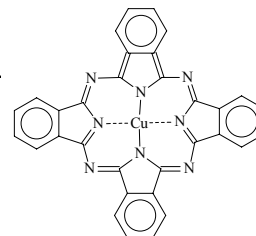
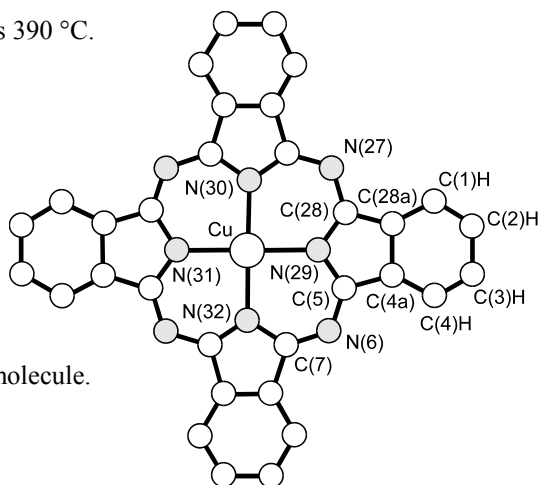


949 **C₃₂H₁₆CuN₈**ED, DFT
calculations**Phthalocyaninatocopper(II)**[29*H*,31*H*-Phthalocyaninato- $\kappa^2N^{29},\kappa^2N^{30},\kappa^2N^{31},\kappa^2N^{32}$]copper**D_{4h}**

<i>r</i> ^{a)}	Å ^{b)}	θ ^{a)}	deg ^{b)}
Cu–N(29)	1.935(22)	C(5)–N(29)–C(28)	104.8(16)
C(5)–N(29)	1.321(21)	N(29)–C(5)–N(6)	127.3(10)
C(5)–C(4a)	1.457(15)	C(4)–C(4a)–C(28a)	120.7(13)
C(4a)–C(28a)	1.397 ^{c)}	C(4a)–C(4)–H	120.0 ^{c)}
C(4a)–C(4)	1.353(12)	N(29)–C(5)–C(4a) ^{d)}	113.8
C(3)–C(4)	1.352 ^{c)}	C(5)–C(4a)–C(28a) ^{d)}	103.8
C(2)–C(3)	1.366 ^{c)}	C(4a)–C(4)–C(3) ^{d)}	117.9
C–H (average)	1.108 ^{f)}	C(5)–N(6)–C(7) ^{d)}	120.2



The temperature of the measurements was 390 °C.

^{a)} Unidentified, possibly r_a and θ_a .^{b)} Twice the estimated standard errors.^{c)} Assumed at the value from DFT calculations [1].^{d)} Dependent parameter.^{e)} Differences between the C(4a)–C(4), C(3)–C(4) and C(2)–C(3) bond lengths were assumed at the values from DFT calculations [1].^{f)} Assumed at the ED value for benzene molecule.Mastryukov, V., Ruan, C.-Y., Fink, M., Wang, Z., Pachter, R.: J. Mol. Struct. **556** (2000) 225.[1] Day, P.N., Wang, Z., Pachter, R.: J. Mol. Struct. (Theochem) **455** (1998) 33.