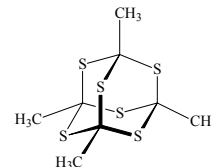


851 **C₈H₁₂S₆**ED, DFT
calculations**1,3,5,7-Tetramethyl-2,4,6,8,9,10-hexathiatricclo-
[3.3.1.1^{3,7}]decane**

1,3,5,7-Tetramethyl-2,4,6,8,9,10-hexathiaadamantane

T_d

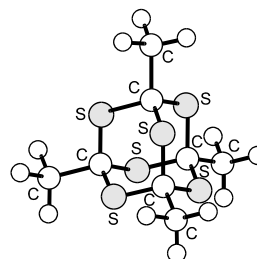
r_g	Å ^{a)}	θ_a	deg ^{a)}
C–S	1.820(4)	C–S–C	102.2(2)
C–C	1.536(4)	H–C–H	109.9(7)
C–H	1.119(5)		



The methyl groups were found to be in the staggered positions with respect to the adjacent C–S bonds. The barrier to the torsion of methyl groups was estimated to be 17 kJ mol^{−1} by the B3LYP/6-31G* method.

The nozzle temperature was about 170 °C.

^{a)} Estimated total errors.



Szász, G., Kovács, A., Hargittai, I., Jeon, I., Miller, G.P.: J. Phys. Chem. A **102** (1998) 484.