Supplementary Material for PCCP

Electronic Supplementary information

Summary tables of calculated energies.

Table 1. Relative energies of the trans and cis tautomers as well as barriers to trans-to-cis tautomerization (in kJ/mol) for molecule **1** in the electronic ground state S_0 and in the first electronic excited state S_1.

	ΔE (B3LYP/6-311G*)[a]	ΔE (TD-B3LYP/6-311G*)[b]
trans tautomer	0.0	0.0
cis tautomer	+40.2	+40.9
barrier to trans-to-cis tautomerization	+58.6	+61.6

[a]: Electronic ground state S_0.
[b]: Electronic excited state S1 time dependent density functional theory.

Table 2. Relative energies (in kJ/mol) of the various conformers and tautomers of molecule **2** (electronic ground state S_0) as obtained at the B3LYP/6-311G* level of theory.

Trans tautomers	ΔE[a]	Cis tautomers	ΔE[a]
up-down-up-down (udud)[c]	0.0		
		udud-cis[1]	+35.2
		udud-cis[2]	+39.8
		udud-cis[3]	+39.9
		udud-cis[4]	+52.3
uduu[c]	+0.2		
		udud-cis[1]	+36.4
		udud-cis[2]	+39.4
		udud-cis[3]	+40.4
		udud-cis[4]	+55.1
uudd[c]	+4.5		
		udud-cis[1]	+34.8
		udud-cis[2]	+39.0
		udud-cis[3]	+40.5
		udud-cis[4]	+54.9
uuuu[c,d]	+4.7		
duud[c,d]	+8.2		
uuud[c,d]	+11.7		

[a]: Relative energies of the 6 trans tautomers (different conformations, see text).
[b]: Relative energies with respect to the corresponding trans form.
[c]: See main text for further details of the various conformers.
[d]: No cis tautomers calculated.

Table 3. Relative energies of the trans and cis tautomers as well as barriers to trans-to-cis tautomerization (in kJ/mol) for molecule **3** in the electronic ground state S_0.

	ΔE (B3LYP/6-311G*)[a]
trans tautomer	0.0
cis tautomer	+37.6
barrier to trans-to-cis tautomerization	+55.2