SUPPORTING INFORMATION

Reply to the 'Comment on "Designing potentially singlet fission materials with an anti-Kasha behaviour"' by K. Jindal, A. Majumdar and R. Ramakrishnan, Phys. Chem. Chem. Phys., 2025, 27, DOI: 10.1039/D4CP02863E

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Table S1. Excitation energies for the ghost states computed at the TD-LC-ωHPBE/6-311G(d,p)//B3LYP/6-311G(d,p) level for substituted azulenes.

Position[a]	Ghost state energy (cm^{-1})	Position[a]	Ghost state energy (cm^{-1})
Azulene	1692.8	OH8b	–3029.2
CN1	4881.7	OH12a	8286.8
CN2	3550.2	OH12b	9337.7
CN6	–5789.9	OH13	–3438.1
CN7	-3700.2	OH48	-4071.2
CN8	–5972.9	OH56a	3769.6
CN12	5473.7	OH56b	12846.7
CN13	7100.4	OH57	5429.4
CN47	–7191.6	OH58	2767.9
CN48	–8209.4	OH68	3893.8
CN57	–4902.7	OH78	5301.9
CN67	–6621.4	OH123	11790.2
CN68	–7870.6	OH456	6045.5
CN78	–6965.7	OH457a	–5286.6
CN123	7196.4	OH458a	10194.2
CN457	–7632.7	OH467	7014.1
CN458	–8939.2	OH468	10569.2
CN467	–8596.5	OH478	9309.4
CN468	–9350.6	OH567	16283.2
CN567	–7098.8	OH568	10894.2
CN678	–8460.2	OH578	1467.8
CN4578	–9290.1	OH678	11241.0
CN4678	–9879.6	OH4567	4981.8
CN5678	-8874.7	OH4568a	8682.8
CN45678	–10149.8	OH4578	7422.2
OH1a	417.0	OH4678	12785.4
OH1b	–3658.3	OH5678	7704.5
OH2	1654.9	OH45678	13359.7
OH6a	7829.5		

[a] In the OH-substituted compounds, isomers a and b are observed; these are relative to the position of the hydrogen in –OH but do not change considerably the final result.