



>>Entry Name: Dichlorobis(triphenylphosphine)nickel, 10Cl, 9Cl

Synonym(s): Bis(triphenylphosphine)nickel(II) dichloride

CAS Registry Number: 14264-16-5

Related CAS Registry Numbers(s): 39716-73-9 53996-95-5

(Ph₃P)₂NiCl₂ (C_{2v})

Molecular Formula: C₃₆H₃₀Cl₂NiP₂

Molecular Weight: 654.176

Accurate Mass: 652.055324

Percentage Composition: C 66.10%; H 4.62%; Cl 10.84%; Ni 8.97%; P 9.47%

Source/Synthesis: Synth. from NiCl₂·6H₂O in H₂O and PPh₃ in HOAc, or from NiCl₂·6H₂O and PPh₃ in refluxing EtOH

Use/Importance: Commercially available. Catalyst for cross-coupling of Grignard reagents; catalyses addn. of RMgX to allylic ethers; hydrosilylations and hydrogenation, oligomerisation and polym. of many unsatd. spp. Undergoes exchange with free PPh₃

Physical Description: Dark blue cryst.

Melting Point: Mp 205-206° (247-250° dec.)

Solubility: Sol. CHCl₃

Other Data: Paramagnetic; μ_{eff} = 3.41 μ_B (300K)

Hazard & Toxicity: Cancer suspect agent

Aldrich: 23711-6

Fluka: 15245

Sigma: T7785

References:

Yamamoto, K., *Bull. Chem. Soc. Jpn.*, 1954, **27**, 501, (*synth*)

Venanzi, L.M., *J. Inorg. Nucl. Chem.*, 1958, **8**, 137, (*synth*)

Venanzi, L.M., *J.C.S.*, 1958, 719, (*synth*)

Cotton, F.A. *et al.*, *J.A.C.S.*, 1961, **83**, 344, (*synth, uv-vis, magnetism*)

Garton, J. *et al.*, *J.C.S.*, 1963, 3625, (*cryst struct*)

LaLancette, E.A. *et al.*, *J.A.C.S.*, 1964, **86**, 5145, (*pmr*)

Gmelin Handbook Inorg. Chem., Syst. No. 57, 1969, **C2**, 1046, (*rev*)

Matienzo, L.J. *et al.*, *Inorg. Nucl. Chem. Lett.*, 1972, **8**, 1085, (*xpe*)

Barnett, K.W., *J. Chem. Educ.*, 1974, **51**, 422, (*synth*)

Felkin, H. *et al.*, *Tetrahedron*, 1975, **31**, 2735, (*use*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 59, (*use*)

Compr. Coord. Chem., Pergamon, 1987, **5**, 108, (*rev*)

Didiuk, M.T. *et al.*, *J.A.C.S.*, 1995, **117**, 7273, (*use, reaction with allylic ethers*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BLS250