CORRECTION

Check for updates

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

Atreyee Majumdar, Komal Jindal, Surajit Das and Raghunathan Ramakrishnan*

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

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 +0.057eV at the CC2-level."

(ii) "From previously reported[9] 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.

Tata Institute of Fundamental Research, Hyderabad 500046, India. E-mail: ramakrishnan@tifrh.res.in

16266 | *Phys. Chem. Chem. Phys.*, 2025, **27**, 16266–16267

This journal is © the Owner Societies 2025

Table 1 For the six azaphenalenes 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 $S_1 = 0.78$ μm^{-1} and $T_1 = 0.75$ μm^{-1} from ref. 28 multiplied by 1.2398 eV μm^{-1}.