>>**Entry Name: Dichlorobis(η^5-2,4-cyclopentadien-1-yl)hafnium,** 9Cl
Synonym(s): Dichlorodi-π-cyclopentadienylhafnium, 8Cl. Bis(cyclopentadienyl)hafnium dichloride. Hafnocene dichloride

CAS Registry Number: 12116-66-4

As Dibromobis(η^5-2,4-cyclopentadien-1-yl)hafnium, BQC51-Q with
X = Cl

Molecular Formula: $C_{10}H_{10}Cl_2Hf$
Molecular Weight: 379.584
Accurate Mass: 379.962499
Percentage Composition: C 31.64%; H 2.66%; Cl 18.68%; Hf 47.02%
Source/Synthesis: Synth. from $HfCl_4$ and NaCp in THF
Use/Importance: Catalyst component with many applications. Catalyses chemoselective redn. of polycarbonyl compds. to hydroxycarbonyls and 1,2-redn. of α,β-unsatd. carbonyl compds. to allylic alcohols by hydrogen transfer from Pr^iOH; reagent for alkyl/alkene and alkene/alkene coupling. Precursor to many Cp_2Hf (*II* or *IV*) compds.
Physical Description: Colourless cryst.
Melting Point: Mp 234-235° (>300°)
Boiling Point: $Bp_{0.01}$ 155°
Solubility: Sol. aromatic solvs., $CHCl_3$; sl. sol. THF, Et_2O; insol. hexane

Aldrich: 11933-4
Fluka: 51315

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1155A, *(ir)*
Druce, P.M. *et al.*, *J.C.S.(A)*, 1969, 2106; 2814, *(ir, ms, nmr, Raman)*
Burmeister, J.L. *et al.*, *Inorg. Chem.*, 1970, **9**, 58, *(ir, uv)*
Samuel, E. *et al.*, *Inorg. Chem.*, 1973, **12**, 881, *(ir)*
Cauletti, C. *et al.*, *J. Electron Spectrosc. Relat. Phenom.*, 1980, **18**, 61, *(pe)*
Nakano, T. *et al.*, *J.O.C.*, 1988, **53**, 3752, *(use)*
Soloveichik, G. *et al.*, *Metalloorg. Khim.*, 1988, **1**, 226, *(cryst struct)*
Ward, S.G. *et al.*, *Appl. Organomet. Chem.*, 1989, **3**, 491, *(tox)*
Swanson, D.R. *et al.*, *J.O.C.*, 1989, **54**, 3521, *(use)*
McLaughlin, M.L. *et al.*, *J.A.C.S.*, 1990, **112**, 8949, *(tox)*
Gassman, P.G. *et al.*, *Organometallics*, 1991, **10**, 1592, *(pe)*
Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **3**, 1660, *(pmr, use)*
Synthetic Methods of Organometallic and Inorganic Chemistry, (ed. Hermann, W.A.), Thieme, 1997, **8**, 31-32, *(synth)*
Lewis, R.J.*, Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HAE500