



>>Entry Name: Zirconium(IV) chloride oxide (ZrCl₂O)

Synonym(s): Dichlorooxozirconium(IV), 11Cl. Zirconyl chloride. Zirconium oxychloride

CAS Registry Number: 7699-43-6

ZrOCl₂

Molecular Formula: Cl₂OZr

Molecular Weight: 178.129

Accurate Mass: 175.837322

Percentage Composition: Cl 39.81%; O 8.98%; Zr 51.21%

Source/Synthesis: Synth. from ZrO₂ in HF and crystallising product from aq. HCl

Use/Importance: Commercially available. Used in v. wide range of applications from the manuf. of refractories to catalysts for many processes, in humidity sensors and antiperspirants

Physical Description: White solid. Forms adducts by direct reaction in EtOH

Aldrich: 46419-8

>>Derivative: Octahydrate

CAS Registry Number: 13520-92-8

Molecular Formula: Cl₂H₁₆O₉Zr

Molecular Weight: 322.25

Accurate Mass: 319.921842

Percentage Composition: Cl 22.00%; H 5.00%; O 44.68%; Zr 28.31%

Use/Importance: Commercially available

Aldrich: 22431-6

Fluka: 96609

>>Derivative: Bis-HMPA complex

Synonym(s): Dichlorobis(hexamethylphosphoric triamide-*O*)oxozirconium(IV), 11Cl

CAS Registry Number: 26499-98-9

Molecular Formula: C₁₂H₃₆Cl₂N₆O₃P₂Zr

Molecular Weight: 536.532

Accurate Mass: 534.07482

Percentage Composition: C 26.86%; H 6.76%; Cl 13.22%; N 15.66%; O 8.95%; P 11.55%; Zr 17.00%

Physical Description: White solid, non-electrolyte

Other Data: 5-Coordinate

>>Derivative: Bis(pyridine-1-oxide) complex

Synonym(s): Dichlorooxobis(pyridine-1-oxide-*O*)zirconium(IV), 11Cl

CAS Registry Number: 77886-08-9

Molecular Formula: C₁₀H₁₀Cl₂N₂O₃Zr

Molecular Weight: 368.33

Accurate Mass: 365.91155

Percentage Composition: C 32.61%; H 2.74%; Cl 19.25%; N 7.61%; O 13.03%; Zr 24.77%

Physical Description: White solid

Solubility: Sol. EtOH, PhNO₂, DMSO; insol. Et₂O

>>Derivative: Bis(benzo[*f*]quinoline) complex

CAS Registry Number: 101944-09-6

Other Data: Paramagnetic, $\mu_{\text{eff}} = 1.68\mu_{\text{B}}$

>>Derivative: Tetrakis(phenylhydrazine) complex

>>Derivative: Tetrakis-Py complex

>>Derivative: Tetrakis-quinoline complex