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Correction: Influence of pseudo-Jahn–Teller activity on the singlet–triplet gap of azaphenalenenes

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Correction for 'Influence of pseudo-Jahn–Teller activity on the singlet–triplet gap of azaphenalenenes' by Atreyee Majumdar *et al.*, *Phys. Chem. Chem. Phys.*, 2024, **26**, 26723–26733, <https://doi.org/10.1039/D4CP02761B>.

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The authors regret that Table 1 of the original article was incorrect. The correct table is shown here.

The associated discussion of Table 1 should read:

(i) “Furthermore, for the D_{3h} structure of 1AP, the vertical STG underestimates the adiabatic transition energy (0–0), which accounts for geometric effects in S_1 and T_1 along with the zero-point vibrational energy, by +0.057 eV at the CC2-level.”

(ii) “From previously reported⁹ CC2-level vertical and 0–0 values of STG, one can correct the TBE of the vertical STG of 5AP from ref. 13 to be –0.07 eV, agreeing with the experimental value of –0.047 eV.³⁰”

Additionally, in the same section, the authors would like to state that the results presented in Tables S1, S2, S3, and S4 of the supplementary information (ESI) of the original article are based on the cc-pVTZ basis set.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.



Table 1 For the six azaphenalenenes shown in Fig. 1, vertical excitation energies of the S_1 and T_1 states with respect to the ground state, S_0 , along with the singlet–triplet gap (S_1-T_1) are given in eV. The excited state energies were calculated using the ADC(2)/aug-cc-pVTZ method using geometries determined with the CCSD(T)/cc-pVTZ method. The barrier for automerization, E^\ddagger (in kJ mol^{-1}), determined using two-point CBS extrapolation of CCSD(T) energies with cc-pVTZ and cc-pVQZ basis sets, is stated for the symmetric saddle point. Results from other studies are included for comparison; 0–0 indicates adiabatic transition energies accounting for the energy of the vibrational ground state

| System | E^\ddagger | S_1 | T_1 | S_1-T_1 | Source |
|------------------|--------------|-------|--------|-------------------|-------------------------|
| 1AP (D_{3h}) | 0.3 | 0.979 | 1.121 | −0.142 | This work |
| 1AP (C_{3h}) | | 1.130 | 1.190 | −0.060 | This work |
| 1AP | | 1.047 | 1.180 | −0.133 | CC2 ⁹ |
| 1AP | | 0.992 | 1.068 | −0.076 | 0–0, CC2 ⁹ |
| 1AP (D_{3h}) | | 0.979 | 1.110 | −0.131 | TBE ¹³ |
| 1AP | | 0.97 | 0.93 | +0.04 | Exp. ^{28 a} |
| 5AP (C_{2v}) | | 2.128 | 2.274 | −0.147 | This work |
| 5AP | | 2.231 | 2.365 | −0.134 | CC2 ⁹ |
| 5AP | | 1.971 | 2.056 | −0.085 | 0–0, CC2 ⁹ |
| 5AP (C_{2v}) | | 2.177 | 2.296 | −0.119 | TBE ¹³ |
| 5AP | | 1.957 | 2.003 | −0.047 | 0–0, exp. ³⁰ |
| 7AP (D_{3h}) | | 2.636 | 2.889 | −0.253 | This work |
| 7AP | | 2.756 | 2.998 | −0.242 | CC2 ⁹ |
| 7AP | | 2.512 | 2.618 | −0.106 | 0–0, CC2 ⁹ |
| 7AP (D_{3h}) | 2.717 | 2.936 | −0.219 | TBE ¹³ | |
| 7AP | | | <0 | Exp. ³ | |
| 2AP (C_{2v}) | 2.1 | 0.838 | 0.941 | −0.102 | This work |
| 2AP (C_s) | | 1.246 | 1.121 | +0.125 | This work |
| 2AP (C_{2v}) | | 0.833 | 0.904 | −0.071 | TBE ¹³ |
| 3AP (C_{2v}) | 5.3 | 0.689 | 0.768 | −0.079 | This work |
| 3AP (C_s) | | 1.335 | 1.061 | +0.274 | This work |
| 3AP (C_{2v}) | | 0.693 | 0.735 | −0.042 | TBE ¹³ |
| 4AP (D_{3h}) | 11.1 | 0.550 | 0.623 | −0.073 | This work |
| 4AP (C_{3h}) | | 1.409 | 1.017 | +0.392 | This work |
| 4AP (D_{3h}) | | 0.554 | 0.583 | −0.029 | TBE ¹³ |

^a Using $S_1 = 0.78 \mu\text{m}^{-1}$ and $T_1 = 0.75 \mu\text{m}^{-1}$ from ref. 28 multiplied by $1.2398 \text{ eV } \mu\text{m}^{-1}$.

