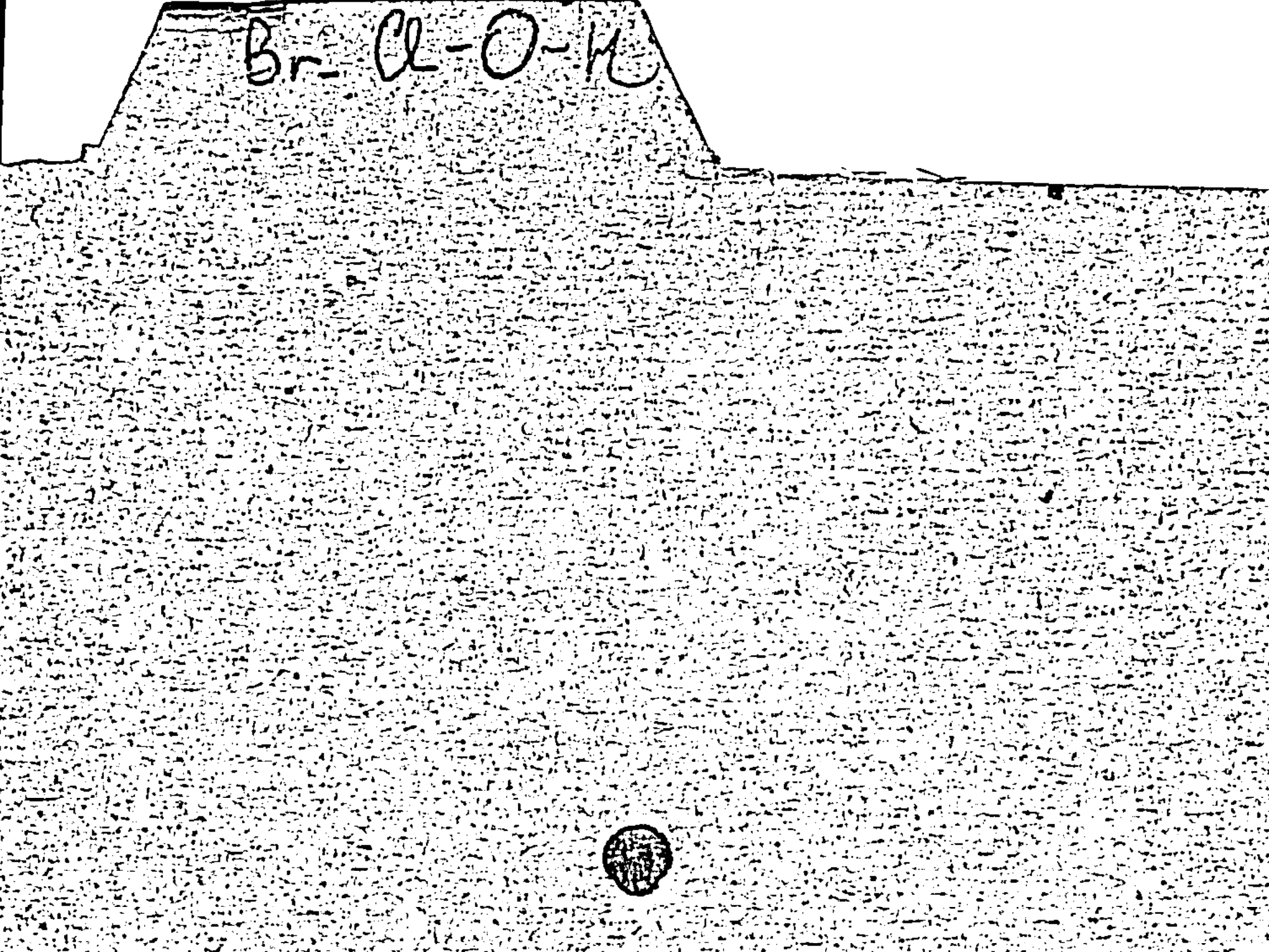
Br-Cl-O-H

$BrClO_3$

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Francisco J. S. et al.,

J. Phys Chem., 1998,

A 102, 2209-2214

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F: Cl--HOBr
P: 3

(of.140833)

2001

134:242939 **Ab Initio Characterization of the Structure, Vibrational, and Energetic Properties of Br--HOCl, Cl--HOBr, and Br--HOBr Anionic Complexes.** Flowers, Bradley A.; Francisco, Joseph S. Department of Chemistry and Department of Earth and Atmospheric Sciences, Purdue University, West Lafayette, IN, USA. J. Phys. Chem. A (2001), 105(2), 494-500. in English.

Ab initio MO methods have been employed to det. mol. structure, vibrational frequencies, and relative energetics of Br--HOCl, Cl--HOBr, and Br--HOBr anionic complexes. These parameters were detd. using second-order Moller-Plesset perturbation theory (MP2) and coupled cluster methods. The min. energy structures for all three complexes are reported. The min. for the mixed halogen conformers place the halogen anion in complexation through the hydrogen. The calcd. binding energies are 23.3, 19.5, and 19.5 kcal mol-1 for Cl--HOBr, Br--HOCl, and Br--HOBr, resp.

F: Br--HOCl
P: 3

[ ot-40833 ]

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