



>>Entry Name: Zirconium(IV) oxide (ZrO₂), 11Cl

Synonym(s): Zirconium dioxide. Zirconia

CAS Registry Number: 1314-23-4

Related CAS Registry Numbers(s): 12164-98-6

Extra CAS Registry Numbers(s): 53801-45-9

ZrO₂

Molecular Formula: O₂Zr

Molecular Weight: 123.223

Accurate Mass: 121.894533

Percentage Composition: O 25.97%; Zr 74.03%

is not pressure sensitive at r.t. Phase changes from monoclinic << >> tetragonal << >> cubic (CaF₂ struct.) occur at 1100 and 2300° respectively. Sol-gel material has amorphous struct. below 300°; annealing at higher temps leads to nanophases cont. both tetragonal (main) and monoclinic forms, with similar crystallite sizes; further annealing results in irreversible transformation of tetragonal into monoclinic phase. Morphology of aerogels dependent on preparative conditions

Source/Synthesis: Synth. of ZrO₂ and 10% Cu-ZrO₂ by forming gels from ZrO(NO₃)₂ or ZrO(NO₃)₂ and Cu(NO₃)₂ and drying supercritically at 533K and 8.1 MPa. Redn. at 575K yields the catalyst: Cu is reduced preferentially. Commercial material may be synth. by hydrol. of any Zr^{IV} compd. Cryst. may be grown by flux methods. Mesoporous, high-surface-area zirconia synth. by controlled heating of surfactant/ZrO₂ composite; latter obt. by reaction of Zr(OCH₂CH₂CH₃)₄ or ZrOCl₂ with e.g. alkyltrimethylammonium halides, dodecyl phosphate or sulfate, or hexadecyl sulfonate. Nanocrystalline zirconia can be prepared by the sol-gel technique, e.g. reaction of Zr[O(CH₂)₃CH₃] with hydrol. catalyst such as HCl, H₂SO₄, C₂H₄O₂ and NH₄OH. Europium-doped crystalline powders can be produced by heating mixt. of co-precipitated hydrated Eu and Zr oxides

Use/Importance: Used in ceramics, enamels and electrical devices. Tends to crack on thermal cycling because of the phase change at 1100°. The cubic form is stabilised by adding MgO or CaO leading to cubic zirconia as a gemstone substit. for diamond. In fibrous form may be used as an insulator. A semiconductor sol, synth. by hydrol. of ZrO(C₂O₄) in water at 90° for 48h, is a sensitizer for uv cleavage of water. Monoclinic form is used as additive to hydroxyapatite as a toughening agent to form a composite for prosthetic applications. Interesting new catalyst systems. Materials had surface areas >250m² g⁻¹. After redn. ZrO₂ hydrogenated CO to form 2-propanol with high selectivity. The Cu-ZrO₂ system is a better MeOH catalyst than Cu-ZnO. Can be used as thermal shield. Doped material finds applications in sensor devices (e.g. for O₂) and in fabrication of fuel cells

Physical Description: White or colourless solid

Melting Point: Mp *ca.* 2710°

Other Data: Ionic conductor when doped with divalent or trivalent cations. Low thermal conductivity at high temps. Porosity and surface area of aerogels dependent on preparative conditions. Luminescent material produced by doping with Eu³⁽⁺⁾

Aldrich: 23069-3

Fluka: 96596

Sigma: Z2500

>>Variant: Mineral-form

Synonym(s): Baddeleyite (ZrO₂)

CAS Registry Number: 12036-23-6

Molecular Formula: O₂Zr

Molecular Weight: 123.223

Accurate Mass: 121.894533

Percentage Composition: O 25.97%; Zr 74.03%

Source/Synthesis: Widespread occurrence

Physical Description: May be almost any colour depending on impurities; dark submetallic cryst.

References:

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