



>>Entry Name: Di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]diiridium, 12Cl, 11Cl, 10Cl, 9Cl

Synonym(s): Bis(1,5-cyclooctadiene- μ -chloroiridium)

CAS Registry Number: 12112-67-3

As Di- μ -bromobis[(1,2,5,6- η)-1,5-cyclooctadiene]diiridium, GKM05-Q with
X = Cl

Molecular Formula: C₁₆H₂₄Cl₂Ir₂

Molecular Weight: 671.711

Accurate Mass: 672.051338

Percentage Composition: C 28.61%; H 3.60%; Cl 10.56%; Ir 57.23%

Source/Synthesis: Synth. from [NH₄]₂[IrCl₆] + cod in PrⁱOH aq. under reflux for 18h; alternatively from IrCl₃.xH₂O + cod either in PrⁱOH aq. at 65-70° for 40h or in EtOH aq. in a microwave oven for 45s, or in EtOH aq. (2:1) at 45° then under reflux for 4h with hydroquinone

Use/Importance: Catalyst for the selective hydrogenation of α,β -unsatd. acids to satd. acids; also, with phosphines, for transfer hydrogenation of α,β -unsatd. aldehydes using 2-propanol, with high selection for allyl alcohols; catalyses [2+2] cyclodimerisation of nbd

Physical Description: Red or orange cryst. (CH₂Cl₂/EtOH). Solid discolours in air after 1 month. In soln. in air [IrCl(cod)]₂(μ -OH)₂(μ -O) is formed

Melting Point: Mp 200 dec.°

Solubility: Sol. CHCl₃, CH₂Cl₂

Other Data: Compds. with X = Br and I also known

Aldrich: 27513-1

Fluka: 14691

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 752C, (nmr)

Winkhaus, G. *et al.*, *Chem. Ber.*, 1966, **99**, 3610, (synth, pmr, ir)

Fraser, A.R. *et al.*, *J.A.C.S.*, 1973, **95**, 597, (use, cyclodimerisation of nbd)

Inorg. Synth., 1974, **15**, 18, (synth)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 113, (use)

Bonnaire, R. *et al.*, *J. Organomet. Chem.*, 1976, **104**, 107, (cmr)

Crabtree, R.H. *et al.*, *J. Organomet. Chem.*, 1977, **135**, 395, (synth, props)

Bezman, S.A. *et al.*, *Inorg. Chem.*, 1980, **19**, 3755, (synth, props)

Sievert, A.C. *et al.*, *Inorg. Chem.*, 1981, **20**, 489, (synth, props)

Crabtree, R.H. *et al.*, *Synth. React. Inorg. Met.-Org. Chem.*, 1982, **12**, 407, (synth, props)

Visintin, M. *et al.*, *J. Mol. Catal.*, 1985, **32**, 349, (use, hydrogenation of unsatd aldehydes)

Cotton, F.A. *et al.*, *Inorg. Chim. Acta*, 1986, **120**, 153, (synth, cryst struct, reactions)

Baghurst, D.R. *et al.*, *J. Organomet. Chem.*, 1989, **368**, C43, (synth)

Wehman-Ooyevaar, I.C.M. *et al.*, *Inorg. Chem.*, 1993, **32**, 3347, (synth, reactions)