Supporting Information

for

1,3,4,6,7,9-Hexamethylbenzo[1,2-*c*:3,4-*c′*:5,6-*c′′*]trithiophene: A Twisted Heteroarene

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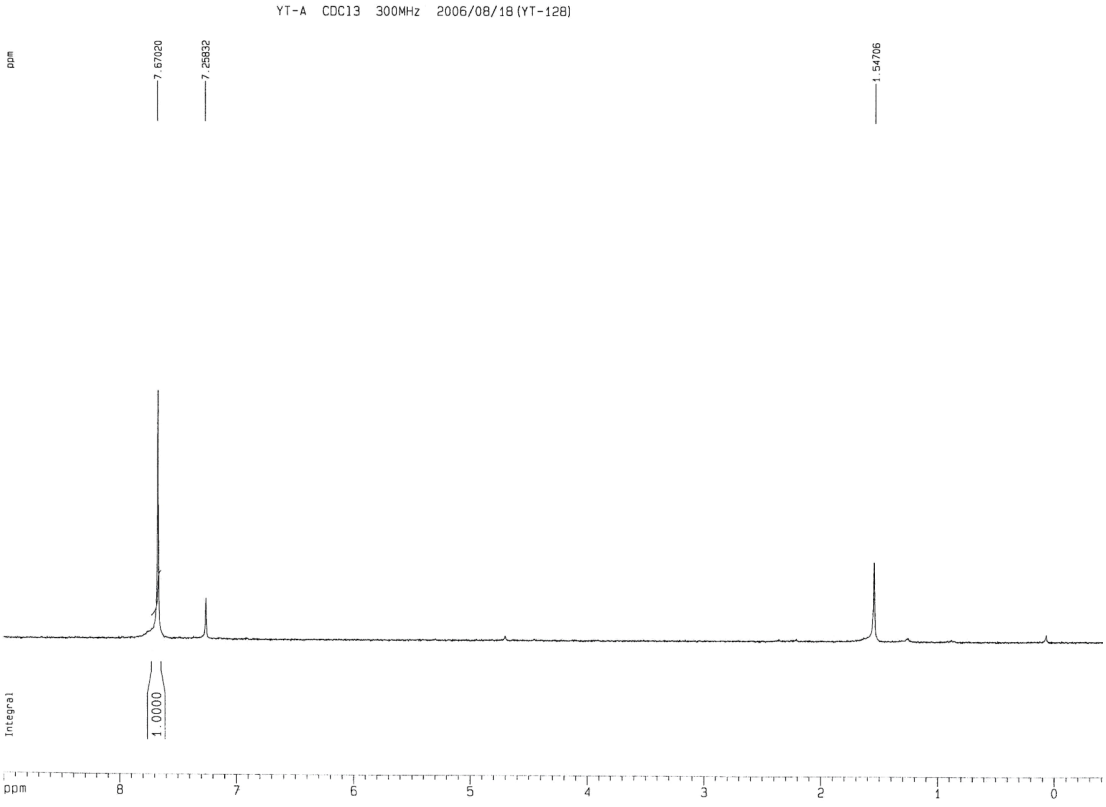
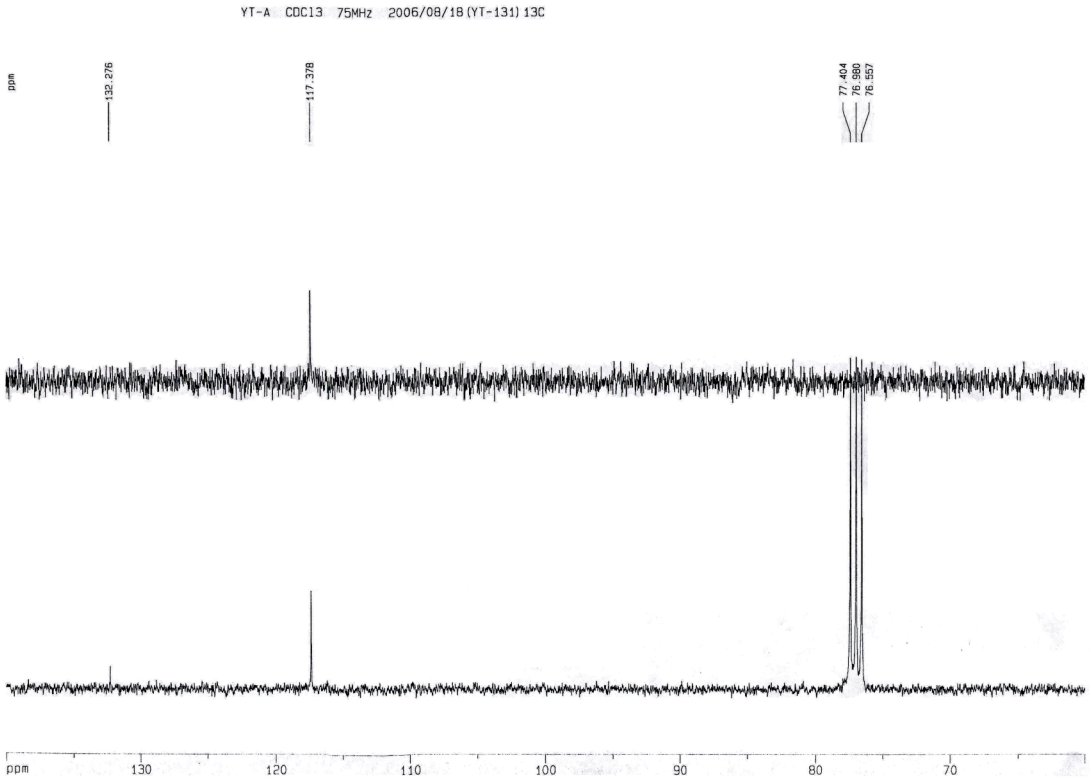
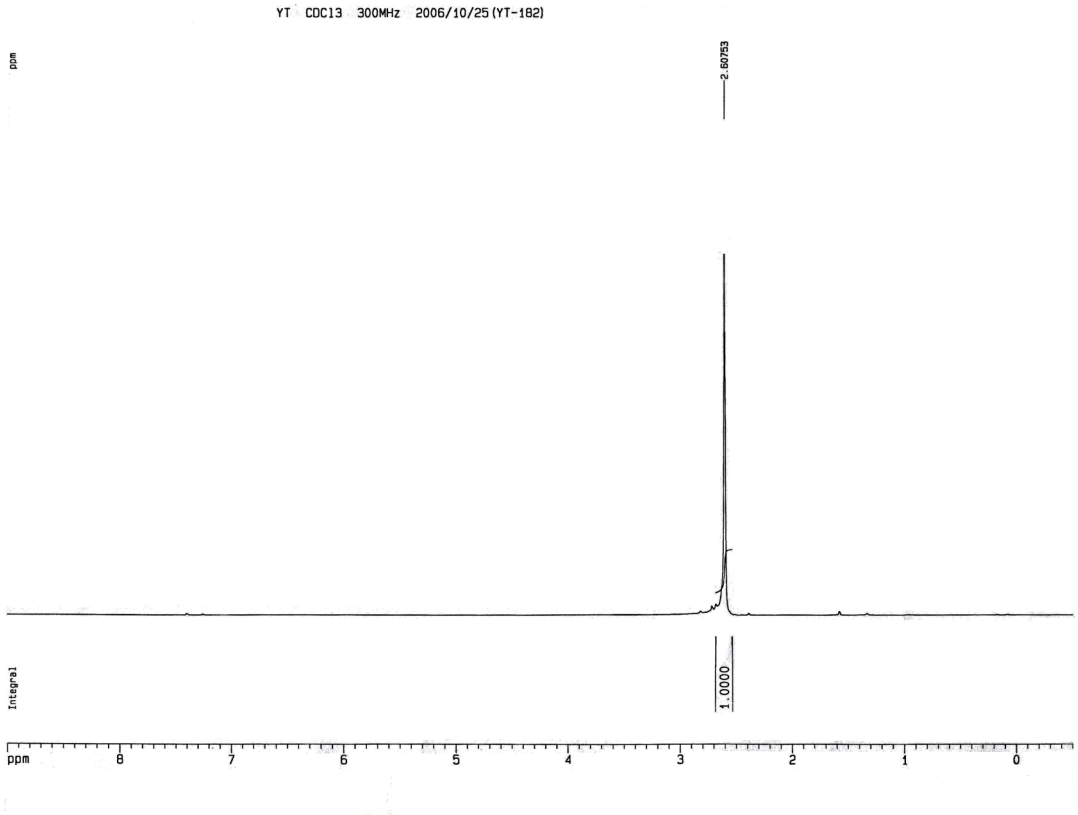
A. NMR Spectra

