## UC Berkeley UC Berkeley Previously Published Works

### Title

Erratum: "Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks" [J. Chem. Phys. 141, 024102 (2014)].

Permalink https://escholarship.org/uc/item/0v00g7sg

**Journal** The Journal of chemical physics, 143(14)

**ISSN** 0021-9606

#### **Authors**

Zuev, Dmitry Jagau, Thomas-C Bravaya, Ksenia B <u>et al.</u>

Publication Date 2015-10-01

## DOI

10.1063/1.4932100

Peer reviewed

# Erratum: "Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks" [J. Chem. Phys. 141, 024102 (2014)]

Dmitry Zuev<sup>a</sup>, Thomas-C. Jagau<sup>a</sup>, Ksenia B. Bravaya<sup>b</sup>, Evgeny Epifanovsky<sup>*a,c,d*</sup>, Yihan Shao<sup>*d*</sup>, Eric Sundstrom<sup>*c*</sup>, Martin Head-Gordon<sup>*c*</sup>, and Anna I. Krylov<sup>*a*</sup>

<sup>a</sup> Department of Chemistry, University of Southern California, Los Angeles, California 90089
<sup>b</sup> Department of Chemistry, Boston University, Boston, Massachusetts 02215
<sup>c</sup> Department of Chemistry, University of California, Berkeley, California 94720
<sup>d</sup> Q-Chem Inc., 6601 Owens Drive, Suite 105, Pleasanton, California 94588

Several values for resonance widths taken from the literature [1, 2] and reported in Tables VIII, IX, and X in Ref. 3 are in fact half-widths. In detail:

- The experimental value for the width of the <sup>2</sup>Π resonance of CO<sup>-</sup> is 0.8 eV [1] and not 0.4 eV (last row of Table VIII in Ref. 3). We note that values for the resonance width of this state obtained with our theoretical approach (CAP-EOM-EA-CCSD) converge to this experimental value of 0.8 eV with increasing size of the one-electron basis set (cf. Table IV in Ref. 3).
- The value for the width of the <sup>2</sup>Π<sub>g</sub> resonance of C<sub>2</sub>H<sub>2</sub><sup>-</sup> obtained using the stabilization method at the TDDFT(HFE\_PBE)/aug-cc-pVTZ+3p level of theory is 1.2 eV [2] and not 0.6 eV (fifth row of Table IX in Ref. 3).
- The value for the width of the <sup>2</sup>B<sub>2g</sub> resonance of C<sub>2</sub>H<sub>4</sub><sup>-</sup> obtained using the stabilization method at the TDDFT(HFE\_PBE)/aug-cc-pVTZ+3p level of theory is 0.62 eV [2] and not 0.31 eV (thirteenth row of Table X in Ref. 3).

#### References

- [1] H. Ehrhardt, L. Langhans, F. Linder, and H. S. Taylor, Phys. Rev. 173, 222 (1968).
- [2] M. F. Falcetta, L. A. DiFalco, D. S. Ackerman, J. C. Barlow, and K. D. Jordan, J. Phys. Chem. A 118, 7489 (2014).
- [3] D. Zuev, T.-C. Jagau, K. B. Bravaya, E. Epifanovsky, Y. Shao, E. Sundstrom, M. Head-Gordon, and A. I. Krylov, J. Phys. Chem. 141, 024102 (2014).