



>>Entry Name: Barium thiocyanate

Synonym(s): Thiocyanuric acid, barium salt, 8Cl

CAS Registry Number: 2092-17-3

Ba(NCS)₂

Molecular Formula: C₂BaN₂S₂

Molecular Weight: 253.494

Accurate Mass: 253.85552

Percentage Composition: C 9.48%; Ba 54.17%; N 11.05%; S 25.30%

Source/Synthesis: Prep. either by reaction of [NH₄]SCN with Ba(OH)₂·8H₂O or by slow neutralisation of BaCO₃ with aq. HSCN. Cryst. as trihydrate which gives anhydrous Ba(SCN)₂ on drying in air

Use/Importance: Reagent for converting metal sulfates to thiocyanates

Physical Description: White solid, highly hygroscopic

Solubility: V. sol. H₂O; sol. Me₂CO, MeOH, EtOH

>>Derivative: Dihydrate

CAS Registry Number: 5908-82-7

Molecular Formula: C₂H₄BaN₂O₂S₂

Molecular Weight: 289.525

Accurate Mass: 289.87665

Percentage Composition: C 8.30%; H 1.39%; Ba 47.43%; N 9.68%; O 11.05%; S 22.15%

Other Data: Incorrectly formulated; structural analysis has shown this species to be the trihydrate

>>Derivative: Trihydrate

CAS Registry Number: 68016-36-4

Molecular Formula: C₂H₆BaN₂O₃S₂

Molecular Weight: 307.54

Accurate Mass: 307.887215

Percentage Composition: C 7.81%; H 1.97%; Ba 44.65%; N 9.11%; O 15.61%; S 20.85%

Use/Importance: Commercially available

Physical Description: Colourless monoclinic cryst., deliquescent. Dec. on heating with H₂O loss

Solubility: Sol. H₂O (4.3 g per 100cm³ at 20°); v. sol. EtOH (35g per 100 cm³ at 20°)

Hazard & Toxicity: Irritant

Aldrich: 33915-6

References:

Inorg. Synth., 1950, **3**, 24, (*synth*)

Zvonkova, Z.V. *et al.*, *Zh. Fiz. Khim.*, 1950, **24**, 1345, (*dihydrate, original cryst struct*)

Tramer, A., *C. R. Hebd. Seances Acad. Sci.*, 1961, **253**, 1679, (*hydrate, ir, Raman*)

Tramer, A., *J. Chim. Phys. Phys.-Chim. Biol.*, 1962, **59**, 637, (*hydrate, ir, Raman*)

Krasser, W. *et al.*, *Naturwissenschaften*, 1967, **54**, 134, (*Raman*)

Kargol, J.A. *et al.*, *Inorg. Chem.*, 1979, **18**, 2532, (*cmr*)

Mereiter, K. *et al.*, *Acta Cryst. B*, 1982, **38**, 382, (*trihydrate, revised cryst struct*)