^{1}H- and ^{13}C-NMR Spectra of benzo[1,2-*c*:3,4-*c*':5,6-*c*'']trithiophene (**C**-H)





^{1}H- and ^{13}C-NMR Spectra of 1,3,4,6,7,9-Hexamethylbenzo[1,2-*c*:3,4-*c*':5,6-*c*'']trithiophene (**C**-Me)



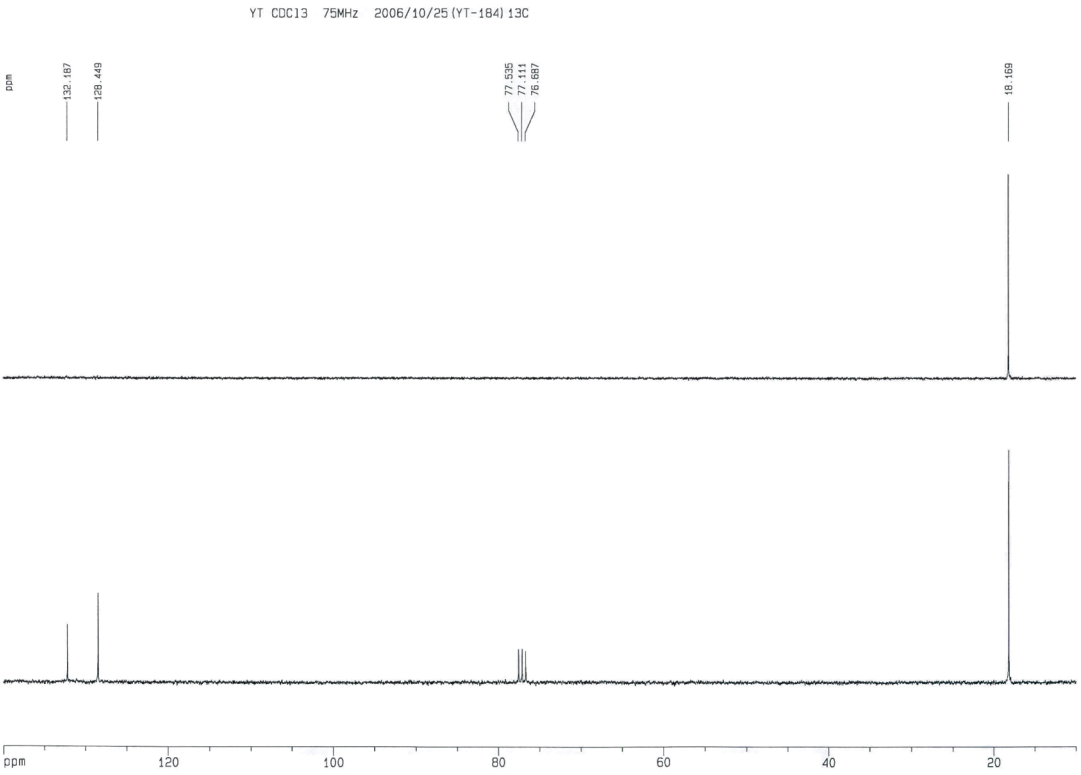


Table S1. Calculated and experimental physical properties of compounds **C**-Me and **C**-H.

Compound		**C**-Me	**C**-H
UV, λ_{max} (nm)	Exp.	264 (4.91),[a] 316 (4.08)	248 (4.88),[a] 257 (4.92), 279 (4.30), 295 (4.07), 307 (4.16), 320 (4.03)
	Cal.[b]	266.7, 274.2, 274.8, 283.1, 293.7, 299.4, 312.4, 317.8, 321.7	256.5, 264.9, 295.9, 309.0
^{1}H NMR (ppm)	Exp.	2.61	7.67
	Cal.	2.45	—
^{13}C NMR (ppm)	Exp.	18.2, 128.4, 132.2	117.4, 132.3
	Cal.	22.3, 129.9, 135.5	—
Ox. Potential, E_{pa} (V)	Exp.	0.79, 1.10	0.84, 1.27
HOMO (eV)	Cal.[b]	−5.36	−5.93
	Exp[c]	−5.38	−5.55
LUMO (eV)	Cal.[b]	−0.87	−1.35
Koopmans	Cal.[b]	−5.36	−5.93
ΔSCF (eV)	Cal.[b]	−6.77	−7.47

[a] lgε ($M^{-1}cm^{-1}$). [b]B3PW91/DZ+(2d,p). [c] $E_{HOMO} = -E_{onset} - 4.8$.

