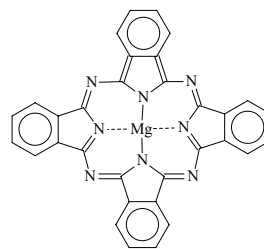


950 **C₃₂H₁₆MgN₈**
ED, DFT
calculations

[29*H*,31*H*-Phthalocyaninato- κ N²⁹, κ N³⁰, κ N³¹, κ N³²]-
magnesium
Phthalocyaninatomagnesium(II)

D_{4h}

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(5)–N(29)	1.386(24)	C(5)–N(29)–C(28)	109.5(26)
C(4a)–C(5)	1.411(28)	N(29)–C(5)–N(6)	125.9(23)
C(4a)–C(28a)	1.468(82)	C(28a)–C(4a)–C(4)	119.2(19)
Mg–N(29)	1.990(15)	C(4a)–C(4)–H	115.0(39)
C(4a)–C(4)	1.400(4)	N(29)–C(5)–C(4a)	108.9 ^{b)}
C(3)–C(4)	1.399 ^{c)}	C(5)–C(4a)–C(28a)	106.3 ^{b)}
C(2)–C(3)	1.412 ^{c)}	C(4a)–C(4)–C(3)	120.3 ^{b)}
C–H(average)	1.121(59)	C(5)–N(6)–C(7)	127.7 ^{b)}

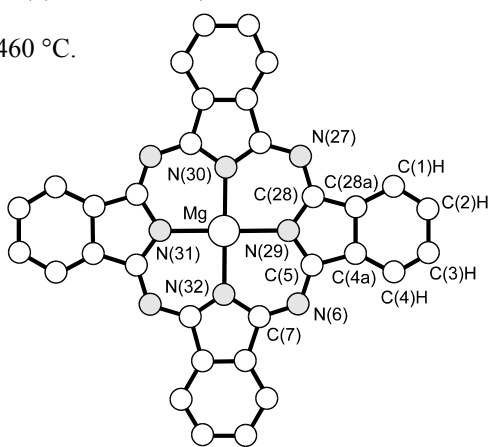


The temperature of the measurements was 460 °C.

^{a)} Twice the estimated standard errors.

^{b)} Dependent parameter.

^{c)} Difference to C(4a)–C(4) bond lengths was assumed at the value from B3LYP/6-31G* calculations.



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