Darstellung und Eigenschaften von Tetra(*n*-butyl)ammonium-*cis*-diacidooxophthalocyaninato(2-)niobaten(V) und -tantalaten(V); Kristallstruktur von ($^{n}Bu_4N$)^{cis}[Nb(F)$_2$Opc^{2-}]

Preparation and Properties of Tetra(*n*-butyl)ammonium *cis*-Diacidooxophthalocyaninato(2-)niobates(V) and -tantalates(V); Crystal Structure of ($^{n}Bu_4N$)^{cis}[Nb(F)$_2$Opc^{2-}]

Karsten Schweiger, Heiner Hückstädt und Heiner Homborg*

Institut für Anorganische Chemie der Christian-Albrechts-Universität,
Olshausenstraße 40, D-24098 Kiel

* Sonderdruckanforderungen an Dr. H. Homborg. Fax: (+49) 431 8801520.
E-mail: homborg@ac.uni-kiel.de

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Phthalocyaninates, Niobium and Tantalum Compounds, Optical Spectra, Vibrational Spectra, Crystal Structure

Tetra(*n*-butyl)ammonium *cis*-diacidooxophthalocyaninato(2-)niobates(V) and -tantalates(V), ($^{n}Bu_4N$)^{cis}[M(X)$_2$Opc^{2-}] (M = Nb, Ta; X = F, Cl, NCS, N_3), are obtained by the reaction of ^{cis}[M(Cl)$_3$pc^{2-}] or ^{cis}[M(Cl)Opc^{2-}] (M = Nb, Ta) with the respective tetra(*n*-butyl)ammonium salt. ($^{n}Bu_4N$)^{cis}[Nb(F)$_2$Opc^{2-}] crystallizes in the monoclinic space group $P2_1/n$ with cell parameters a = 13.460(5), b = 13.820(5), c = 23.360(5) Å, β = 92.640(5)°, Z = 4. The heptacoordinated Nb(V) atom is surrounded by four isoindole nitrogen atoms (N_{iso}) of the pc^{2-} ligand, two fluorine atoms and one oxygen atom in a distorted square-base-trigonal-cap polyhedron. Nb(V) is displaced out of the centre of the (N_{iso})$_4$ plane (Ct(N_{iso})) towards the acido ligands (d(Nb-Ct(N_{iso})) = 1.241 Å). The average (Nb-N_{iso}), (Nb-F), and (Nb-O) distances are 2.300, 1.957, and 1.720(5) Å, the (F-Nb-F) and the average (O-Nb-F) angles are 79.8(2) and 91.8°, respectively. The pc^{2-} ligand is concavely distorted. Typical π-π*-transitions of the pc^{2-} ligand are observed in the UV/Vis spectra at *ca.* 14500 and 29300 cm^{-1}. Vibration frequencies $\nu_{as,s}$(M-X), ν(M-O) and δ(X-M-O) have been assigned.