Computational Results:

M06-2X/D95(2d,p)

Molecule	*Exo*	*Endo*	Δ(*Exo-Endo*)	Symmetry	Character
D	1.4203	1.3988	0.02	Flat/D3H	PD
C-H	1.4589	1.4389	0.02	Flat/D3H	PD
B-F	1.469	1.418	0.05	Nonplanar/C2	PD
B-F	1.4608	1.4181	0.04	Nonplanar/D3	PD
Triphenylene	1.4641	1.4106	0.05	Flat/D3H	PD
B-Me	1.4768	1.4235	0.05	Nonplanar/C2	PD
B-Me	1.4691	1.4191	0.05	Nonplanar/D3	PD
C-Me	1.4686	1.4508	0.02	Nonplanar/C2	PD
C-Me	1.4642	1.4516	0.01	Nonplanar/D3	PD
C-Me	1.4608	1.4508	0.01	Nonplanar/C1	PD

Compound **C**-H looks essentially like 3 independent thiophenes, whereas, compound 10 looks like an aromatic central ring and isolated double bonds in the flanking rings. The former is more radialene-like. As such, the latter is more stable by 9.2 kcal/mol.

Molecule	E+ZPE	Δ(Energy)	Symmetry	Character
D	-1655.143889	0.0	Flat/D3H	PD
D np_opt	No change		Flat/d3h=C2	PD
C-H	-1655.129201	9.22	Flat/D3H	PD
C-H at **C**-Me C2,opt	No change		Flat/d3h=C2	
B-F	-1883.628061	26.96	Flat/D3H	MNE
B-F	-1883.671017	0.0	Nonplanar/C2	PD
B-F	-1883.663274	4.86	Nonplanar/D3	PD
B-F	-1883.628057	26.96	Nonplanar/Cs	MNE
Triphenylene	-692.761130	--	Flat/D3H	PD
Triphenylene np_opt	No change			
B-Me	-928.361084	0.0	Nonplanar/C2	PD
B-Me	-928.354067	4.40	Nonplanar/D3	PD
B-Me	-928.338703	14.04	Nonplanar/CsTS	MNE
C-Me	-1890.758203	0.0	Nonplanar/C2 ➔ same as C1	PD
C-Me	-1890.748970	6.4	Nonplanar/D3	PD
C-Me	-1890.755192	--	Nonplanar/Cs	2NE
C-Me	-1890.742735	--	Nonplanar/Cs	3NE
C-Me	-1890.759193	0.0	Nonplanar/C1 ➔ same as C2	PD
C-Me	-1890.744274	--	Nonplanar/C2	2NE
C-Me C2 to D3 TS	-1890.747569	7.3	Nonplanar/C2	1NE
C-Me C2 to C2 TS	-1890.754415	3.0	Nonplanar/C1	1NE

'np' == nonplanar

M06-2X/DZ(2d,op) structures

D structure:

C	1.2316074111	-0.6575914661	0.
C	-0.0463036635	1.3953457369	0.
C	-1.2607589273	0.6589910741	0.
C	0.0596277869	-1.4213264272	0.
C	1.2011441683	0.7623623465	0.
C	-1.1853059034	-0.737804863	0.
S	2.6336439621	-1.6658448338	0.
S	0.1257840378	3.1136800002	0.
C	-2.6141530997	1.1290518493	0.
C	0.3292304899	-2.8283799066	0.
C	2.2848077737	1.6995462352	0.
S	-2.7594793945	-1.4479549427	0.
C	1.6656452547	-3.0945401204	0.
C	1.8471112056	2.9897023626	0.
C	-3.5128498383	0.1046768246	0.
H	-2.8938498529	2.1751581671	0.
H	-0.4368117549	-3.593714795	0.
H	3.3306466031	1.4188551553	0.
H	2.1468501449	-4.0617758021	0.
H	2.4441220488	3.8900845735	0.
H	-4.5911084525	0.1714788318	0.

C-H structure:

C	1.2518726435	-0.7294293704	0.
C	0.0057680433	1.4488681968	0.
C	-1.2576406798	0.7194388387	0.
C	0.0057680291	-1.4488681969	0.
C	1.2518726506	0.7294293582	0.
C	-1.2576406868	-0.7194388264	0.
C	2.3325874987	-1.5748649555	0.
C	0.1975793096	2.8075125081	0.
C	-2.5301667963	1.2326475774	0.
C	0.1975792821	-2.8075125101	0.
C	2.3325875141	1.5748649326	0.
C	-2.5301668083	-1.2326475527	0.
S	1.8557939946	-3.2143295234	0.
S	1.8557940261	3.2143295052	0.
S	-3.7115880207	0.0000000182	0.
H	3.3809943637	-1.3170910612	0.
H	-0.5498628638	3.5865725397	0.
H	-2.8311314778	2.2694815062	0.
H	-0.5498628989	-3.5865725343	0.
H	3.3809943766	1.3170910281	0.
H	-2.8311315	-2.2694814785	0.

