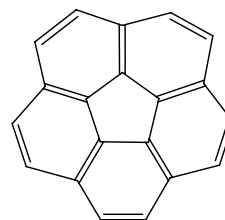


941 $\text{C}_{20}\text{H}_{10}$
ED, *ab initio* and
DFT calculations

Dibenzo[ghi,mno]fluoranthene
Corannulene

C_{5v} assumed

r_g	$\text{\AA}^a)$	θ_α	$\text{deg}^a)$
C–H	1.136(17)	C(20)–C(6)–C(7)	131.5(23)
C(1)–C(2)	1.414(6)	C(2)–C(1)–C(6)	122.4(6)
C(1)–C(6)	1.414(20)	C(1)–C(6)–C(7)	113.9(6)
C(6)–C(7)	1.447(16)	C(6)–C(7)–C(8)	122.4(4)
C(7)–C(8)	1.380(16)	C(6)–C(7)–H	119.2(2)
		C(8)–C(7)–H	118.2(2)
		φ_1 (1,6;5,1,2) ^{b)}	24.4(21)
		φ_2 (6,1;20,6,7) ^{c)}	–8.8(84)
		φ_3 (7,21;6,7,8) ^{d)}	–4.8 ^{e)}
		$\delta^f)$	0.5 ^{e)}
		φ_4 (5,1,2;6,1,2) ^{g)}	29.3(23)
		φ_5 (6,1,2;6,7,8) ^{h)}	13.8(56)
		φ_6 (6,7,8;21,7,8) ⁱ⁾	–5.4 ^{e)}



The average C–C bond distance was found to be *ca.* 0.022 Å shorter than that in C_{60} .
The vapor temperature was 303 °C.

^{a)} Twice the estimated standard errors.

^{b)} Angle between the C(1)–C(6) bond and the C(5)C(1)C(2) plane.

^{c)} Angle between the C(6)–C(1) bond and the C(20)C(6)C(7) plane.

^{d)} Angle between the C(7)–H bond and the C(6)C(7)C(8) plane.

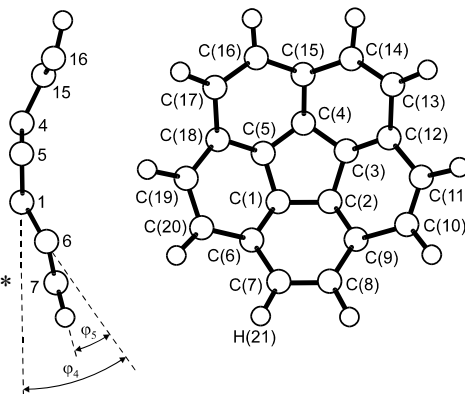
^{e)} Assumed at the value from B3LYP/6-31G* calculations.

^{f)} Angle between the bisector of the C–C–C angle and the projection of the C–H bond onto the CCC plane.

^{g)} Dihedral angle between the C(5)C(1)C(2) and C(6)C(1)C(2) planes, see figure.

^{h)} Dihedral angle between the C(6)C(1)C(2) and C(6)C(7)C(8) planes, see figure.

ⁱ⁾ Dihedral angle between the C(6)C(7)C(8) and H(21)C(7)C(8) planes.



Hedberg, L., Hedberg, K., Cheng, P.-C., Scott, L.T.: J. Phys. Chem. A **104** (2000) 7689.