SUPPORTING INFORMATION

Table 1
CCSD(T)/cc-pVTZ optimized geometry (XYZ) of **1** - **4** (Å).

C	0.000000	0.000000	1.229555
C	0.933168	0.000000	0.000000
C	-0.933168	0.000000	0.000000
C	0.000000	1.064826	-0.614778
C	0.000000	-1.064826	-0.614778
H	2.012453	0.000000	0.000063
H	-2.012453	0.000000	0.000063
H	0.000000	-0.900420	1.832256
H	0.000000	0.900420	1.832256
H	0.000000	2.036990	-0.136342
H	0.000000	1.136570	-1.695914
H	0.000000	-1.136570	-1.695914
H	0.000000	-2.036990	-0.136342

(a) **1**

C	0.000000	0.000000	1.287184
C	0.785860	0.000000	0.000000
C	-0.785860	0.000000	0.000000
C	0.000000	1.114734	-0.643592
C	0.000000	-1.114734	-0.643592
H	0.000000	-0.911996	1.857511
H	0.000000	0.911996	1.857511
H	0.000000	2.064650	-0.138944
H	0.000000	1.152654	-1.718568
H	0.000000	-1.152654	-1.718568
H	0.000000	-2.064650	-0.138944

(b) **2**

C	0.000000	0.000000	0.000000
C	0.970944	0.000000	1.180749
C	-0.970944	0.000000	1.180749
C	0.000000	0.725382	2.087256
C	0.000000	-0.725382	2.087256
H	0.000000	0.898487	-0.608947
H	0.000000	-0.898487	-0.608947
H	2.040857	0.000000	1.125579
H	-2.040857	0.000000	1.125579
H	0.000000	1.500262	2.816969
H	0.000000	-1.500262	2.816969

(c) **3**

C	0.000000	0.000000	0.000000
C	0.832127	0.000000	1.257920
C	-0.832127	0.000000	1.257920
C	0.000000	0.752211	2.206382
C	0.000000	-0.752211	2.206382
H	0.000000	0.911927	-0.575028
H	0.000000	-0.911927	-0.575028
H	0.000000	1.613809	2.826302
H	0.000000	-1.613809	2.826302

(d) **4**

Table 2
CCSD(T)/cc-pVTZ optimized geometry (XYZ) of **5** - **8** (Å).

C	0.000000	0.000000	0.000000
C	1.019694	0.000000	1.283519
C	0.000000	-1.019694	1.283519
C	-1.019694	0.000000	1.283519
C	0.000000	1.019694	1.283519
H	2.075549	0.000000	1.139117
H	0.000000	-2.075549	1.139117
H	-2.075549	0.000000	1.139117
H	0.000000	2.075549	1.139117

(a) **5**

C	0.000000	0.000000	0.000000
C	0.902712	0.000000	1.563543
C	-0.902712	0.000000	1.563543
C	0.000000	1.043078	1.042362
C	0.000000	-1.043078	1.042362
H	0.000000	2.105883	1.042362
H	0.000000	-2.105883	1.042362

(b) **6**

C	0.000000	0.000000	0.000000
C	1.147647	0.000000	0.954069
C	-0.573823	0.993891	0.954069
C	-0.573823	-0.993891	0.954069
C	0.000000	0.000000	1.908138

(c) **7**

C	0.000000	0.000000	1.000000
C	0.000000	1.171666	1.928525
C	0.000000	-1.171666	1.928525
C	0.000000	0.731655	3.199471
C	0.000000	-0.731655	3.199471
H	0.875199	0.000000	0.352596
H	-0.875199	0.000000	0.352596
H	0.000000	2.192653	1.603796
H	0.000000	-2.192653	1.603796
H	0.000000	1.342351	4.080669
H	0.000000	-1.342351	4.080669

(d) **8**

Table 3
CASPT2(4,4)/cc-pVTZ optimized geometry (XYZ) of TS (Å).

C	-0.115021	-0.868436	-0.888100
C	0.400135	-0.752738	0.514033
C	-0.106817	0.617537	-1.134565
C	0.321289	0.837466	0.320013
C	-0.540979	0.098026	1.240369
H	-1.038775	1.101449	-1.426454
H	0.676605	0.898276	-1.842254
H	-0.749921	-1.641108	-1.298257
H	-0.596596	0.213247	2.311366
H	1.025476	1.583775	0.659761
H	1.176471	-1.343595	0.979153

Table 4

Complete frequency table for **1**.

