469.225152	761.313984	930.677568	1298.2776	3062.530848	
618.709824	788.964288	951.478848	1427.379744	3071.647104	

Rotational constants (GHZ)
8.61816 4.11581 2.78552

TS(C4Y-1→C4Y-2)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.671868	-0.042943	-0.118890
2	6	-1.464369	-0.017794	0.013580
3	6	-0.074668	-0.010055	0.208760
4	6	1.022665	-1.022691	0.002106
5	6	1.958198	-0.046549	-0.187959
6	6	0.970284	1.032574	-0.004274
7	1	0.858426	2.063402	-0.320218
8	1	0.341526	0.777362	1.194272
9	1	3.039683	-0.038152	-0.245584
10	1	1.046927	-2.095067	0.154262
11	1	-3.728013	-0.062796	-0.262666

Vibrational frequencies

*i*2009.295072	507.958272	742.693056	1071.380928	1470.197856	3132.48
173.871168	552.32928	785.185536	1157.422368	1782.397152	3353.744
186.929376	612.949728	900.427296	1217.495328	2084.79984	
451.669248	619.844352	938.397984	1241.206176	3103.041504	
485.227008	690.074208	1030.646304	1307.001312	3113.959488	

Rotational constants (GHZ)
13.4654883 2.4135626 2.0943642

Non interacting fragments

n-C_4H_3 (HCCH cis)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.366892	1.837239	0
2	6	0.000000	0.684294	0
3	6	0.491565	-0.654865	0
4	6	-0.258487	-1.745096	0
5	1	-0.712754	2.845806	0
6	1	1.584260	-0.764289	0
7	1	-0.068626	-2.810945	0

Vibrational frequencies

219.418848	655.618368	1587.461088
336.851904	783.442848	2136.807168
515.575968	791.53584	2927.133216
563.78112	987.587328	3135.62544
610.963776	1232.056896	3355.79472

Rotational constants (GHZ)
68.27530 4.79182 4.47757

n-C_4H_3 (HCCH trans)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.508960	1.752290	0
2	6	0.000000	0.653920	0
3	6	0.622118	-0.633177	0
4	6	-0.054251	-1.771344	0
5	1	-0.972453	2.712548	0
6	1	1.714349	-0.653322	0
7	1	-1.095344	-2.069363	0

Vibrational frequencies

207.093408	675.605184	1572.720384
347.061984	838.873632	2127.573024
494.91264	850.152	3000.764832
557.890272	967.968096	3133.400544
603.970176	1234.965696	3355.365216

Rotational constants (GHZ)
50.36687 5.08031 4.61483

i-C_4H_3

Structure

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	0.003969	1.874992	0
2	6	0.000000	0.565280	0
3	6	-0.000166	-0.756261	0
4	6	-0.011747	-1.993025	0
5	1	-0.918898	2.458946	0
6	1	0.930607	2.453019	0
7	1	0.035954	-3.057882	0

Vibrational frequencies

48.036	601.67808	1743.710016
133.855392	846.552576	1952.67888
241.163232	874.016256	2971.860384
430.627296	957.14496	3027.860928
555.138048	1407.275712	3346.41024

Rotational constants (GHZ)

292.76519 4.14018 4.08245

C_2H_2

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0	0	0.602476
2	6	0	0	-0.602476
3	1	0	0	-1.669118
4	1	0	0	1.669118

Vibrational frequencies

513.479904	3303.926592
513.479904	3400.104768
744.205632	
744.205632	
2004.712896	

Rotational constants (GHZ)
35.274675

l-C_6H_4 (cis)

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.351008	-2.064098	0
2	6	-1.229882	-0.858963	0
3	6	-1.14797	0.5559	0
4	6	0	1.27537	0
5	6	1.309084	0.732422	0
6	6	2.44663	0.316434	0
7	1	-1.431578	-3.127319	0
8	1	-2.091577	1.098426	0
9	1	-0.076546	2.361144	0
10	1	3.438575	-0.074644	0

Vibrational frequencies

104.125152	544.188576	714.763776	1208.278368	3042.075456
227.488896	568.360512	751.30992	1379.363808	3057.628704
252.213216	593.398272	864.442368	1584.320544	3355.366944
366.188544	601.94736	924.925056	2120.548608	3355.762368
431.289696	606.012288	1006.830048	2138.452416	