C-H (nonplanar = C2)

C	0.0951231433	-0.723141753	1.2607557507
C	-0.1886634648	1.4365701864	0.0144772486
C	-0.0935677203	0.7133977877	-1.2488433108
C	0.1886634648	-1.4365701864	0.0144772485
C	-0.0951231433	0.7231417529	1.2607557508
C	0.0935677202	-0.7133977876	-1.2488433109
S	0.4188426031	-3.1869365311	1.864597048
S	-0.4188426031	3.186936531	1.8645970482
S	0	0.0000000002	-3.7028175837
C	0.2052243979	-1.5612527785	2.341545338
C	-0.3658505422	2.7835869124	0.2061374981
C	-0.1602374641	1.2223810138	-2.5212612074
C	0.3658505422	-2.7835869124	0.2061374979
C	-0.2052243979	1.5612527783	2.3415453381
C	0.1602374641	-1.2223810136	-2.5212612075
H	0.1716366924	-1.3053928838	3.3899748797
H	-0.4673312003	3.5558403343	-0.5414117406
H	-0.2950433322	2.2505433509	-2.8218544252
H	0.4673312003	-3.5558403342	-0.5414117409
H	-0.1716366924	1.3053928835	3.3899748798
H	0.2950433321	-2.2505433507	-2.8218544254

B-F structure (D3H):

C	0.7242590271	1.2810712663	0.
C	0.7473107471	-1.2677623495	0.
C	-0.7473107465	-1.2677623499	0.
C	-0.7242590277	1.2810712659	0.
C	1.4715697742	-0.013308916	0.
C	-1.4715697742	-0.0133089168	0.
C	1.3568987222	2.5466851299	0.
C	1.5270446569	-2.4484513287	0.
C	-1.5270446556	-2.4484513295	0.
C	-1.3568987235	2.5466851292	0.
C	2.8839433791	-0.0982337997	0.
C	-2.883943379	-0.0982338012	0.
C	0.6810661505	3.7530328796	0.
C	2.9096887397	-2.4663370277	0.
C	-2.9096887384	-2.4663370292	0.
C	-0.6810661524	3.7530328792	0.
C	3.5907548908	-1.28669585	0.
C	-3.5907548902	-1.2866958518	0.
F	1.3586726724	4.8860326938	0.
F	3.5520921004	-3.6196613966	0.
F	-3.5520920985	-3.6196613984	0.
F	-1.3586726749	4.8860326931	0.
F	4.9107647734	-1.2663712947	0.
F	-4.9107647727	-1.2663712972	0.
F	2.660152161	2.7794967855	0.
F	1.0770387454	-3.6935077421	0.
F	-1.0770387436	-3.6935077427	0.
F	-2.6601521624	2.7794967841	0.
F	3.737190906	0.9140109585	0.
F	-3.7371909065	0.9140109566	0.

B-F structure (D3)

C	-1.2500815484	-0.7076786997	0.0495179973
C	1.2379085058	-0.7287630278	0.0495179973
C	0.0121730425	-1.4364417275	-0.0495179973
C	1.2379085058	0.7287630278	-0.0495179973
C	-1.2500815484	0.7076786997	-0.0495179973
C	0.0121730425	1.4364417275	0.0495179973
C	-2.4778947715	-1.3420450264	0.3017746811
C	2.4011924716	-1.4748973068	0.3017746811
C	0.0767022998	-2.8169423332	-0.3017746811
C	2.4011924716	1.4748973068	-0.3017746811
C	-2.4778947715	1.3420450264	-0.3017746811
C	0.0767022998	2.8169423332	0.3017746811
C	-3.6780187169	-0.6682562257	0.1850992729
C	2.4177362262	-2.8511295316	0.1850992729
C	1.2602824907	-3.5193857573	-0.1850992729
C	2.4177362262	2.8511295316	-0.1850992729
C	-3.6780187169	0.6682562257	-0.1850992729
C	1.2602824907	3.5193857573	0.1850992729
F	-2.547752295	2.5914295748	-0.7426162578
F	-0.9703676965	-3.5021329974	-0.7426162578
F	3.5181199914	-0.9107034226	0.7426162578
F	-0.9703676964	3.5021329974	0.7426162578
F	-2.547752295	-2.5914295748	0.7426162578
F	3.5181199914	0.9107034226	-0.7426162578
F	-4.8210922304	-1.293371469	0.4100759535
F	3.5306386639	-3.5285026111	0.4100759535
F	1.2904535665	-4.82187408	-0.4100759535
F	3.5306386639	3.528502611	-0.4100759535
F	-4.8210922304	1.293371469	-0.4100759535
F	1.2904535666	4.82187408	0.4100759535

B-F structure (C2)

C	-0.7257433075	0.0827340849	1.2707028775
C	0.7257433075	-0.0827340849	1.2707028775
C	-1.4315913399	-0.1127730066	0.0567105768
C	1.4315913399	0.1127730066	0.0567105768
C	-0.6696622994	-0.2392036365	-1.1931898342
C	0.6696622994	0.2392036365	-1.1931898342
C	-2.8112310616	0.1163409478	0.0618735004
C	2.8112310616	-0.1163409478	0.0618735005
C	-1.4149192895	0.5252747087	2.3994632929
C	1.4149192895	-0.5252747087	2.3994632929
C	-2.7925716164	0.6625694798	2.3972464124
C	2.7925716164	-0.6625694798	2.3972464124
C	-3.4922380533	0.4473055321	1.2230957955
C	3.4922380533	-0.4473055321	1.2230957955
C	-0.5944232331	-0.3559426317	-3.6119482398
C	0.5944232331	0.3559426317	-3.6119482398
C	-1.2209697363	-0.6471821803	-2.4098102783
C	1.2209697363	0.6471821803	-2.4098102783
F	-3.5300621965	0.1428153217	-1.0528228888
F	3.5300621965	-0.1428153217	-1.0528228888
F	-0.7782872958	0.92320231	3.4934219772
F	0.7782872958	-0.92320231	3.4934219772
F	-3.4278153477	1.0683419058	3.483127393
F	3.4278153477	-1.0683419058	3.483127393
F	-4.7983810876	0.6504596627	1.1878470282
F	4.7983810876	-0.6504596627	1.1878470282
F	-1.1449667368	-0.7229138468	-4.7565665187
F	1.1449667368	0.7229138468	-4.7565665187
F	-2.3346526094	-1.3638543393	-2.4724510954
F	2.3346526094	1.3638543393	-2.4724510954

B-Me structure (D3)

