



>>Entry Name: Sodium borohydride

ENTRY UNDER REVIEW

Synonym(s): Tetrahydroborate sodium salt, 8Cl. Sodium tetrahydroborate(III)

CAS Registry Number: 16940-66-2

NaBH₄

Molecular Formula: BH₄Na

Molecular Weight: 37.832

Accurate Mass: 38.030372

Percentage Composition: B 28.58%; H 10.66%; Na 60.77%

Source/Synthesis: Commercially available either as solid, supported on alumina or silica gel or in soln. in diglyme, triglyme or aq. NaOH. Manuf. by reaction of NaH with boron hydrides (B₂H₆) or boron trihalides (BF₃) in ethereal solvs.

Use/Importance: Versatile reducing agent

Physical Description: White cubic cryst. Dec. on heating into constituent elements

Melting Point: Mp 497°

Solubility: V. sol H₂O (56 g per 100 cm³ at 24°); mod. sol. EtOH, MeOH; spar. sol. Py; insol. Et₂O; sol. liq. NH₃

Other Data: Dissolves in cold H₂O to cryst. as the dihydrate; at higher temps. hydrolysis occurs. $\Delta H_f^\circ -191.8 \text{ kJ mol}^{-1}$; $\Delta G_f^\circ -127.1 \text{ kJ mol}^{-1}$; $S^\circ 101.4 \text{ J K}^{-1} \text{ mol}^{-1}$

Hazard & Toxicity: Flammable solid, corrosive

Aldrich: 20097-2

Fluka: 71321

Sigma: S9125

>>Derivative: Tetra-deutero deriv.

Synonym(s): Sodium borodeuteride. Sodium tetradeuteroborate

CAS Registry Number: 15681-89-7

Molecular Formula: BD₄Na

Molecular Weight: 41.857

Source/Synthesis: Synth. by reaction of Na[B(OMe)₄] with B₂D₆

Use/Importance: Versatile deuterating agent

Physical Description: White cubic cryst.

Solubility: V. sol. H₂O; mod. sol. EtOH, MeOH; spar. sol. Py; insol. Et₂O; sol. liq. NH₃

Aldrich: 38856-4

Fluka: 71309

Sigma: S2882

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 1249B, (*ir*)
Ford, P.T. *et al.*, *Acta Cryst.*, 1954, **7**, 604, (*cryst struct*)
Emery, A.R. *et al.*, *J. Chem. Phys.*, 1958, **28**, 1029, (*NaBD₄*, *synth*, *Raman*)
Taylor, R.C. *et al.*, *J.A.C.S.*, 1958, **80**, 27, (*Raman*)
Onak, T.P. *et al.*, *J. Phys. Chem.*, 1959, **63**, 1533, (*B-11 nmr*)
Davies, R.E. *et al.*, *J.A.C.S.*, 1960, **82**, 5950, (*NaBD₄*, *hydrolysis*)
Schutte, C.J.H., *Spectrochim. Acta*, 1960, **16**, 1054, (*ir*)
Gmelin Handbook Inorg. Chem., Syst. No.21, 1964, **1**, 257; 1966, **3**, 1212; 1230, (*rev*, *bibl*)
Canadian Pat., 1967, 762 843; *CA*, **67**, 110184, (*manuf*, *NaBD₄*)
Pyykko, P., *Turun Yliopiston Julk.*, *Sar. A*, 1967, **103**, 46; *CA*, 1968, **68**, 118370, (*NaBD₄*, *D-2 nmr*)
Smith, B.E. *et al.*, *Inorg. Chem.*, 1977, **16**, 2057, (*NaBD₄*, *B-11 nmr*)
Buechner, W. *et al.*, *Pure Appl. Chem.*, 1977, **49**, 733, (*rev*, *bibl*, *uses*)
Bernstein, M.A. *et al.*, *J.A.C.S.*, 1979, **101**, 2744, (*uses*, *NaBD₄*)
Francois, P. *et al.*, *Inf. Chim.*, 1985, **258**, 115, (*rev*)
Chase, M.W. *et al.*, *J. Phys. Chem. Ref. Data*, 1985, **14**, 234, (*thermochem data*)
Davis, R.L. *et al.*, *J. Solid State Chem.*, 1985, **59**, 393, (*NaBD₄*, *cryst struct*)
Tabeta, R., *Bull. Chem. Soc. Jpn.*, 1986, **59**, 1957, (*Na-23 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2533
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, SFF500