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Corrigendum

Corrigendum to "Theoretical study of the electronic (hyper)polarizabilities of amino acids in gaseous and aqueous phases" [Comput. Theor. Chem. 976 (2011) 188–190]

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The author regrets that the range of ⟨α⟩ values in Fig. 4 was incorrectly presented in the published article. Fig. 4 is correctly reproduced below (with the range for the ⟨α⟩ values at 40–130 a.u. instead of 0–100 a.u.).

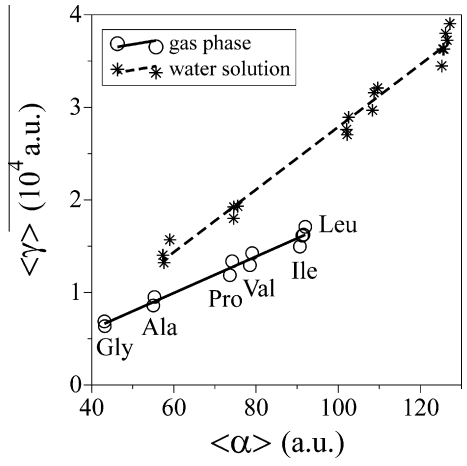

Fig. 4. Relationship between ⟨γ⟩ and ⟨α⟩ values of the aliphatic amino acids computed at the MP2/aug-cc-pVDZ level. Gas phase ⟨α⟩ values are taken from Ref. [1]. Gas phase: ⟨γ⟩ = −0.186 + 0.020 · ⟨α⟩, r = 0.99. Water solution: ⟨γ⟩ = −0.594 + 0.034 · ⟨α⟩, r = 0.99.

Reference

[1] S. Millefiori, A. Alparone, A. Millefiori, A. Vanella, Electronic and vibrational polarizabilities of the twenty naturally occurring amino acids, Biophys. Chem. 132 (2008) 139–147 (and references therein).

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