C	0.62685	1.13959	-0.61292
C	0.802	-1.12297	0.40436
C	-0.65329	-1.12789	0.60767
C	-0.77775	1.13737	-0.41081
C	1.43503	0.08686	0.01722
C	-1.43341	-0.11319	-0.00542
C	1.17966	2.12428	-1.46867
C	1.59763	-2.29013	0.51556
C	-1.30994	-2.06604	1.44222
C	-1.4771	2.36198	-0.54712
C	2.81011	0.25037	0.31694
C	-2.80148	-0.37978	-0.25948
C	0.41051	3.24285	-1.77438
C	2.97851	-2.14408	0.60542
C	-2.69236	-2.18834	1.34116
C	-0.85207	3.41016	-1.21552
C	3.55827	-0.8801	0.63058
C	-3.405	-1.43921	0.41089
H	0.82594	4.00392	-2.42912
H	3.59699	-3.03319	0.69198
H	-3.20473	-2.90575	1.97622
H	-1.38046	4.35309	-1.32595
H	4.61376	-0.76503	0.86128
H	-4.45396	-1.65129	0.2232
C	2.48867	1.96764	-2.20932
C	1.06387	-3.69812	0.37745
C	-0.63288	-2.83187	2.55646
C	-2.7946	2.66723	0.1293
C	3.48911	1.59111	0.48379
C	-3.61322	0.30346	-1.33683
H	2.28766	2.08505	-3.27863
H	2.94007	0.98699	-2.05987
H	3.21872	2.73294	-1.93159
H	1.61235	-4.18901	-0.43238
H	0.00388	-3.72166	0.12529
H	1.22029	-4.29359	1.28114
H	-1.16423	-2.61311	3.48783
H	0.40925	-2.54273	2.69058
H	-0.67743	-3.91396	2.40528
H	-2.65919	3.56279	0.74347
H	-3.12691	1.86088	0.78284
H	-3.59077	2.88453	-0.58812
H	3.93302	1.62237	1.48358
H	2.79391	2.42625	0.40073
H	4.29994	1.73992	-0.23469
H	-4.00794	-0.46948	-2.00343
H	-3.01769	0.99074	-1.93751
H	-4.46992	0.84835	-0.93071

B-Me structure (C2)

C	-0.7279429689	0.107781859	1.2789984605
C	0.7279429689	-0.107781859	1.2789984605
C	-1.4317883992	-0.168545459	0.0726932177
C	1.4317883992	0.168545459	0.0726932177
C	-0.6290725354	-0.3325858668	-1.1590483525
C	0.6290725354	0.3325858668	-1.1590483525
C	-2.8273507458	0.0572355673	0.0195796945
C	2.8273507458	-0.0572355673	0.0195796945
C	-1.3922429916	0.6588381514	2.3879271859
C	1.3922429916	-0.6588381514	2.3879271859
C	-2.7824319397	0.7541036449	2.3473951578
C	2.7824319397	-0.7541036449	2.3473951578
C	-3.4811360868	0.4410537433	1.1938912054
C	3.4811360868	-0.4410537433	1.1938912054
C	-0.48175707	-0.5019363111	-3.5525753201
C	0.48175707	0.5019363111	-3.5525753201
C	-1.0725634635	-0.9182766167	-2.356655958
C	1.0725634635	0.9182766167	-2.356655958
C	-3.6766226387	0.0819215994	-1.2299899521
C	3.6766226387	-0.0819215994	-1.2299899521
C	-0.6992287757	1.2926439081	3.5710194685
C	0.6992287757	-1.2926439081	3.5710194685
C	-2.0528123909	-2.065011523	-2.3788426055
C	2.0528123909	2.065011523	-2.3788426055
H	-3.3104508774	1.1557942063	3.2078156764
H	3.3104508774	-1.1557942063	3.2078156764
H	-4.5558026805	0.5954372627	1.1623758484
H	4.5558026805	-0.5954372627	1.1623758484
H	-0.8242042792	-0.9338491084	-4.4888883805
H	0.8242042792	0.9338491084	-4.4888883805
H	-4.480525767	0.8091576938	-1.0953734306
H	4.480525767	-0.8091576938	-1.0953734306
H	-3.1003562705	0.3737780644	-2.1095411816
H	3.1003562705	-0.3737780644	-2.1095411816
H	-4.1447331573	-0.8836118815	-1.439130056
H	4.1447331573	0.8836118815	-1.439130056
H	-1.1204756393	2.2897836979	3.7291727691
H	1.1204756393	-2.2897836979	3.7291727691
H	0.3743698002	1.400502372	3.4169318318
H	-0.3743698002	-1.400502372	3.4169318318
H	-0.8612585565	0.7233722441	4.4911406776
H	0.8612585565	-0.7233722441	4.4911406776
H	-2.4348239518	-2.2899608004	-1.3820423583
H	2.4348239518	2.2899608004	-1.3820423583
H	-1.5290508249	-2.9562585273	-2.7401280875
H	1.5290508249	2.9562585273	-2.7401280875
H	-2.8960447507	-1.8844834295	-3.0514255024
H	2.8960447507	1.8844834295	-3.0514255024

Triphenylene (FLAT – contrary to the reviewer)

C	0.7052965476	1.2524745332	0.
C	0.7320264896	-1.237041994	0.
C	-0.7320264896	-1.237041994	0.
C	-0.7052965476	1.2524745332	0.
C	1.4373230372	-0.0154325392	0.
C	-1.4373230372	-0.0154325392	0.
C	1.3818129613	2.4874419588	0.
C	1.4632814461	-2.4404061071	0.
C	-1.4632814461	-2.4404061071	0.
C	-1.3818129613	2.4874419588	0.
C	2.8450944074	-0.0470358516	0.
C	-2.8450944074	-0.0470358516	0.
C	0.7004183151	3.6890079476	0.
C	2.8445654399	-2.451084028	0.
C	-2.8445654399	-2.451084028	0.
C	-0.7004183151	3.6890079476	0.
C	3.544983755	-1.2379239197	0.
C	-3.544983755	-1.2379239197	0.
H	1.2499818903	4.623988887	0.
H	3.3795008978	-3.3945105148	0.
H	-3.3795008978	-3.3945105148	0.
H	-1.2499818903	4.623988887	0.
H	4.6294827881	-1.2294783722	0.
H	-4.6294827881	-1.2294783722	0.
H	2.4627307787	2.5151049429	0.
H	0.9467793843	-3.3903398885	0.
H	-0.9467793843	-3.3903398885	0.
H	-2.4627307787	2.5151049429	0.
H	3.409510163	0.8752349456	0.
H	-3.409510163	0.8752349456	0.

