Benchmark values of chemical potential and chemical hardness for atoms and atomic ions (including unstable anions) from the energies of isoelectronic series

Por: Cardenas, C (Cardenas, Carlos)[1,2] ; Heidar-Zadeh, F (Heidar-Zadeh, Farnaz)[3,4,5] ; Ayers, PW (Ayers, Paul W.)[3]

PHYSICAL CHEMISTRY CHEMICAL PHYSICS
Volumen: 18
Número: 36
Páginas: 25721-25734
DOI: 10.1039/c6cp04533b
Fecha de publicación: SEP 28 2016
Ver información de revista

Resumen

We present benchmark values for the electronic chemical potential and chemical hardness from reference data for ionization potentials and electron affinities. In cases where the energies needed to compute these quantities are not available, we estimate the ionization potential of the metastable (di) anions by extrapolation along the isoelectronic series, taking care to ensure that the extrapolated data satisfy reasonable intuitive rules to the maximum possible extent. We also propose suitable values for the chemical potential and chemical hardness of zero-electron species. Because the values we report are faithful to the trends in accurate data on atomic energies, we believe that our proposed values for the chemical potential and chemical hardness are ideally suited to conceptual studies of chemical trends across the periodic table. The critical nuclear charge (Z critical) of the isoelectronic series with $2 < N < 96$ has also been reported for the first time.

Palabras clave

KeyWords Plus: DENSITY-FUNCTIONAL THEORY; HARD/SOFT-ACID/BASE PRINCIPLE; FRONTIER-ELECTRON THEORY; MAXIMUM HARDNESS; SOFT ACIDS; ELECTRONEGATIVITY EQUALIZATION; HSAB PRINCIPLE; GROUND-STATE; VARIATIONAL-PRINCIPLES; PERTURBATION-THEORY

Información del autor

Dirección para petición de copias: Cardenas, C (autor para petición de copias)

+ Univ Chile, Fac Ciencias, Dept Fis, Casilla 653, Santiago 7800024, Chile.

Dirección para petición de copias: Cardenas, C (autor para petición de copias)

Ctr Desarrollo Nanociencia & Nanotecnol CEDENNA, Avda Ecuador 3493, Santiago 9170124, Chile.

Direcciones:

+ [1] Univ Chile, Fac Ciencias, Dept Fis, Casilla 653, Santiago 7800024, Chile

[2] Ctr Desarrollo Nanociencia & Nanotecnol CEDENNA, Avda Ecuador 3493, Santiago 9170124, Chile

[3] McMaster Univ, Dept Chem & Chem Biol, Hamilton, ON L8S 4M1, Canada

[4] Univ Ghent, Dept Inorgan & Phys Chem, Krijgslaan 281 S3, B-9000 Ghent, Belgium

[5] Univ Ghent, Ctr Mol Modeling, Technol Pk 903, B-9052 Ghent, Belgium

Direcciones de correo electrónico:cardena@macul.ciencias.uchile.cl

Financiación

Entidad financiadora	Número de concesión
FONDECYT	1140313
Centers Of Excellence With Basal/Conicyt Financing	FB0807
NSERC	
Compute Canada	
Vanier Canada Graduate Scholarship	

Ver texto de financiación

Editorial

ROYAL SOC CHEMISTRY, THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS, ENGLAND

Categorías / Clasificación

Áreas de investigación: Chemistry; Physics

Categorías de Web of Science: Chemistry, Physical; Physics, Atomic, Molecular & Chemical

Información del documento

Tipo de documento: Article

Idioma: English

Número de acceso: WOS:000384249300104

ID de PubMed: 27711480

ISSN: 1463-9076

eISSN: 1463-9084

Información de la revista

- **Impact Factor:** Journal Citation Reports®

Otra información

Número IDS: DX3CB

Referencias citadas en la Colección principal de Web of Science: 83

Veces citado en la Colección principal de Web of Science: 0