



Erratum:

“Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework”

Coriani, Sonia; Koch, Henrik

Published in:

Journal of Chemical Physics

Link to article, DOI:

<http://dx.doi.org/10.1063/1.4964714>

Publication date:

2016

Document Version

Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):

Coriani, S., & Koch, H. (2016). Erratum: “Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework”. *Journal of Chemical Physics*, 145. <https://doi.org/10.1063/1.4964714>

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Erratum: “Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework” [J. Chem. Phys. 143, 181103 (2015)]

Sonia Coriani¹ and Henrik Koch¹

Citation: *The Journal of Chemical Physics* **145**, 149901 (2016); doi: 10.1063/1.4964714

View online: <http://dx.doi.org/10.1063/1.4964714>

View Table of Contents: <http://aip.scitation.org/toc/jcp/145/14>

Published by the *American Institute of Physics*



**COMPLETELY
REDESIGNED!**

**PHYSICS
TODAY**

Physics Today Buyer's Guide
Search with a purpose.

Erratum: “Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework” [J. Chem. Phys. **143**, 181103 (2015)]

Sonia Coriani^{1,2,a)} and Henrik Koch^{3,4,b)}

¹*Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste, I-34127 Trieste, Italy*

²*Aarhus Institute of Advanced Studies, Aarhus University, DK-8000 Århus C, Denmark*

³*Department of Chemistry, Norwegian University of Science and Technology, 7491 Trondheim, Norway*

⁴*Department of Chemistry and the PULSE Institute, Stanford University, Stanford, California 94305, USA*

(Received 20 September 2016; accepted 29 September 2016; published online 13 October 2016)

[<http://dx.doi.org/10.1063/1.4964714>]

Due to an unfortunate error, an exchange contribution was missing in the computed core-ionization potentials collected in Table III of Ref. 1. The revised values of the ionization potentials are collected in Table I below. Even though the revision does not alter the main conclusions of our previous study, it does deteriorate the agreement between CCSD results and experiment. We note that this is not due to the core-valence separation itself, as we verified by applying the perturbative correction to the ionization potentials.

TABLE I. CVS-CCSD core ionisation potentials (eV).

System	Basis	Ionization	CCSD	Δ UGA-SUMRCC ²	Expt.
H ₂ O	cc-pVDZ	O 1s ⁻¹	543.34 ^a	541.97	539.78
	cc-pVTZ		540.68 ^a	539.02	
	cc-pCVTZ		541.15 ^a	539.24	
CO	cc-pVTZ	C 1s ⁻¹	296.98 ^a	295.25	296.2 ^b
	cc-pCVTZ		297.54 ^a	295.67	
	cc-pVTZ	O 1s ⁻¹	543.71 ^a		542.5 ^b
	cc-pCVTZ		544.18 ^a		
N ₂	cc-pVTZ	N 1s ⁻¹	410.52		409.9 ^b
	cc-pCVTZ		411.04		
HF	cc-pVTZ	F 1s ⁻¹	695.02 ^a	693.40	693.80
	cc-pCVTZ		695.44 ^a		
	cc-pVTZ		694.86 ^c		
	cc-pCVTZ		695.27 ^c		

^aAt ground-state geometry of Ref. 2.

^bFrom the compilations in Refs. 3 and 4.

^cAt ionized-state geometry of Ref. 2.

¹S. Coriani and H. Koch, *J. Chem. Phys.* **143**, 181103 (2015).

²S. Sen, A. Shee, and D. Mukherjee, *Mol. Phys.* **111**, 2625 (2013).

³J. Stöhr, *NEXAFS Spectroscopy* (Springer, Berlin, 1992).

⁴A. A. Bakke, H.-W. Chen, and W. L. Jolly, *J. Electron Spectrosc. Relat. Phenom.* **20**, 333 (1980).

^a)Electronic mail: coriani@units.it

^b)Electronic mail: henrik.koch@ntnu.no