C-Me structure (C2)

C	-0.2319139844	-0.6926087307	1.2911088471
C	0.2184153193	1.4377395135	0.0462345849
C	-0.0638377174	0.7252692299	-1.2068935356
C	-0.2184153193	-1.4377395135	0.0462345849
C	0.2319139844	0.6926087307	1.2911088471
C	0.0638377174	-0.7252692299	-1.2068935356
S	-1.2826173345	-2.952686705	1.8081364183
S	1.2826173345	2.952686705	1.8081364183
S	0.	0.	-3.6542286653
C	-0.8110099468	-1.3837737788	2.3268214986
C	0.7806784014	2.687686979	0.1845793098
C	-0.2408593714	1.2339662294	-2.4709683215
C	-0.7806784014	-2.687686979	0.1845793098
C	0.8110099468	1.3837737788	2.3268214986
C	0.2408593714	-1.2339662294	-2.4709683215
C	-1.2311532842	-0.9164221535	3.6889238292
C	1.1972376321	3.7004590229	-0.83975756
C	-0.7413975881	2.577761129	-2.9156525128
C	-1.1972376321	-3.7004590229	-0.83975756
C	1.2311532842	0.9164221535	3.6889238292
C	0.7413975881	-2.577761129	-2.9156525128
H	-2.1908298281	-1.364912479	3.9611040979
H	2.0217592149	4.3069674917	-0.4558725385
H	-1.5646608642	2.4442292534	-3.6241544052
H	-2.0217592149	-4.3069674917	-0.4558725386
H	2.1908298281	1.364912479	3.9611040979
H	1.5646608642	-2.4442292534	-3.6241544052
H	-1.3564764762	0.1693376495	3.6783520828
H	1.5467938722	3.1853440979	-1.7392054755
H	0.0213297275	3.1901746837	-3.4062037844
H	-1.5467938722	-3.1853440979	-1.7392054755
H	1.3564764762	-0.1693376495	3.6783520828
H	-0.0213297275	-3.1901746837	-3.4062037844
H	-0.5108221645	-1.1694588262	4.4728755682
H	0.3914669223	4.3813860999	-1.1281136036
H	-1.1300147803	3.1274690149	-2.0567476417
H	-0.3914669223	-4.3813860999	-1.1281136036
H	0.5108221645	1.1694588262	4.4728755682
H	1.1300147803	-3.1274690149	-2.0567476417

C-Me structure (D3):

C	1.2580090366	-0.730520385	-0.0480720973
C	0.0036446931	1.4547279764	-0.0480720973
C	-1.2616537297	0.7242075914	0.0480720973
C	0.0036446931	-1.4547279764	0.0480720973
C	1.2580090366	0.730520385	0.0480720973
C	-1.2616537297	-0.7242075914	-0.0480720973
S	1.8541056479	-3.2114051848	0.
S	1.8541056479	3.2114051848	0.
S	-3.7082112958	0.	0.
C	2.335765023	-1.5740091538	-0.2166643882
C	0.1952494015	2.809836424	-0.2166643882
C	-2.5310144244	1.2358272703	0.2166643882
C	0.1952494015	-2.809836424	0.2166643882
C	2.335765023	1.5740091538	0.2166643882
C	-2.5310144244	-1.2358272703	-0.2166643882
C	3.7243569517	-1.3157886312	-0.7284229215
C	-0.7226720952	3.8832820485	-0.7284229215
C	-3.0016848565	2.5674934174	0.7284229215
C	-0.7226720952	-3.8832820485	0.7284229215
C	3.7243569517	1.3157886312	0.7284229215
C	-3.0016848565	-2.5674934174	-0.7284229215
H	4.0128814618	-2.1188992669	-1.4124041072
H	-0.1714201378	4.5347069218	-1.4124041072
H	-3.8414613241	2.4158076549	1.4124041072
H	-0.1714201378	-4.5347069218	1.4124041072
H	4.0128814618	2.1188992669	1.4124041072
H	-3.8414613241	-2.4158076549	-1.4124041072
H	3.7428640519	-0.3794645105	-1.2891774511
H	-1.54280612	3.4311476071	-1.2891774511
H	-2.2000579319	3.0516830966	1.2891774511
H	-1.54280612	-3.4311476071	1.2891774511
H	3.7428640519	0.3794645105	1.2891774511
H	-2.2000579319	-3.0516830966	-1.2891774511
H	4.4827424183	-1.2644093623	0.0578827905
H	-1.1463605806	4.514373494	0.0578827905
H	-3.3363818377	3.2499641317	-0.0578827905
H	-1.1463605806	-4.514373494	-0.0578827905
H	4.4827424183	1.2644093623	-0.0578827905
H	-3.3363818377	-3.2499641317	0.0578827905

C2 to C2 TS

C	-1.27982	0.08622	0.72165
C	1.22841	-0.22787	0.74547
C	1.22727	-0.23315	-0.74199
C	-1.27946	0.08896	-0.71984
C	-0.00176	0.17895	1.42109
C	-0.00042	0.17731	-1.41865
S	-3.65771	-0.47576	-0.00013
S	1.80146	0.24334	3.20319
S	1.80021	0.21519	-3.20306
C	-2.5072	-0.23305	1.25543
C	2.27622	-0.30208	1.64007
C	2.27241	-0.32594	-1.63877
C	-2.50711	-0.22809	-1.25475
C	0.18437	0.55351	2.72828
C	0.187	0.54209	-2.72911
C	-2.90382	-0.5848	2.65812
C	3.7211	-0.7092	1.54509
C	3.70289	-0.78269	-1.54896
C	-2.90489	-0.57531	-2.65824
C	-0.73103	1.2951	3.65749
C	-0.72212	1.29019	-3.65951
H	-3.69333	-1.34097	2.64776
H	4.34853	0.09518	1.15255
H	4.31461	-0.11656	-0.94011
H	-3.69971	-1.3259	-2.6495
H	-0.1896	2.12195	4.12654
H	-0.17436	2.11375	-4.12708
H	-2.04096	-1.0019	3.1848
H	3.85475	-1.59531	0.92706
H	3.77651	-1.79467	-1.14598
H	-2.04455	-0.99779	-3.18483
H	-1.56322	1.71769	3.09055
H	-1.55221	1.71835	-3.09376
H	-3.27066	0.27148	3.23176
H	4.09601	-0.95096	2.54375
H	4.14296	-0.80241	-2.54967
H	-3.26521	0.28416	-3.23118
H	-1.13919	0.66958	4.45703
H	-1.13324	0.66801	-4.46014

B3PW91/DZ(2d,p) Structures:

C-Me-C_1:

