

Erratum: “The chemical bond in external electric fields: Energies, geometries, and vibrational Stark shifts of diatomic molecules” [J. Chem. Phys.139, 144101 (2013)]

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Erratum: “The chemical bond in external electric fields: Energies, geometries, and vibrational Stark shifts of diatomic molecules” [J. Chem. Phys. 139, 144101 (2013)]

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In Table IV, as published in the original paper (Ref. 1, p. 9), we have mistakenly used c_2 values calculated for homo-nuclear diatomics (the top four c_2 values in Table III of Ref. 1 (p. 8)) to estimate the bond lengths of the four hetero-nuclear diatomics [from Eqs. (10) to (12)] instead of using the correct c_2 values (the last four entries in Table III). This resulted in discrepancies between the estimated bond lengths compared to those calculated directly (with the field-including hamiltonian) for hetero-nuclear diatomics, discrepancies that are more visible at stronger field strengths in Table IV. Upon the use of the correct c_2 values, these discrepancies practically vanish for hetero-nuclear diatomics (as they do for homo-nuclear diatomics) for all field strengths and orientations. Table IV should be replaced by the corrected one presented in this Erratum.

TABLE IV. Directly calculated equilibrium internuclear separations (bond lengths) in Å under different fields and those obtained from the regression parameters listed in Table III using Eq. (10).^a

E ($\times 10^9$ V m ⁻¹) ^{b,c}	H ₂	N ₂	O ₂	F ₂	Cl ₂	H←F	H←Cl	C→O	N→O
-10.28 (←)						0.92115	1.28281	1.13556	1.15560
						0.92116	1.28281	1.13557	1.15554
-5.14 (←)						0.00	0.00	0.00	-0.01
						0.91759	1.27746	1.13174	1.15266
						0.91758	1.27745	1.13174	1.15271
-3.60 (←)						0.00	0.00	0.00	0.00
						0.91663	1.27615	1.13070	1.15192
						0.91662	1.27614	1.13070	1.15197
-2.57 (←)						0.00	0.00	0.00	0.00
						0.91601	1.27536	1.13003	1.15145
						0.91601	1.27535	1.13004	1.15150
-1.54 (←)						0.00	0.00	0.00	0.00
						0.91542	1.27462	1.12939	1.15102
						0.91541	1.27461	1.12940	1.15105
-0.51 (←)						0.00	0.00	0.00	0.00
						0.91484	1.27394	1.12877	1.15061
						0.91484	1.27394	1.12877	1.15063
0						0.00	0.00	0.00	0.00
	0.74262	1.09752	1.19947	1.39376	1.99741	0.91456	1.27362	1.12847	1.15042
	0.74262	1.09752	1.19947	1.39376	1.99741	0.91456	1.27362	1.12847	1.15042
0.51 (→)						0.00	0.00	0.00	0.00
	0.74263	1.09752	1.19947	1.39376	1.99743	0.91429	1.27331	1.12817	1.15023
	0.74262	1.09752	1.19947	1.39377	1.99743	0.91429	1.27332	1.12817	1.15022
1.54 (→)						0.00	0.00	0.00	0.00
	0.74267	1.09754	1.19951	1.39381	1.99760	0.91376	1.27275	1.12758	1.14987
	0.74266	1.09754	1.19951	1.39381	1.99759	0.91375	1.27276	1.12759	1.14983
	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	

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TABLE IV. (Continued).

E ($\times 10^9$ V m $^{-1}$) ^{b,c}	H ₂	N ₂	O ₂	F ₂	Cl ₂	H←F	H←Cl	C→O	N→O
2.57 (→)	0.74274	1.09757	1.19959	1.39391	1.99793	0.91324	1.27224	1.12702	1.14952
	0.74274	1.09757	1.19959	1.39391	1.99792	0.91324	1.27225	1.12703	1.14947
	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3.60 (→)	0.74286	1.09761	1.19971	1.39405	1.99842	0.91275	1.27178	1.12648	1.14920
	0.74286	1.09761	1.19971	1.39405	1.99842	0.91275	1.27180	1.12649	1.14912
	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
5.14 (→)	0.74310	1.09771	1.19997	1.39436	1.99948	0.91205	1.27121	1.12570	1.14873
	0.74310	1.09771	1.19997	1.39436	1.99947	0.91205	1.27123	1.12571	1.14863
	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01
10.28 (→)	0.74456	1.09827	1.20147	1.39620	2.00591	0.91003	1.27024	1.12342	1.14722
	0.74456	1.09827	1.20147	1.39620	2.00591	0.91003	1.27022	1.12342	1.14731
	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01

^aAll data are based on calculations at the (U)QCISD/6-311++G(3df,2pd) level of theory.

^bThe direction of the field with respect to the permanent molecular dipole moment is indicated by the arrow, while the permanent dipole moment is indicated by the arrow between the atomic symbols.

^cFor every field there are three rows: The top row is the value calculated directly from the Gaussian 09 program, the middle row is the value obtained from using the regression parameters c_1 and c_2 listed in Table III and obtained from a fitting of bond lengths using Eq. (10), and the third row is the signed % error of the fitted value.

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