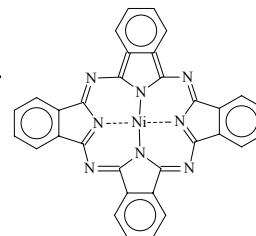
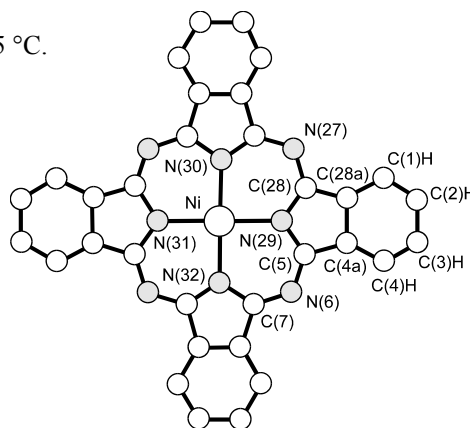


951 **C₃₂H₁₆N₈Ni**ED, DFT
calculations**Phthalocyaninatonicel(II)**[29*H*,31*H*-Phthalocyaninato- $\kappa\text{N}^{29},\kappa\text{N}^{30},\kappa\text{N}^{31},\kappa\text{N}^{32}$]nickel**D_{4h}**

<i>r</i> ^{a)}	Å ^{b)}	θ ^{a)}	deg ^{b)}
Ni–N(29)	1.871(13)	C(5)–N(29)–C(28)	106.3(13)
C(5)–N(29)	1.391(16)	N(29)–C(5)–N(6)	127.9(15)
C(5)–C(4a)	1.460(18)	C(4)–C(4a)–C(28a)	120.2(12)
C(4a)–C(28a)	1.470(31)	C(4a)–C(4)–H	122(6)
C(4a)–C(4)	1.374(8)	N(29)–C(5)–C(4a) ^{c)}	111.8
C(3)–C(4)	1.375 ^{d)}	C(5)–C(4a)–C(28a) ^{c)}	105.0
C(2)–C(3)	1.379 ^{d)}	C(4a)–C(4)–C(3) ^{c)}	117.4
C–H (average)	1.083(37)	C(5)–N(6)–C(7) ^{c)}	120.5
C(5)–N(6) ^{c)}	1.296		



The temperature of the measurements was 475 °C.

^{a)} Unidentified, possibly r_a and θ_a .^{b)} Twice the estimated standard errors.^{c)} Dependent parameter.^{d)} Differences between the C(4a)–C(4), C(3)–C(4) and C(2)–C(3) bond lengths were assumed at the values from VWN/DNP calculations.Mastryukov, V., Ruan, C.-Y., Fink, M.,
Wang, Z., Pachter, R.: J. Mol. Struct. **556** (2000) 225.