C	0.004602	1.440540	0.190791
C	-1.186070	-0.710614	-0.267193
C	0.083494	-1.438460	-0.188472
C	1.268197	0.762965	-0.035197
C	-1.222650	0.643724	0.271689
C	1.307891	-0.692462	0.039252
S	1.718642	3.242891	-0.411875
S	-3.653957	-0.097264	-0.001254
S	1.895861	-3.144402	0.408081
C	0.107495	2.808988	0.007382
C	-2.443671	-1.176495	-0.596339
C	0.263053	-2.799631	-0.009802
C	2.284413	1.619803	-0.406660
C	-2.503524	1.043049	0.598193
C	2.370226	-1.492371	0.408419
C	-0.927415	3.887633	-0.075318
C	-2.877478	-2.321407	-1.462329
C	-0.708943	-3.935678	0.067883
C	3.655558	1.344037	-0.943081
C	-2.995652	2.160334	1.468726
C	3.724163	-1.142003	0.944991
H	-0.555874	4.726877	-0.672032
H	-3.633705	-1.977033	-2.177299
H	-0.278920	-4.766670	0.636096
H	3.917250	2.077095	-1.713543
H	-3.688344	1.764061	2.220383
H	4.025192	-1.859341	1.715899
H	-1.828715	3.505035	-0.564394
H	-2.032199	-2.698353	-2.041690
H	-0.999469	-4.327508	-0.912874
H	3.682121	0.353083	-1.404731
H	-2.162107	2.616228	2.005930
H	3.696496	-0.150921	1.406221
H	-1.218955	4.287311	0.902282
H	-3.315663	-3.157554	-0.905528
H	-1.618957	-3.615460	0.585255
H	4.439111	1.381762	-0.177617
H	-3.526956	2.947360	0.921075
H	4.508831	-1.137264	0.179727

C-Me-C_2 (the one that is essentially the energy of C_1):

C	0.1485561015	-0.7135929126	1.2891154304
C	-0.0355273305	1.4516727302	0.0442018657
C	0.1614932089	0.7108590582	-1.2046263676
C	0.0355273305	-1.4516727302	0.0442018657
C	-0.1485561015	0.7135929126	1.2891154304
C	-0.1614932089	-0.7108590582	-1.2046263676
S	0.8984361196	-3.0935842815	1.8074385168
S	-0.8984361196	3.0935842815	1.8074385168
S	0.	0.	-3.6550293467
C	0.6416757162	-1.4758330061	2.3285176464
C	-0.4260817737	2.7724753373	0.1847637696
C	0.4187271798	1.1890634294	-2.4742643043
C	0.4260817737	-2.7724753373	0.1847637696
C	-0.6416757162	1.4758330061	2.3285176464
C	-0.4187271798	-1.1890634294	-2.4742643043
C	1.122040449	-1.0857345523	3.6928419009
C	-0.6787188939	3.8529330009	-0.8203367825
C	1.1017354544	2.4409546033	-2.9374855256
C	0.6787188939	-3.8529330009	-0.8203367825
C	-1.122040449	1.0857345523	3.6928419009
C	-1.1017354544	-2.4409546033	-2.9374855256
H	1.9910719019	-1.6887468141	3.9767710075
H	-1.3848795305	4.5875049509	-0.4201980009
H	1.886128194	2.1869627487	-3.6598749693
H	1.3848795305	-4.5875049509	-0.4201980009
H	-1.9910719019	1.6887468141	3.9767710075
H	-1.886128194	-2.1869627487	-3.6598749693
H	1.431378744	-0.0367970442	3.6937473287
H	-1.1209269547	3.4259127191	-1.7259922157
H	1.5861821344	2.9407467041	-2.0964881105
H	1.1209269547	-3.4259127191	-1.7259922157
H	-1.431378744	0.0367970442	3.6937473287
H	-1.5861821344	-2.9407467041	-2.0964881105
H	0.3653332758	-1.2159157805	4.4750121767
H	0.2265270815	4.3966747063	-1.1119571592
H	0.4311623222	3.1571360688	-3.4261673497
H	-0.2265270815	-4.3966747063	-1.1119571592
H	-0.3653332758	1.2159157805	4.4750121767
H	-0.4311623222	-3.1571360688	-3.4261673497

C-Me-TS structure:

C	-0.2309007661	0.6853455136	1.2422212987
C	-0.1398174361	0.7233983616	-1.2930372393
C	0.1398174361	-0.7233983616	-1.2930372393
C	0.2309007661	-0.6853455136	1.2422212987
C	-0.2391808984	1.4214465215	-0.0158665825
C	0.2391808984	-1.4214465215	-0.0158665825
S	0.	0.	3.6918051384
S	-0.3842022293	3.2224894157	-1.8083540029
S	0.3842022293	-3.2224894157	-1.8083540029
C	-0.54221791	1.1364048281	2.5147112281
C	-0.3132364629	1.5976755786	-2.3588667743
C	0.3132364629	-1.5976755786	-2.3588667743
C	0.54221791	-1.1364048281	2.5147112281
C	-0.2597095729	2.8007782821	-0.1544148083
C	0.2597095729	-2.8007782821	-0.1544148083
C	1.3917548108	-2.2786135639	2.9865468677
C	-0.5552859062	1.4335027487	-3.8322895382
C	0.5552859062	-1.4335027487	-3.8322895382
C	-1.3917548108	2.2786135639	2.9865468677
C	-0.0043069447	3.9055460383	0.8261935956
C	0.0043069447	-3.9055460383	0.8261935956
H	2.0746407152	-1.9284028376	3.7686567504
H	-0.9224951249	2.376978099	-4.2488693683
H	0.9224951249	-2.376978099	-4.2488693683
H	-2.0746407152	1.9284028376	3.7686567504
H	0.5663908398	4.7049581209	0.341445082
H	-0.5663908398	-4.7049581209	0.341445082
H	2.0037446913	-2.6585825695	2.1657905714
H	0.3417669914	1.1647563499	-4.3956923092
H	-0.3417669914	-1.1647563499	-4.3956923092
H	-2.0037446913	2.6585825695	2.1657905714
H	-0.9152936036	4.3595562904	1.231645586
H	0.9152936036	-4.3595562904	1.231645586
H	0.8215188736	-3.1153058501	3.4060983372
H	-1.3238852411	0.6801356123	-4.0250874399
H	1.3238852411	-0.6801356123	-4.0250874399
H	-0.8215188736	3.1153058501	3.4060983372
H	0.5924141782	3.5358486017	1.6640474446
H	-0.5924141782	-3.5358486017	1.6640474446

imaginary mode to move the methyl/methyl class is -40.1 cm-1

C-Me-D_3 structure:

