Erratum: Deorbitalization strategies for meta-generalized-gradient-approximation exchange-correlation functionals [Phys. Rev. A 96, 052512 (2017)]

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We have discovered a transcription error in one entry of Table V. The mean absolute error for MVS-L with the CRopt deorbitalizer is 7.83 kcal/mol (not 6.20). The corrected version is shown below.

The conclusions of Sec. IV remain unaltered with one modest exception. In particular, the striking result of best-performing deorbitalization is unchanged. The one exception is that the last sentence of that section, "On the test sets considered, MVS-L delivers performance quite similar to the highly sophisticated SCAN mGGA functional," must be modified to change "quite similar" to "closer than expected."

The conclusions of the rest of the paper are unaltered.

We thank Héctor Francisco R. for identifying the problem with the original Table V.

TABLE V. Performance of the deorbitalized versions of the MVS exchange-correlation functional. Heat of formation errors are in kcal/mol, bond length errors are in Å, and frequency errors are in cm^{-1}.

		PC	PCopt	TFLreg	TFLopt	CRloc	CRopt	MVS
Heats of formation	ME	24.00	−15.37	18.27	19.18	2.71	2.89	−17.33
	MAE	25.53	15.94	19.09	19.91	7.53	7.83	18.34
Bonds	ME	0.0069	−0.0025	0.0092	0.0072	0.0025	0.0049	−0.0016
	MAE	0.0137	0.0127	0.0139	0.0139	0.0121	0.0130	0.0139
Frequencies	ME	2.9	39.3	9.6	20.0	25.3	28.7	46.2
	MAE	29.4	46.0	34.7	37.7	37.0	42.6	52.0