	CCSD(T)/cc-pVTZ		MP2/cc-pVTZ	
Symmetry of vibration	Harm. Frequency (cm^{-1})	IR Intensity (km/mol)	Harm. Frequency (cm^{-1})	Raman Activity $Å^4$/AMU
e'	546.8054	0.1181	542.0722	0.3718
e''	814.0839	0.0000	817.1278	5.2986
a_2''	860.9906	5.4408	870.0394	0.0000
a_1'	918.7447	0.0000	913.7645	4.6593
e'	935.2339	0.3951	932.3916	3.4895
a_2'	969.9064	0.0000	970.1281	0.0000
a_1''	1015.8324	0.0000	1018.2241	0.0000
e''	1044.7555	0.0000	1041.3212	14.5908
e'	1126.5167	0.6411	1124.8727	0.5616
e''	1151.0153	0.0000	1154.5174	2.2080
a_1'	1151.7798	0.0000	1147.1555	36.5053
e''	1242.1427	0.0001	1232.6661	0.1532
a_2''	1252.6803	37.0231	1258.3539	0.0000
e'	1295.3325	2.3511	1277.8349	6.1802
e'	1510.4434	0.6187	1514.8117	4.6680
a_1'	1560.3663	0.0000	1565.3778	4.4460
e'	3080.2401	72.6371	3096.5721	0.3641
a_1'	3085.2965	0.0000	3098.7185	351.8356
a_2'	3118.7567	0.0000	3158.7069	0.0000
e'	3122.8828	59.3926	3161.8833	112.2368
a_2''	3133.5073	109.0816	3145.0481	0.0000
a_1'	3152.5392	0.0000	3164.0198	376.9150

Table 5
Complete frequency table for **2**.

	CCSD(T)/cc-pVTZ		MP2/cc-pVTZ	
Symmetry of vibration	Harm. Frequency (cm^{-1})	IR Intensity (km/mol)	Harm. Frequency (cm^{-1})	Raman Activity $Å^4$/AMU
e'	535.5610	0.2041	533.0724	0.7270
a_2''	647.6564	121.9259	671.0530	0.0000
e''	759.5454	0.0000	771.8552	0.6878
a_1'	933.3213	0.0000	930.6276	6.5086
a_1''	938.5267	0.0000	931.1258	0.0000
a_2'	972.5866	0.0000	965.5999	0.0000
e''	1082.6437	0.0000	1085.0224	0.6747
e'	1120.4133	0.5933	1119.5275	4.0317
a_2''	1131.6029	24.3155	1133.4470	0.0000
a_1'	1169.1848	0.0000	1165.4594	50.6262
e''	1178.0155	0.0000	1166.2945	8.1836
e'	1241.9389	2.0501	1233.3774	5.2110
e'	1505.8312	2.7811	1505.8330	2.8585
a_1'	1552.0135	0.0000	1552.2633	2.3806
e'	3174.5602	19.4091	3181.4309	0.0134
a_1'	3178.4583	0.0000	3183.7196	297.4588
a_2'	3231.5823	0.0000	3261.1582	0.0000
e'	3233.2511	8.8817	3262.9618	81.6115

Table 6
Complete frequency table for **3**.

