

Correction to "A Fresh Look at Resonances and Complex Absorbing Potentials: Density Matrix-Based Approach"

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In Table 1, the experimental value for the width of the ${}^2\Pi$ resonance of CO⁻ taken from ref 1 is in fact a half-width. Thus, the corresponding entry in Table 1 should read 0.8 eV and not 0.4 eV. Although this correction does not affect the main conclusions of the paper, the agreement of the theoretical values for the resonance width computed with our approach (CAP-EOM-EA-CCSD) with the corrected experimental value is unsatisfactory. This is likely due to using an insufficient basis set as further computations illustrate.²

The reference value for the ${}^2\Pi_{\sigma}$ resonance of N_2^- has been taken from ref 3 and is not affected.

REFERENCES

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- (2) Zuev, D.; Jagau, T.-C.; Bravaya, K. B.; Epifanovsky, E.; Shao, Y.; Sundstrom, E.; Head-Gordon, M.; Krylov, A. I. Complex Absorbing Potentials within EOM-CC Family of Methods: Theory, Implementation, and Benchmarks. J. Chem. Phys. 2014, 141, 024102.
- (3) Berman, M.; Estrada, H.; Cederbaum, L. S.; Domcke, W. Nuclear Dynamics in Resonant Electron-Molecule Scattering beyond the Local Approximation: The 2.3-eV Shape Resonance in N2. Phys. Rev. A: At., Mol., Opt. Phys. 1983, 28, 1363-1381.



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