



>>Entry Name: Cyanogen bromide

Synonym(s): Bromine cyanide. Bromocyanogen. Bromocyan

CAS Registry Number: 506-68-3

$\text{BrC}\equiv\text{N}$ ($C_{(\infty)}$)_v

Molecular Formula: CBrN

Molecular Weight: 105.922

Accurate Mass: 104.94141

Percentage Composition: C 11.34%; Br 75.44%; N 13.22%

General Statement: Interatomic distances: Br-C 179, C-N 115.7 pm

Use/Importance: Commercially available. Used in the Von Braun reaction, cleavage of thioethers, synth. of heterocycles, synth. of *trans* olefins, synth. of disulfides, phenol dehydroxylation, synth. of 1,2-aminocarbonates, synth. of cyanatobenzene

Physical Description: Cryst.

Melting Point: Mp 52°

Boiling Point: Bp 61-62°

Solubility: Sol. Et₂O, H₂O, EtOH

Density: d²⁰ 2.01

Hazard & Toxicity: Potentially unstable on storage. Eye, skin, respiratory tract, and mucous membrane irritant

Aldrich: 34189-4

Fluka: 16774

Sigma: C6388

References:

Cook, R.P., *J.C.S.*, 1935, 1001, (*synth, props*)

Org. Synth., Coll. Vol., 2, 1943, 150, (*synth*)

Tyler, J.K. *et al.*, *Trans. Faraday Soc.*, 1963, **59**, 2661, (*struct*)

Rabalais, J.W. *et al.*, *Chem. Rev.*, 1971, **71**, 73, (*uv, ir*)

Brauer, G., *Handbuch Prap. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **2**, 632, (*synth*)

Müller, J., *Z. Naturforsch., B*, 1979, **34**, 437, (*N-15 nmr, cmr*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1981, **9**, 127, (*use*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, COO500

Bretherick, L., *Handbook of Reactive Chemical Hazards*, 4th edn., Butterworths, 1990, 0298