

Erratum to “Geometries and Vertical Excitation Energies in Retinal Analogues Resolved at the CASPT2 Level of Theory: Critical Assessment of the Performance of CASSCF, CC2, and DFT Methods”

Elżbieta Walczak, Borys Szefczyk, and Tadeusz Andruniów*

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Supporting Information

Recently, we have found an error in Local CC2 (LCC2) calculations that affected LCC2-based geometries, excitation energies, and properties published in the original paper: “Geometries and vertical excitation energies in retinal analogues resolved at the CASPT2 level of theory: Critical assessment of the performance of CASSCF, CC2, and DFT methods” (*J. Chem. Theory Comput.* 2013, 9, 4915–4927).

Tables 1 and 2 summarize the corrected data. The mean absolute error of bond length alternation (BLA) obtained at

Table 1. Erratum to Tables 1 and 6—BLA and Vertical Excitation Energies ($S_0 \rightarrow S_1$) Calculated at LCC2/cc-pVTZ Level of Theory^a

	BLA [Å]	ΔE [eV]
9,13-dimethyl	0.049	2.82 (2.81)
9-methyl	0.046	2.77 (2.76)
13-methyl	0.049	2.90 (2.89)
9,10-dimethyl (<i>twist</i>)	0.051	2.79 (2.78)
9,10-dimethyl (C_s)	0.047	2.81 (2.81)
9,10,13-trimethyl (<i>twist</i>)	0.049	2.61 (2.61)
9,10,13-trimethyl (C_s)	0.049	2.70 (2.69)
<i>locked-11.5</i>	0.050	2.79 (2.79)
<i>locked-11.7</i>	0.045	2.79 (2.78)
<i>locked-11.8</i>	0.051	2.67 (2.66)
<i>locked-11.8-b1</i>	0.047	2.72 (2.71)
<i>locked-11.8-b2</i>	0.046	2.67 (2.66)
mean absolute error	0.004	0.02 (0.02)
max absolute error	0.007	0.05 (0.05)
min absolute error	0.000	0.00 (0.00)

^aExcitation energies were calculated using extended domains. Values calculated using standard domains are presented in parentheses.

LCC2, compared to MP2 is 0.004 Å, not 0.002 Å as specified in the original text. The stability of the two conformers, 9,10-dimethyl (C_s) and 9,10-dimethyl (*twist*), is different: the relative energy is 0.30 kcal/mol instead of −0.06 kcal/mol, the dihedral angle centered at the C10–C11 bond is −169.1° instead of −165.9°, and the dihedral angle centered at the C11–C12 bond is 8.0° instead of 11.6° (Table 2 in the original paper). The relative energy of 9,10,13-trimethyl (C_s) with respect to 9,10,13-trimethyl (*twist*) is 7.00 kcal/mol instead of 6.50 kcal/mol. The dihedral angle centered at the C10–C11 bond is −161.4° instead of −157.8°, and the dihedral angle centered at the C11–C12 bond is 26.3° instead of 24.0°. Relative energies of *locked-11.8* and *locked-11.8-b2* with respect

Table 2. Erratum to Tables 7 and 8—Oscillator Strength and Change in (Unrelaxed) Dipole Moment upon the $S_0 \rightarrow S_1$ Transition for RPSB Analogues Calculated at LCC2/cc-pVTZ Level of Theory Using Extended Domains^a

	f	$\Delta\mu^b$ [D]
9,13-dimethyl	1.53 (1.52)	5.25 (5.30)
9-methyl	1.39 (1.38)	4.60 (4.68)
13-methyl	1.57 (1.56)	5.89 (5.90)
9,10-dimethyl (<i>twist</i>)	1.50 (1.49)	4.20 (4.27)
9,10-dimethyl (C_s)	1.57 (1.56)	4.52 (4.58)
9,10,13-trimethyl (<i>twist</i>)	1.26 (1.26)	4.69 (4.73)
9,10,13-trimethyl (C_s)	1.47 (1.46)	6.11 (6.16)
<i>locked-11.5</i>	0.86 (0.86)	2.89 (2.91)
<i>locked-11.7</i>	1.41 (1.41)	5.40 (5.42)
<i>locked-11.8</i>	1.15 (1.14)	5.11 (5.16)
<i>locked-11.8-b1</i>	1.29 (1.28)	5.19 (5.22)
<i>locked-11.8-b2</i>	1.29 (1.28)	4.86 (4.89)

^aValues calculated using standard domains are presented in parentheses. ^bIn Table 8 of the original paper CC2-derived changes in dipole moments are calculated based on unrelaxed dipole moments.

to *locked-11.8-b1* (Table 3 in the original paper) are 1.46 and 0.52 kcal/mol, respectively.

The corrected vertical excitation energies are closer to the CASPT2/ANO-L-VDZP set, yielding mean average error of 0.02 eV, therefore identical with canonical CC2. Similarly, the corrected dipole moments (Table 2). This invalidates our conclusion that the LCC2 method is unable to describe the charge transfer character of the $S_0 \rightarrow S_1$ excitation in retinal analogues.

The Supporting Information includes corrections to Table S7, Figure S2, and the Cartesian coordinates of LCC2-optimized structures.

In conclusion, LCC2 method provides BLAs, vertical excitation energies, oscillator strengths, and dipole moments very close to the corresponding values obtained from canonical CC2 calculations.

ASSOCIATED CONTENT

Supporting Information

Corrected Table S7, Figure S2, and Cartesian Coordinates of LCC2-optimized structures. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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