

ชื่อบทความ : ภาษาไทย โครงสร้างซูปรามอเลคิวลาร์ของสารประกอบเชิงซ้อนสี่โคออร์ดิเนตนิเกิล
บิสฟอสฟีน
: ภาษาอังกฤษ SUPRAMOLECULAR STRUCTURES OF FOUR-COORDINATE
NICKEL BIS(TRIPHENYLPHOSPHINE) COMPLEXES
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The multiple phenyl-phenyl edge-to-face (*ef*) C-H \cdots π attractive interactions of the concerted sextuple phenyl embrace (6PE) give a sum of interaction energy sufficient to make it a dominant supramolecular motif for triphenylphosphine (TPP) complexes (Dance & Scudder, *Chem. Comm.*1995, 1039-40). The title complexes Ni(X)(Y)(P(C₆H₅)₃)₂, with X = NCS⁻, N₃⁻, or Cl⁻; Y= NO while closely related have quite different supramolecular structures.

The primary extended interactions in the isothiocyanato complex are the expected 6PE between adjacent TPP ligands which occur in parallel chains made up of alternating; d[P-P] = 7.087Å, colinearity = 176.9° and d[P-P] = 7.246Å, colinearity = 173.0° 6PE. Adjacent chains are joined by four phenyl ring regions to form layers dominated by *ef* C-H \cdots π interactions. Layers are joined together by nitrosyl-phenyl and phenyl-phenyl interactions.

The chloro complex contains a benzene solvate which can be viewed as lying within a cavity with one end inserted into the cleft of a bis-TPP nickel fragment located on a pseudo two-fold axis utilizing one complex-to-benzene *ef* and one benzene-to-complex *ef* interaction to each of the TPP ligands. The central region of the cavity is occupied by six additional *ef* interactions, and the cavity is completed by the chloro and nitrosyl ligands of another molecule. Thus, the benzene molecule, able to form considerably more C-H \cdots π interactions, becomes the major link between surrounding molecules.

The shortest intermolecular P-P distances in the azido complex are 7.411Å and 7.825Å with colinearities of 86.9° and 117.7°, thus not 6PE. The strongest nonbonded interaction is a 2.493Å *intramolecular* C-H \cdots N interaction to the lone pair on the N bonded to Ni destroying the pseudo three-fold symmetry of one TPP ligand, while another strong *intramolecular* C-H \cdots N interaction to the azido ligand π cloud involves the other TPP ligand, thus disrupting the both possibilities to form 6PEs. The azido ligand is also involved in intermolecular nonbonded interactions. Thus, as the strongest hydrogen bond acceptor, the azido ligand becomes the most important determiner of the supramolecular structure.

Crystals of NiCl₂(P(C₆H₅)₃)₂ were prepared as starting material in the preparation of chloro nitrosyl complex. Data were collected on a BV Nonius KappaCCD diffractometer equipped with a fine focus molybdenum x-ray source, graphite crystal monochromator, 0.5 mm *ifg* capillary colimator, and Oxford Cryosystems 600 low temperature device. Structure solution and refinement utilized SIR92, and the SHELXTL system.

Crystal data: C₃₆H₃₀NiCl₂P₂, *M_r* = 654.16 Daltons, olive green square plate, 0.16 X 0.25 X 0.29 mm, T = 200 K; monoclinic, P2/c (No. 13) *a* = 11.6298(3) Å, *b* = 8.1224(2) Å, *c* = 17.2972(4) Å, β = 107.0943(12)°, *V* = 1561.74(7) Å³, *Z* = 2, *d*_{calc} = 1.391 Mg/m³, $\lambda_{MoK\alpha}$ = 0.71073 Å, μ = 9.2 cm⁻¹, 24,324 data collected, 3890 unique data, multiscan absorption correction, 3,316 unique observed data (*F_o* > 4 σ (*F_o*)), *F*(000) = 676., *R*_{merge} (sym) = 0.042, *R*₁ (obs) = 0.0370, *wR*₂ (all) 0.0971, max *c/c* = 0.002, max correlation coefficient = 0.563, ρ_{max} = 0.52 e/Å³, ρ_{min} = -0.51 e/Å³, ρ_{error} 0.07 e/Å³

