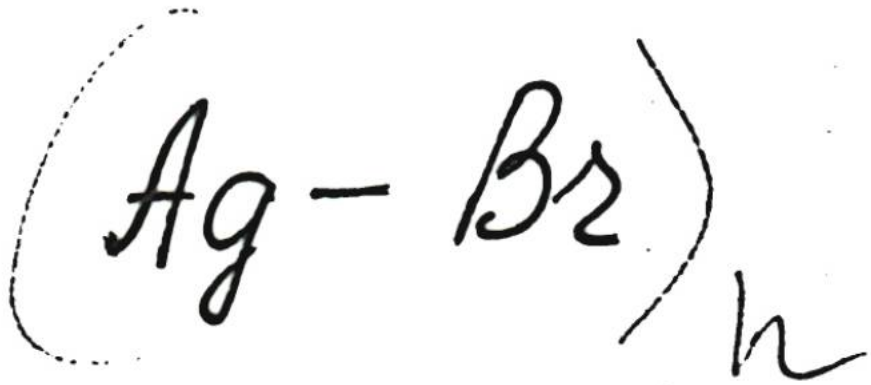
Ag – Br
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$(AgBr)_3$ | ommuch 10995 | 1981.

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J. Electr. Spectrosc. and Relat. Phenom., 1981, 22, 1-25.

2000

F: Ag2Br+
P: 3
133:325865 Ab initio pseudopotential study of M2As- and M2Br+ (M = Cu, Ag, Au). Zhao, Yongfang; Jing, Xiaogong; Zhang, Mingyu Department of Physics, Harbin Institute of Technology Harbin 150001, Peop. Rep. China Int. J. Quantum Chem., 80(1), 38-43 (English) 2000. The equil. geometries and the vibration frequencies of Cu2As-, Ag2As-, Au2As-, Cu2Br+, Ag2Br+, and Au2Br+ were calcd. at the Hartree- Fock (HF)

and the second-order Moller-Plesset (MP2) levels with pseudopotentials. The species have a bent C2v structure. The electron correlation corrections to geometries were investigated at the MP2 level; the bond angles were reduced by 10.degree.-20.degree.. The electron correlation effects on the geometry of Au2As- were studied at MP2, MP3, MP4, CCSD and CCSD(T) levels. A comparison of the species contg. Ag and Au shows that relativistic effects slightly shorten the bond lengths. A bonding state is predicted for Au2As-.

F: Ag2Br+
P: 3

2001

134:331878 **Ab initio pseudopotential study of M2As- and M2Br+ (M = Cu, Ag, Au).** Zhao, Yong-fang; Jing, Xiao-gong; Zhang, Ming-yu. Institute of Atomic and Molecular Physics, Jilin University, Changchun, Peop. Rep. China. Yuanzi Yu Fenzi Wuli Xuebao (2001), 18(1), 76-79. in Chinese.

The equil. geometries and the vibration frequencies of M2As- and M2Br+ (M = Cu, Ag, Au) were calcd. at the HF and the MP2 levels with pseudopotentials. The calcd. results indicated that the species had a bent structure (C2v). The electron correlation corrections to the geometries were investigated at the MP2 level; the bond angles were reduced by 10°-20° for the considered species. The electron correlation effects on the geometry of the Au2As- were studied particularly at MP2, MP3, MP4, CCSD and CCSD(T) levels. A comparison between the species contg. Ag and Au showed that the relativistic effects slightly shortened the bond lengths. The bonding state of Au2As- was predicted.