	CCSD(T)/cc-pVTZ		MP2/cc-pVTZ	
Symmetry of vibration	Harm. Frequency (cm^{-1})	IR Intensity (km/mol)	Harm. Frequency (cm^{-1})	Raman Activity $Å^4$/AMU
b_2	463.7504	2.3557	478.6811	0.0530
a_1	599.2228	6.9709	576.3431	1.3879
a_2	776.0172	0.0000	783.4607	1.5042
b_2	788.2577	61.4246	795.5729	2.7171
a_1	831.8670	3.1658	830.3337	6.2369
a_2	844.1329	0.0000	861.3330	7.6890
b_1	857.3506	10.2025	866.4718	0.0724
a_1	926.4524	1.3850	939.3031	2.4711
b_1	929.1361	0.0013	933.7365	15.0826
b_2	939.6999	0.0105	961.9075	0.3852
a_2	1035.2151	0.0000	1059.4986	1.0194
a_1	1075.0336	0.9817	1052.5046	5.6076
b_2	1082.2838	0.7349	1084.0933	0.3579
a_2	1118.7458	0.0000	1128.9102	4.8240
b_2	1135.1508	9.8041	1130.5248	13.1589
b_1	1157.9013	1.5457	1179.0080	1.0737
b_1	1175.9878	5.1409	1196.5797	1.0344
a_1	1214.9544	4.4196	1231.2336	33.3268
b_1	1296.8065	7.5076	1290.7796	0.9775
a_1	1418.9216	2.0537	1417.0524	22.6127
a_1	1512.9615	0.0181	1519.0243	6.5076
a_1	3087.1112	68.5499	3089.3373	157.6319
b_2	3136.2517	42.1857	3149.7662	88.4243
b_1	3269.1382	28.0376	3247.7634	1.3559
a_1	3270.3150	0.6079	3248.3793	237.7724
b_2	3348.9658	0.1670	3330.6994	81.8025
a_1	3369.2152	0.0031	3349.3687	155.0679

Table 7
Complete frequency table for **4**.

	CCSD(T)/cc-pVTZ		MP2/cc-pVTZ	
Symmetry of vibration	Harm. Frequency (cm^{-1})	IR Intensity (km/mol)	Harm. Frequency (cm^{-1})	Raman Activity $Å^4$/AMU
b_1	443.1635	2.9431	443.3068	0.3631
b_2	653.8769	104.8464	687.9623	0.4869
a_2	787.4903	0.0000	778.8847	0.0195
a_1	789.6608	26.0283	739.9580	0.2648
a_1	818.9116	4.0453	813.9419	10.8483
b_1	898.3684	4.1802	865.5368	0.0499
a_2	940.0110	0.0000	904.3048	1.9502
a_1	954.2393	0.0450	942.6155	4.0361
b_2	966.3807	18.6072	947.0298	2.8988
b_1	1073.8516	3.0596	1069.1523	1.8484
b_2	1083.1670	11.0951	1096.3345	3.0043
a_2	1111.9021	0.0000	1099.0674	6.7171
a_1	1145.3453	5.9208	1146.9129	27.6445
b_1	1189.7191	1.4556	1179.2893	13.5438
b_2	1190.9973	0.3976	1186.1429	4.6517
a_1	1421.0058	0.6205	1411.4646	28.2467
a_1	1509.7018	0.0810	1513.3651	3.7769
a_1	3164.5822	21.3343	3162.4525	125.9621
b_1	3222.6836	5.7932	3243.0746	65.1533
b_1	3354.1046	7.4444	3359.5275	63.5741
a_1	3371.9570	1.8309	3376.1956	124.5844

Table 8

Complete frequency table for **5**.

	CCSD(T)/cc-pVTZ		MP2/cc-pVTZ	
Symmetry of vibration	Harm. Frequency (cm^{-1})	IR Intensity (km/mol)	Harm. Frequency (cm^{-1})	Raman Activity $Å^4$/AMU
e	471.6586	5.5622	507.4323	6.4006
b_2	485.9052	0.0000	433.0632	10.0577
a_1	750.4253	48.0146	754.9300	6.9166
e	848.2197	24.4321	822.9034	1.0574
b_2	918.4933	0.0000	894.7214	1.5440
e	1012.6440	11.6161	1008.0648	1.3932
b_1	1025.1792	0.0000	1022.1475	15.2480
b_2	1030.0743	0.0000	1021.0629	3.6441
a_1	1083.0891	95.6725	1073.0145	24.5439
a_2	1201.6064	0.0000	1194.0396	0.0000
b_1	1307.0140	0.0000	1305.1525	1.1400
a_1	1334.5317	1.0783	1327.0822	53.7827
e	1407.9405	1.1373	1396.6255	1.6257
b_2	3292.2298	0.0000	3304.7223	131.5936
e	3311.3721	1.0683	3321.3378	0.5162
a_1	3332.1208	0.4316	3340.8555	213.1994

Table 9

Complete frequency table for **6**.