Rotational constants (GHZ)
7.29418 2.46626 1.84309

b-C_6H_4

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0	1.800137	0
2	6	0	0.449318	0
3	6	1.222291	-0.303351	0
4	6	-1.222321	-0.303313	0
5	6	-2.238067	-0.958893	0
6	6	2.238113	-0.958809	0
7	1	0.930938	2.356378	0
8	1	-0.93094	2.356373	0
9	1	-3.137565	-1.531573	0
10	1	3.137468	-1.531715	0

Vibrational frequencies

131.832768	561.185088	658.626912	1236.276768	3061.316256
225.57408	561.445824	707.799264	1382.383296	3151.462752
239.052576	566.816352	731.514912	1585.975392	3354.745152
345.22128	604.843392	890.988	2137.440864	3355.696704
468.718944	606.996576	922.999872	2143.979328	

Rotational constants (GHZ)

6.20344 2.84460 1.95029

o-C_6H_4

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.20607	-0.684496	0
2	6	-1.291023	0.697581	0
3	6	0	1.271037	0
4	6	1.17189	0.492174	0
5	6	1.143081	-0.920202	0
6	6	-0.164081	-1.376989	0
7	1	-2.195451	1.297429	0
8	1	0.08937	2.355309	0
9	1	2.136954	0.994438	0
10	1	2.046339	-1.52181	0

Vibrational frequencies

379.548288	725.47872	968.39232	1276.663392	3050.74176
389.982336	810.18528	1043.816256	1381.315488	3065.79168
419.677536	836.457216	1072.36464	1428.172704	3086.549952
572.231808	877.798272	1126.045824	1442.779008	3090.45024
597.890208	924.131616	1234.916736	1945.324224	

Rotational constants (GHZ)

7.01034 5.70136 3.14423

m-C_6H_4

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.237596	-1.32409	0
2	6	-1.023915	-0.187738	0
3	6	-1.347249	1.122734	0
4	6	0	1.040956	0
5	6	1.259557	0.47249	0
6	6	1.12036	-0.933628	0
7	1	-2.183295	1.819224	0
8	1	2.198827	1.013147	0
9	1	1.957516	-1.631249	0
10	1	-0.599998	-2.345472	0

Vibrational frequencies

304.770336	734.235264	941.905152	1262.248416	3050.190528
388.274112	773.996832	1040.455296	1349.606208	3055.88304
546.307968	784.816704	1043.643072	1378.23792	3100.234176
562.990848	796.281408	1051.186944	1520.815296	3104.41488
593.318784	877.2312	1125.890688	1780.89792	

Rotational constants (GHZ)
8.74431 5.02713 3.19203

p-C_6H_4

Structure

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.193477	-0.739677	0
2	6	0	-1.363524	0
3	6	1.193476	-0.739678	0
4	6	1.193477	0.739679	0
5	6	0	1.363521	0
6	6	-1.193477	0.739679	0
7	1	2.176944	-1.196464	0
8	1	2.176945	1.196461	0
9	1	-2.176944	1.196463	0
10	1	-2.176943	-1.196465	0

Vibrational frequencies

295.1794	708.0429	898.0662	1254.2500	3223.3673
456.6870	722.4179	958.0332	1331.8126	3227.5864
480.1184	740.2519	1090.1669	1423.6920	3242.3032
492.1130	835.0702	1110.1843	1489.3906	3243.3376
555.6788	857.2096	1180.0726	1716.4369	

