

Structure Data of Free Polyatomic Molecules

61	BCIS	Boron chloride sulfide	C_{∞v}
IR		Chlorothioxoborane	Cl-B=S

r_e	Å ^{a) b)}
Cl-B	1.6842(8)
B=S	1.6014(8)
Cl...S	3.2856(1)

^{a)} The bond lengths were determined by a weighted least-squares fit to the calculated B_e values of the three isotopomers.

^{b)} Uncertainties were unidentified, probably estimated standard errors.

McNaughton, D., Tay-Lim, R.: J. Mol. Spectrosc. **202** (2000) 89.

MW

r_e	Å
Cl-B	1.680567(89)
B=S	1.604923(90)

r_0	Å
Cl-B	1.6819(22)
B=S	1.6063(22)

r_m^p	Å ^{a)}
Cl-B	1.6805(20)
B=S	1.6048(20)

^{a)} Estimated standard errors.

Bizzocchi, L., Degli Esposti, C., Puzzarini, C.: J. Mol. Spectrosc. **216** (2002) 177.

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