

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

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Citation: *The Journal of Chemical Physics* **143**, 149901 (2015); doi: 10.1063/1.4932100

View online: <http://dx.doi.org/10.1063/1.4932100>

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

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(Received 11 September 2015; accepted 20 September 2015; published online 9 October 2015)

[<http://dx.doi.org/10.1063/1.4932100>]

Several values for resonance widths taken from the literature<sup>1,2</sup> and reported in Tables VIII–X in Ref. 3 are erroneous.

- Different values for the width of the  $^2\Pi$  resonance of  $\text{CO}^-$  have been extracted from the same experimental data.<sup>1</sup> In Ref. 1, a value of 0.40 eV has been determined from the width of the peaks of the  $v'=0$  channel in the elastic differential cross section and the  $v=1$  channel in the inelastic absolute cross section for e-CO scattering. However, in Refs. 4 and 5, fits of complex model potentials to the same experimental cross sections yielded values of 0.80 eV and 0.75 eV, respectively, for the resonance width. The values obtained with our theoretical approach (equation-of-motion electron-attachment coupled-cluster singles and doubles augmented by a complex absorbing potential) seem to converge rather to 0.75 or 0.80 eV than to 0.40 eV with increasing size of the one-electron basis set (cf. Table IV in Ref. 3).
- The value for the width of the  $^2\Pi_g$  resonance of  $\text{C}_2\text{H}_2^-$  obtained using the stabilization method and time-dependent density-functional theory(HFE\_PBE)/aug-cc-pVTZ+3p is 1.2 eV<sup>2</sup> and not 0.6 eV (fifth row of Table IX in Ref. 3).
- The value for the width of the  $^2B_{2g}$  resonance of  $\text{C}_2\text{H}_4^-$  obtained using the stabilization method and time-dependent density-functional theory(HFE\_PBE)/aug-cc-pVTZ+3p is 0.62 eV<sup>2</sup> and not 0.31 eV (thirteenth row of Table X in Ref. 3).

<sup>1</sup>H. Ehrhardt, L. Langhans, F. Linder, and H. S. Taylor, *Phys. Rev.* **173**, 222 (1968).

<sup>2</sup>M. F. Falcetta, L. A. DiFalco, D. S. Ackerman, J. C. Barlow, and K. D. Jordan, *J. Phys. Chem. A* **118**, 7489 (2014).

<sup>3</sup>D. Zuev, T.-C. Jagau, K. B. Bravaya, E. Epifanovsky, Y. Shao, E. Sundstrom, M. Head-Gordon, and A. I. Krylov, *J. Chem. Phys.* **141**, 024102 (2014).

<sup>4</sup>M. Zubek and C. Szmytkowski, *J. Phys. B* **10**, L27 (1977).

<sup>5</sup>M. Zubek and C. Szmytkowski, *Phys. Lett.* **74A**, 60 (1979).