	CCSD(T)/cc-pVTZ		MP2/cc-pVTZ	
Symmetry of vibration	Harm. Frequency (cm^{-1})	IR Intensity (km/mol)	Harm. Frequency (cm^{-1})	Raman Activity $Å^4$/AMU
e'	506.5588	55.3045	378.5691	10.2226
e''	815.2592	0.0000	852.3533	4.3631
a_1'	860.5216	0.0000	922.9654	51.6431
e'	871.9929	20.8376	848.4582	9.2148
e''	1055.9389	0.0000	1022.3063	6.1565
e'	1156.5161	7.2133	1103.8212	1.7492
a_2''	1315.7098	22.6615	1344.5902	0.0000
a_1'	1329.8253	0.0000	1336.8158	55.4359
a_1'	3362.2020	0.0000	3387.1365	143.9967
a_2''	3362.8458	13.6338	3383.4595	0.0000

Table 10
Complete frequency table for **7**.

	CCSD(T)/cc-pVTZ		MP2/cc-pVTZ	
Symmetry of vibration	Harm. Frequency (cm^{-1})	IR Intensity (km/mol)	Harm. Frequency (cm^{-1})	Raman Activity $Å^4$/AMU
e'	540.6797	26.1603	490.9806	22.5626
e''	629.9240	0.0000	1106.9855	6.6986
a_1'	715.9170	0.0000	781.3500	277.4928
a_2''	915.7923	43.7461	1071.7738	0.0000
e'	989.4218	5.1264	959.3700	6.4888
a_1'	1256.7496	0.0000	1279.2486	35.0316

Table 11

^{1}H and ^{13}C NMR shielding tensors of **1** - **7** and methane (ppm): principal components (σ_{11}, σ_{22}, σ_{33}), isotropic NMR shieldings (σ_{iso}) and anisotropies ($\Delta\sigma$).

Str.	Atom(s)	σ_{11}	σ_{22}	σ_{33}	σ_{iso}	$\Delta\sigma$
1	C(2), C(4), C(5)	137.57	144.71	155.42	145.90	14.27
	C(1), C(3)	151.97	151.97	186.07	163.34	34.10
	H(6), H(7), H(8), H(9), H(10), H(11)	25.87	27.83	36.46	30.05	9.62
	H(12), H(13)	24.96	24.96	38.94	29.62	13.98
2	C(2), C(4), C(5)	76.70	139.83	159.87	125.47	51.61
	C(1), C(3)	165.75	212.93	212.93	197.20	23.59
	H(6), H(7), H(8), H(9), H(10), H(11)	24.46	25.32	40.59	30.12	15.70
3	C(1), C(3)	145.78	150.37	230.71	175.62	82.63
	C(2), C(4)	109.98	214.12	216.07	180.05	54.02
	C(5)	126.54	153.44	154.42	144.80	14.43
	H(10), H(11)	24.79	25.19	40.91	30.30	15.92
	H(6), H(7)	23.55	25.11	36.20	28.29	11.87
	H(8), H(9)	25.77	26.43	37.05	29.75	10.95
4	C(1), C(3)	183.01	203.86	237.38	208.08	43.94
	C(2), C(4)	48.58	219.75	222.90	163.74	88.74
	C(5)	-62.12	134.14	153.81	75.28	117.80
	H(6), H(7)	21.75	24.70	36.52	27.66	13.29
	H(8), H(9)	19.76	24.82	36.46	27.01	14.17
5	C(1), C(2), C(3), C(4)	98.15	130.63	159.50	129.43	45.11
	C(5)	245.54	257.99	257.99	253.84	6.22
	H(6), H(7), H(8), H(9)	22.72	24.21	39.24	28.72	15.78
6	C(1), C(3), C(5)	143.34	250.62	303.85	232.60	106.88
	C(2), C(4)	64.52	64.52	126.75	85.26	62.23
	H(6), H(7)	21.31	21.31	35.60	26.07	14.29
7	C(1), C(3), C(5)	166.68	218.24	287.71	224.21	95.25
	C(2), C(4)	70.31	229.50	229.50	176.43	79.60
CH(4)	C	200.28	200.28	200.28	200.28	0.0
	H	28.22	28.22	38.31	31.58	10.09