C	0.725004	1.259994	0.049091
C	0.728684	-1.257869	0.049091
C	-0.728684	-1.257869	-0.049091
C	-0.725004	1.259994	-0.049091
C	1.453688	-0.002125	-0.049091
C	-1.453688	-0.002125	0.049091
S	0.000000	3.709748	0.000000
S	3.212736	-1.854874	0.000000
S	-3.212736	-1.854874	0.000000
C	1.237613	2.536334	0.223368
C	1.577723	-2.339971	0.223368
C	-1.577723	-2.339971	-0.223368
C	-1.237613	2.536334	-0.223368
C	2.815336	-0.196362	-0.223368
C	-2.815336	-0.196362	0.223368
C	2.561987	3.026323	0.728890
C	1.339879	-3.731908	0.728890
C	-1.339879	-3.731908	-0.728890
C	-2.561987	3.026323	-0.728890
C	3.901867	0.705584	-0.728890
C	-3.901867	0.705584	0.728890
H	2.408010	3.895439	1.377548
H	2.169544	-4.033117	1.377548
H	-2.169544	-4.033117	-1.377548
H	-2.408010	3.895439	-1.377548
H	4.577554	0.137678	-1.377548
H	-4.577554	0.137678	1.377548
H	3.048634	2.253933	1.329048
H	0.427647	-3.767161	1.329048
H	-0.427647	-3.767161	-1.329048
H	-3.048634	2.253933	-1.329048
H	3.476280	1.513228	-1.329048
H	-3.476280	1.513228	1.329048
H	3.255179	3.333602	-0.061947
H	1.259395	-4.485868	-0.061947
H	-1.259395	-4.485868	0.061947
H	-3.255179	3.333602	0.061947
H	4.514573	1.152267	0.061947
H	-4.514573	1.152267	-0.061947

C-Me-C_s structure (2 modes of -39.4 cm-1)

C	-1.276342	0.075958	0.721229
C	1.228185	-0.220356	0.741189
C	1.228185	-0.220356	-0.741189
C	-1.276342	0.075958	-0.721229
C	-0.001501	0.187974	1.417742
C	-0.001501	0.187974	-1.417742
S	-3.652629	-0.509199	0.000000
S	1.805092	0.247728	3.201048
S	1.805092	0.247728	-3.201048
C	-2.507388	-0.253586	1.258159
C	2.278839	-0.309740	1.642415
C	2.278839	-0.309740	-1.642415
C	-2.507388	-0.253586	-1.258159
C	0.189381	0.572812	2.728847
C	0.189381	0.572812	-2.728847
C	-2.920469	-0.591176	2.657089
C	3.710693	-0.755620	1.561489
C	3.710693	-0.755620	-1.561489
C	-2.920469	-0.591176	-2.657089
C	-0.708087	1.326514	3.662740
C	-0.708087	1.326514	-3.662740
H	-3.723321	-1.335665	2.648380
H	4.112163	-0.887200	2.571541
H	4.112163	-0.887200	-2.571541
H	-3.723321	-1.335665	-2.648380
H	-0.154937	2.149572	4.129305
H	-0.154937	2.149572	-4.129305
H	-2.073332	-1.019395	3.201372
H	3.811959	-1.715861	1.051179
H	3.811959	-1.715861	-1.051179
H	-2.073332	-1.019395	-3.201372
H	-1.541930	1.763129	3.108186
H	-1.541930	1.763129	-3.108186
H	-3.282818	0.272985	3.225665
H	4.350929	-0.025630	1.057855
H	4.350929	-0.025630	-1.057855
H	-3.282818	0.272985	-3.225665
H	-1.119021	0.711327	4.471498
H	-1.119021	0.711327	-4.471498

C-Me-C_2 (the one that is essentially D_3):

C	0.7250852605	1.2604489672	0.0490292178
C	0.7286559165	-1.257270771	0.0489927846
C	-0.7286559165	-1.257270771	-0.0489927846
C	-0.7250852605	1.2604489672	-0.0490292178
C	1.4538751489	-0.0017429325	-0.0491462725
C	-1.4538751489	-0.0017429325	0.0491462725
S	0.	3.7102328981	0.
S	3.2123682604	-1.8553233254	-0.0001179048
S	-3.2123682604	-1.8553233254	0.0001179048
C	1.2377776026	2.5368414282	0.222563889
C	1.5771846805	-2.339775586	0.2227249877
C	-1.5771846805	-2.339775586	-0.2227249877
C	-1.2377776026	2.5368414282	-0.222563889
C	2.8155295559	-0.1965378118	-0.2229656889
C	-2.8155295559	-0.1965378118	0.2229656889
C	2.5626235016	3.0266865757	0.727087117
C	1.3383817658	-3.7318823433	0.7275734952
C	-1.3383817658	-3.7318823433	-0.7275734952
C	-2.5626235016	3.0266865757	-0.727087117
C	3.9028455508	0.7050671239	-0.7273158911
C	-3.9028455508	0.7050671239	0.7273158911
H	2.4094079859	3.8950112542	1.3769680293
H	2.1690269239	-4.0350938023	1.37402491
H	-2.1690269239	-4.0350938023	-1.37402491
H	-2.4094079859	3.8950112542	-1.3769680293
H	4.5799392251	0.1366152332	-1.3739908975
H	-4.5799392251	0.1366152332	1.3739908975
H	3.0500772498	2.2536410916	1.3256328452
H	0.4275430324	-3.7660849448	1.3298122888
H	-0.4275430324	-3.7660849448	-1.3298122888
H	-3.0500772498	2.2536410916	-1.3256328452
H	3.4781920437	1.511944486	-1.3290854747
H	-3.4781920437	1.511944486	1.3290854747
H	3.2548573879	3.3347391842	-0.0643399935
H	1.2546112613	-4.485146076	-0.0635883764
H	-1.2546112613	-4.485146076	0.0635883764
H	-3.2548573879	3.3347391842	0.0643399935
H	4.5138311632	1.1527467997	0.0642694105
H	-4.5138311632	1.1527467997	-0.0642694105