



>>Entry Name: Chromium carbonyl ($\text{Cr}(\text{CO})_6$), 12Cl, 8Cl

Synonym(s): Hexacarbonylchromium. Chromium hexacarbonyl

CAS Registry Number: 13007-92-6

Related CAS Registry Numbers(s): 25875-16-5 25941-09-7 53042-53-8 53108-98-8 53108-99-9 53109-00-5 53109-01-6 53109-02-7 53109-11-8 53109-12-9 58167-58-1

$\text{Cr}(\text{CO})_6 (O_h)$

Molecular Formula: C_6CrO_6

Molecular Weight: 220.059

Accurate Mass: 219.909999

Percentage Composition: C 32.75%; Cr 23.63%; O 43.62%

Source/Synthesis: Synth. from $\text{CrCl}_3 + \text{CO} + \text{Mg}$ or K

Use/Importance: Catalyst for hydrogenation, isomerisation, water gas shift reaction and alkylation of aromatic hydrocarbons

Physical Description: Colourless cryst. (methylcyclohexane or by subl.)

Melting Point: Mp 152-155°

Solubility: Sl. sol. CCl_4 ; insol. H_2O , EtOH , Et_2O

Other Data: Lower carbonyls $\text{Cr}(\text{CO})_n$ ($n = 5-1$) have been isolated e.g. by matrix isolation as unstable species

Hazard & Toxicity: Explodes at 210°

Aldrich: 40437-3

Fluka: 27091

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1299B, (ir)

Podall, H.E. *et al.*, *J.A.C.S.*, 1961, **83**, 2057, (synth)

Whitaker, A. *et al.*, *Acta Cryst.*, 1967, **23**, 977, (cryst struct)

Rieke, R. *et al.*, *J.O.C.*, 1974, **76**, C19, (synth)

Jost, A. *et al.*, *Acta Cryst. B*, 1975, **31**, 2649, (nd)

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Calhorda, M.J. *et al.*, *J. Organomet. Chem.*, 1984, **262**, 305, (thermochem)

Ziegler, T. *et al.*, *J.A.C.S.*, 1987, **109**, 4825, (calcd bond energies)

Magomedov, G.K. *et al.*, *Zh. Obshch. Khim.*, 1988, **58**, 497, (synth)

Vasil'ev, A.A. *et al.*, *Zh. Org. Khim.*, 1991, **27**, 966, (catal)

Nilsson, A. *et al.*, *J. Chem. Phys.*, 1992, **96**, 8770, (pe)

Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **4**, 2633-2636, (rev, use)

Braga, D. *et al.*, *J.C.S. Dalton*, 1995, 1215, (cryst struct)

Synthetic Methods of Organometallic and Inorganic Chemistry, (ed. Hermann, W.A.), Thieme, 1997, **7**, 8-10, (synth, ir, cmr)

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