F: SgBr
P: 3
132:55059 Structures and Stabilities for Halides and Oxides of Transactin Elements Rf, Db, and Sg

by Relativistic Effective Core Potenti Calculated Han, Young-Kyu; Son, Sang-Kil; Choi, Yoon Methods. Jeong; Lee, Yoon Sup Department of Chemistry and Center for Molecular Science, KAIST Taejon 305-701, S. J. Phys. Chem. A, 103(45), 9109-9115 (English) 1999 The ground states of the halides and oxides contq. transactinide elements Rf (element 104), Db (element 105), and Sq (element 106) were calcd. at t MP2, QCISD, CCSD, and CCSD(T) levels of theory using one- and twocompone relativistic effective core potentials. Spinorbit effects are rather sm geometries, harmonic vibrational frequencies, charge distributions, overl

C-A-2000, 132

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F: SqBr P: 3 Structures and Stabilities for Halides 132:55059 and Oxides of Transactinide Elements Rf, Db, and Sq Calculated by Relativistic Effective Core Potential Han, Young-Kyu; Son, Sang-Kil; Choi, Methods. Yoon Jeong; Lee, Yoon Sup Department of Chemistry Taejon and Center for Molecular Science, KAIST 305-701, S. Korea J. Phys. Chem. A, 103(45), 9109-9115 (English) 1999 The ground states of the halides and oxides contg. transactinide elements Rf (element 104), Db (element 105), and Sg (element 106) were calcd. at the HF, MP2, QCISD, CCSD, and CCSD(T) levels of theory using one- and two-component relativistic effective core potentials. Spin-orbit effects are rather small for geometries, harmonic vibrational frequencies, charge distributions, overlap populations, and dipole moments, but

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F: SQCI P: 3 Structures and Stabilities for Halides 132:55059 and Oxides of Transactinide Elements Rf, Db, and Sg Calculated by Relativistic Effective Core Potential Han, Young-Kyu; Son, Sang-Kil; Choi, Methods. Yoon Jeong; Lee, Yoon Sup Department of Chemistry and Center for Molecular Science, KAIST Taejon 305-701, S. Korea J. Phys. Chem. A, 103(45), 9109-9115 (English) 1999 The ground states of the halides and oxides contg. transactinide elements Rf (element 104), Db (element 105), and Sg (element 106) were calcd. at the HF, MP2, QCISD, CCSD, and CCSD(T) levels of theory using one- and two-component relativistic effective core potentials. Spin-orbit effects are rather small for geometries, harmonic vibrational frequencies, charge distributions, overlap populations, and dipole moments, but considerable for atomization energies. Electron

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F: SgF P: 3

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F: Sg

131:121173 Ionization potentials of seaborgium.

Johnson, E.; Pershina, V. Fricke, B. (Florida Agricultural Mechanical University, Tallahassee, FL, GSI-Rep., 99-01, 16 (English) 1999. Ionization potentias were calcd. of neutral atoms and pos. ions of Sg, C Mo, and W. The calcns. were performed within the multiconfiguration Dira approxn.

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(m 40 146) Sg(1+) Johnson E', Pershina V. et al., Sg (24) g. Phys. Chem. A1999, 103, 8458-62. Sg (St) Ionitation Potentials D Sg (6t) Seaborgium

1)m 40042

F: Sg(CO)6

P: 3

132:55063 Prediction of the Bond Lengths, Vibrational Frequencies, and Bond Dissociation Energy of Octahedral Seaborgium Hexacarbonyl, Sq(CO)6.

Nash, Clinton S.; Bursten, Bruce E. Glenn T. Seaborg Institute for Transactinium Science, Lawrence Livermore National Laboratory Livermore, CA 94550, USA J. Am. Chem. Soc., 121(46), 10830-10831 (English) 1999 The authors calcd. geometries and energies of pentacarbonyls and hexacarbonyls of Mo, W, and Sg as well as dissocn. energies and vibrational frequencies of the hexacarbonyls Mo(CO)6, W(CO)6, and Sg(CO)6 in the frameworks of HF, MP2, and CCD, CCSD, CCSD(T) methods.

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