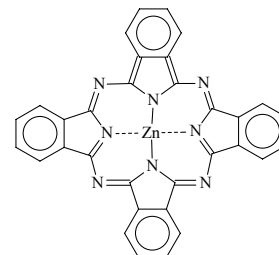


953 **C₃₂H₁₆N₈Zn**ED, DFT
calculations**[29*H*,31*H*-Phthalocyaninato- κ N²⁹, κ N³⁰, κ N³¹, κ N³²]zinc**
Phthalocyaninatozinc(II)**D_{4h}**

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(5)–N(29)	1.374(23)	C(5)–N(29)–C(28)	106.9(46)
C(4a)–C(5)	1.420(27)	N(29)–C(5)–N(6)	125.7(32)
C(4a)–C(28a)	1.55(10)	C(28a)–C(4a)–C(4)	117.2(22)
Zn–N(29)	1.954(29)	C(4a)–C(4)–H	117(11)
C(4a)–C(4)	1.370(14)	N(29)–C(5)–C(4a)	113.0 ^{b)}
C(3)–C(4)	1.369 ^{c)}	C(5)–C(4a)–C(28a)	103.5 ^{b)}
C(2)–C(3)	1.383 ^{c)}	C(4a)–C(4)–C(3)	121.6 ^{b)}
C–H(average)	1.122(82)	C(5)–N(6)–C(7)	125.6 ^{b)}

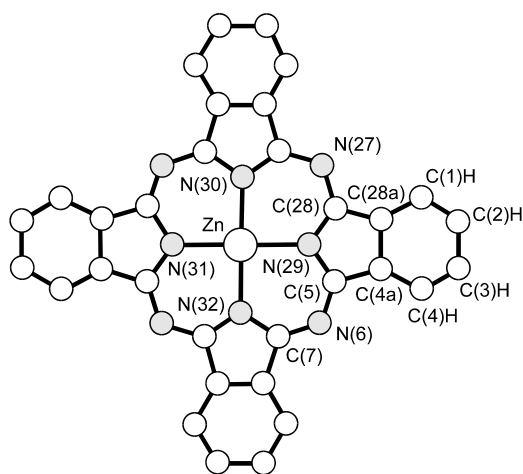


Reanalysis of experimental data from [1].
The nozzle temperature was *ca.* 400 °C.

^{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.

[1] Mihill, A., Buell, W., Fink, M.: J. Chem. Phys. **99** (1993) 6416.

Replaces [II/25D \(3, 2921\)](#)