



>>Entry Name: Zirconate ( $\text{ZrO}_3^{2(-)}$ ), 13Cl, 12Cl, 11Cl

CAS Registry Number: 128337-33-7  
 $[\text{ZrO}_3]^{2(-)}$

Molecular Formula:  $\text{O}_3\text{Zr}^{2(-)}$

Molecular Weight: 139.222

Accurate Mass: 137.889448

Percentage Composition: O 34.48%; Zr 65.52%  
 $2(-)$  ions

>>Derivative: Di-Li salt

Synonym(s): Lithium zirconium(*IV*) oxide ( $\text{Li}_2\text{ZrO}_3$ ), 9Cl. Lithium zirconate

CAS Registry Number: 12031-83-3

Molecular Formula:  $\text{Li}_2\text{O}_3\text{Zr}$

Molecular Weight: 153.104

Accurate Mass: 151.921454

Percentage Composition: Li 9.07%; O 31.35%; Zr 59.58%

Source/Synthesis: Synth. by heating  $\text{Li}_2\text{CO}_3$  and  $\text{ZrO}_2$  to  $900^\circ$

Use/Importance: Used in humidity sensors

Physical Description: White solid

Other Data: Other alkali metal salts are known. Struct. related to NaCl with O and Li in distorted ccp arrangement

Aldrich: 40092-0

>>Derivative: Di-Na salt

Synonym(s): Sodium zirconium(*IV*) oxide ( $\text{Na}_2\text{ZrO}_3$ ), 9Cl. Sodium zirconate

CAS Registry Number: 12201-48-8

Molecular Formula:  $\text{Na}_2\text{O}_3\text{Zr}$

Molecular Weight: 185.202

Accurate Mass: 183.868982

Percentage Composition: Na 24.83%; O 25.92%; Zr 49.26%

Source/Synthesis: Synth. by reacting  $\text{ZrO}_2$  with  $\text{Na}_2\text{CO}_3$ , Na tartrate or wet or dry NaOH; also from  $\text{ZrO}(\text{NO}_3)_2$  and  $\text{Na}_2\text{CO}_3$   $<180^\circ$

Use/Importance: Commercially available

Physical Description: Colourless cryst.

Other Data: Dimorphic. One form has the  $\text{Li}_2\text{SnO}_3$  struct.

Aldrich: 40066-1

>>Derivative: Mg salt

Synonym(s): Magnesium zirconium(*IV*) oxide ( $\text{MgZrO}_3$ ), 9Cl. Magnesium zirconate

CAS Registry Number: 12032-31-4

Molecular Formula:  $\text{MgO}_3\text{Zr}$

Molecular Weight: 163.527

Accurate Mass: 161.87449

Percentage Composition: Mg 14.86%; O 29.35%; Zr 55.79%

Source/Synthesis: Synth. by sintering MgO and ZrO at high pressure, or by hydrol. of  $\text{Mg}(\text{NO}_3)_2$  and  $\text{ZrO}(\text{NO}_3)_2$  in  $\text{NH}_3/(\text{NH}_4)_2\text{CO}_3$  and sintering at  $500^\circ$

Use/Importance: Commercially available. Used as a heat and corrosion resistant coating for e.g. boiler tubes and also as an  $\text{O}_2$  sensor

Physical Description: Colourless cryst.

Aldrich: 39617-6

>>Derivative: Ca salt

Synonym(s): Calcium zirconium(*IV*) oxide ( $\text{CaZrO}_3$ ). Calcium zirconate

CAS Registry Number: 12013-47-7

Extra CAS Registry Numbers(s): 11129-15-0

Molecular Formula:  $\text{CaO}_3\text{Zr}$

Molecular Weight: 179.3

Accurate Mass: 177.852039

Percentage Composition: Ca 22.35%; O 26.77%; Zr 50.88%

Aldrich: 39619-2