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

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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 $^2\Pi$ resonance of CO^- 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 $^2\Pi_g$ resonance of C_2H_2^- 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 $^2B_{2g}$ resonance of C_2H_4^- 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

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- [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).