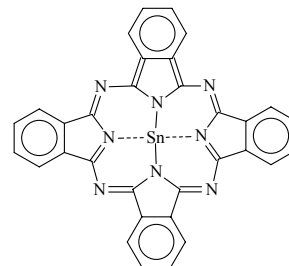


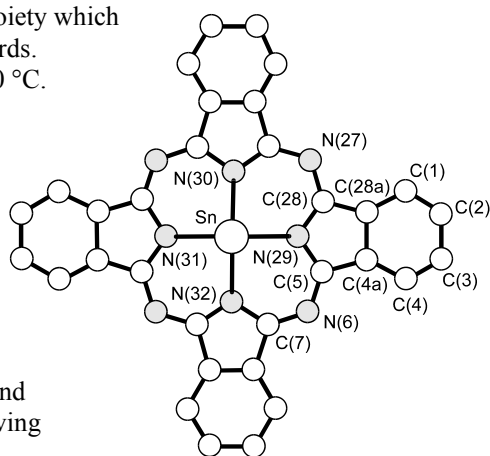
952
ED $\text{C}_{32}\text{H}_{16}\text{N}_8\text{Sn}$ **[29*H*,31*H*-Phthalocyaninato- κN^{29} , κN^{30} , κN^{31} , κN^{32}]tin**
Phthalocyaninatotin(II) C_{4v}

r_a	\AA^a	θ_a	deg a
C(5)–N(29)	1.409(31)	C(5)–N(29)–C(28)	110.5(30)
C(4a)–C(5)	1.438(47)	N(29)–C(5)–N(6)	125.5(28)
C(4a)–C(28a)	1.53(10)	C(28a)–C(4a)–C(4)	118.2(21)
X...N(29) b	1.979(29)	C(4a)–C(4)–H	120.1(78)
h c	1.01(10)	N(29)–C(5)–C(4a)	107.1 d
Sn–N(29)	2.201 d	C(5)–C(4a)–C(28a)	106.1 d
C–C e	1.392(10)	C(4a)–C(4)–C(3)	121.9 d
C–H(average)	1.099(46)	C(5)–N(6)–C(7)	124.6 d
		t f	3.9(52)



The Sn atom lies above the phthalocyanine moiety which is also slightly nonplanar, being bent downwards. The temperature of the measurements was 420 °C.

- a) Twice the estimated standard errors.
 b) Distance from the center of planar phthalocyanine skeleton X to N(29) atom.
 c) Distance from Sn atom to the center of planar phthalocyanine skeleton.
 d) Dependent parameter.
 e) Average value of C(4a)–C(4), C(3)–C(4) and C(2)–C(3) bond lengths.
 f) Angle of rotation of the isoindole units around the C(5)–N(6) and C(28)–N(27) bonds, leaving these atoms in the original plane.



Ruan, C.-Y., Mastryukov, V., Fink, M.: J. Chem. Phys. **111** (1999) 3035.