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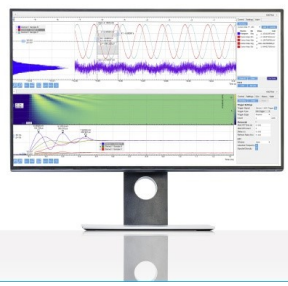

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Erratum: "Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework" [J. Chem. Phys. 143, 181103 (2015)]

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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	ΔUGA-SUMRCC[2]	Expt.
H_2O	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]		693.80
	cc-pCVTZ		695.44[a]	693.40	
	cc-pVTZ		694.86[c]		
	cc-pCVTZ		695.27[c]		

[a]At ground-state geometry of Ref. 2.
[b]From the compilations in Refs. 3 and 4.
[c]At ionized-state geometry of Ref. 2.

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