Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for: Polycyclic Aliphatic Hydrocarbons: Is Tetrahedrane Present in UIR Spectra?

Mode	^{2}H	^{13}C
ω_1	3371.7	3392.7
ω_2	3344.3	3358.8
ω_3	3343.5	3343.7
ω_4	2478.4	3335.4
ω_5	1414.7	1430.4
ω_6	1145.1	1146.2
ω_7	1143.7	1144.5
ω_8	1121.1	1129.5
ω_9	886.0	964.1
ω_{10}	864.6	883.1
ω_{11}	860.3	861.1
ω_{12}	822.9	846.2
ω_{13}	822.4	817.3
ω_{14}	769.7	801.5
ω_{15}	705.2	772.9
ω_{16}	670.4	662.4
ω_{17}	552.0	583.7
ω_{18}	504.3	399.8
ZPT	12231.6	12748.5
ν_1	3234.0	3255.1
ν_2	3211.0	3219.1
ν_3	3211.1	3209.2
ν_4	2405.2	3200.3
ν_5	1378.4	1390.4
ν_6	1090.2	1091.9
ν_7	1093.4	1101.2
ν_8	1076.9	1086.3
ν_9	849.2	932.3
ν_{10}	829.0	848.4
ν_{11}	819.9	820.6
ν_{12}	790.1	817.7
ν_{13}	792.7	795.9
ν_{14}	753.6	767.1
ν_{15}	678.7	757.5
ν_{16}	629.3	627.0
ν_{17}	497.9	520.8
ν_{18}	450.8	373.3

Table S1: F12-TZ vibrational frequencies of singly-isotopically-substituted tetrahedrane (in cm^{-1})

	^{2}H		^{13}C	
Const.	Units	Value	Units	Value
A_e	MHz	13770.4	MHz	13770.4
C_e	MHz	12454.1	MHz	13462.9
A_0	MHz	13661.4	MHz	13673.6
C_0	MHz	12364.8	MHz	13362.0
A_1	MHz	13629.4	MHz	13638.9
C_1	MHz	12345.5	MHz	13342.7
A_2	MHz	13631.6	MHz	13643.0
C_2	MHz	12346.1	MHz	13339.8
A_3	MHz	13630.9	MHz	13641.9
C_3	MHz	12346.2	MHz	13340.9
A_4	MHz	13657.2	MHz	13662.5
C_4	MHz	12314.6	MHz	13332.1
A_5	MHz	13628.7	MHz	13643.1
C_5	MHz	12343.0	MHz	13340.8
A_6	MHz	13673.8	MHz	13687.5
C_6	MHz	12366.6	MHz	13380.6
A_7	MHz	13676.6	MHz	13696.9
C_7	MHz	12351.6	MHz	13335.9
A_8	MHz	13642.0	MHz	13646.6
C_8	MHz	12376.5	MHz	13376.8
A_9	MHz	13647.4	MHz	13665.6
C_9	MHz	12392.3	MHz	13381.2
A_{10}	MHz	13683.5	MHz	13702.5
C_{10}	MHz	12371.9	MHz	13408.1
A_{11}	MHz	13681.1	MHz	13745.4
C_{11}	MHz	12375.3	MHz	13380.6
A_{12}	MHz	15894.0	MHz	13636.6
C_{12}	MHz	12355.4	MHz	13325.4
A_{13}	MHz	12315.5	MHz	13696.7
C_{13}	MHz	11811.2	MHz	13371.7
A_{14}	MHz	13658.6	MHz	13598.3
C_{14}	MHz	12370.8	MHz	13303.7
A_{15}	MHz	13704.3	MHz	13635.7
C_{15}	MHz	12347.5	MHz	13323.6
A_{16}	MHz	13668.5	MHz	13660.6
C_{16}	MHz	12340.3	MHz	13338.7
A_{17}	MHz	13652.2	MHz	13633.4
C_{17}	MHz	12358.0	MHz	13336.9
A_{18}	MHz	13615.1	MHz	13696.4
C_{18}	MHz	12373.8	MHz	13355.6
Δ_J	kHz	6.178	kHz	7.570
Δ_K	kHz	−5.725	kHz	−22.567
Δ_{JK}	kHz	6.988	kHz	22.702
δ_J	Hz	−2.040	Hz	131.778
δ_K	kHz	−1.111	kHz	−24.388
Φ_J	mHz	3.076	mHz	−410.516
Φ_K	Hz	2.628	Hz	7.150
Φ_{JK}	Hz	1.140	Hz	3.323
Φ_{KJ}	Hz	−3.768	Hz	−10.160
ϕ_j	μHz	55.520	mHz	159.200
ϕ_{jk}	mHz	−10.235	Hz	1.134
ϕ_k	Hz	84.391	Hz	6.915
μ	D	0.2	D	0.1

Table S2: F12-TZ rotational constants and dipole moments of singly-isotopically-substituted tetrahedrane