Rotational constants (GHZ)
6.59303 5.77740 3.07916

Relative Gibbs free energies

n-C_4H_3 + C_2H_2	300 K	600 K	900 K	1200 K	1500 K	1800 K	2100 K
n-C_4H_3,C_2H_2 (cis)	380.42	335.97	287.40	237.70	187.59	137.33	86.98
n-C_4H_3,C_2H_2 (trans)	384.10	341.23	294.31	246.28	197.88	149.32	100.70
lctt	246.39	231.90	215.33	198.20	180.87	163.46	146.00
lctc	243.63	229.41	213.07	196.15	179.01	161.79	144.52
lcct	256.16	241.41	224.57	207.16	189.54	171.84	154.10
lccc	254.71	239.95	223.04	205.53	187.79	169.96	152.07
C4Y-1	215.38	205.21	193.10	180.39	167.44	154.40	141.31
FLV-1	118.82	114.84	109.90	104.64	99.25	93.81	88.34
Phenyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
l-C_6H_4,H	355.20	319.48	279.36	237.74	195.46	152.84	110.01
TS(n-C_4H_3,C_2H_2 (cis) → lctt)	412.61	385.00	354.70	324.12	293.77	263.75	234.08
TS(n-C_4H_3,C_2H_2 (cis) → lcct)	419.10	393.27	364.76	335.98	307.42	279.20	251.32
TS(n-C_4H_3,C_2H_2 (trans) → ltct)	437.37	420.26	401.01	381.20	361.18	341.07	320.92
TS(lctt → lctc)	261.84	248.06	233.01	218.11	203.59	189.47	175.72
TS(lctt → lcct)	259.61	248.85	237.21	225.82	214.84	204.27	194.07
TS(lctc → lccc)	260.95	249.93	237.96	226.20	214.84	203.89	193.29
TS(lcct → lccc)	270.70	256.61	241.22	225.96	211.07	196.58	182.44
TS(lctc → l-C_6H_4+H)	409.05	390.12	368.23	345.72	323.18	300.80	278.62
TS(lccc → l-C_6H_4+H)	404.31	383.50	359.76	335.40	311.01	286.78	262.77
TS(lccc → C4Y-1)	396.89	387.27	376.48	365.79	355.42	345.40	335.71
TS(lccc → FLV-1)	269.39	260.66	250.95	241.40	232.23	223.44	215.00
TS(lccc → phenyl)	281.95	274.89	267.06	259.48	252.30	245.51	239.08
i-C_4H_3+ C_2H_2							
i-C_4H_3,C_2H_2	338.88	294.91	246.67	197.26	147.44	97.45	47.37
bcc	254.17	236.83	217.06	196.62	175.94	155.16	134.32
bct	255.51	239.71	221.55	202.76	183.75	164.65	145.50
Btt	248.38	233.99	217.30	200.00	182.47	164.87	147.22
Btc	248.80	234.37	217.58	200.15	182.49	164.74	146.93
C4Y-2	177.95	168.06	156.52	144.50	132.30	120.00	107.66
C4	247.39	239.51	230.10	220.20	210.12	199.96	189.74
FLV-2	141.88	137.81	133.01	128.00	122.91	117.78	112.64
b-C_6H_4,H	376.74	356.66	333.45	309.58	285.66	261.90	238.36
TS(i-C_4H_3+C_2H_2→ bct)	387.25	360.00	330.13	300.02	270.14	240.60	211.41
TS(bct → btt)	262.82	252.23	240.54	229.05	217.96	207.27	196.95
TS(bct → bcc)	269.15	251.08	231.43	211.84	192.60	173.74	155.24
TS(btt → btc)	263.68	249.72	234.23	218.82	203.77	189.10	174.79
TS(bcc → btc)	263.18	252.39	240.43	228.64	217.22	206.21	195.56
TS(bcc → b-C_6H_4+ H)	410.74	390.65	367.45	343.57	319.66	295.90	272.36
TS(btc → b-C_6H_4+ H)	390.40	366.81	339.96	312.40	284.81	257.36	230.13
TS(bcc → C4Y-2)	359.95	350.28	339.46	328.76	318.41	308.43	298.80
TS(btc → C4)	326.82	316.89	305.75	294.72	284.03	273.72	263.76
TS(btc → FLV-2)	306.13	298.81	290.60	282.57	274.93	267.69	260.80
Hydrogen shifts	300.00	600.00	900.00	1200.00	1500.00	1800.00	2100.00
TS(FLV-1 → FLV-2)	371.45	366.56	361.20	355.86	350.70	345.79	341.13
TS(C4Y-1 → C4Y-2)	402.11	394.09	384.89	375.58	366.45	357.57	348.96