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Modulating the thermal isomerization barriers of quadricyclane to norbornadiene through cross-conjugative patterns

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Computations show that thermal isomerizations of quadricyclane to norbornadiene can be modulated by heteroarene substitution. Heteroarenes that are non-cross-conjugated to the norbornadiene double bond increase delocalization of the transition state structure and lower the thermal activation enthalpy (ΔH^{\ddagger}), while cross-conjugated analogs increase ΔH^{\ddagger} without significantly impacting the storage enthalpy ($\Delta H_{\text{storage}}$).

Molecular solar thermal energy storage (MOST) systems are photoswitchable molecules that store solar energy by converting light into chemical energy. These systems typically exist as pairs of isomers that can reversibly convert through light-induced bond cleavage, bond rotation, or conformational changes. Common MOST frameworks include the E/Z-azobenzenes, 2,3 dihydroazulene-vinylheptafulvene, 4-6 dimetal fulvalene complexes, 7,8 and notably, the norbornadiene-quadricyclane (NBD-QC) pair. 9,10 A schematic illustration of the NBD-QC pair functioning as a MOST system is shown in Fig. 1a. Upon photoexcitation, NDB converts to the metastable QC. The energy difference of the two is the stored energy ($\Delta H_{\text{storage}}$), which can then be released spontaneously or by external stimuli (e.g., heat, light, 2,3 or electric potential 11,12) through a thermal back reaction barrier (ΔH^{\ddagger}). Thermal relaxation of QC to NBD proceeds via a concerted, asynchronous, retro-[2+2] cycloaddition, and the transition state structure exhibits high diradical character. 13-15 Efficient MOST systems must meet several criteria: (I) absorption within the solar window; (II) a high photoisomerization quantum yield; (III) a high energy density; (IV) a high energy storage, and (V) a long thermal half-life for the metastable isomer (i.e., a suitable thermal back reaction barrier, ΔH^{\ddagger}). 9,16 These features can be modified through structural designs of the MOST framework, but often, improving some criteria comes at the expense of others.

Norbornadiene stands out among common MOST systems for its low molecular weight and high energy density (0.97 MJ $\,\mathrm{kg}^{-1}$), ¹⁷ but its absorption maximum lies outside of the solar window. ¹⁸

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Structural modifications of NBD–QC have been explored to improve performance, for example, by placing donor (D) and acceptor (A) pairs through-space, ¹⁶ (Fig. 1b) or through-bond ¹⁹ (Fig. 1c), placing bulky substituents at the C7 bridge, (Fig. 1d)²⁰ or by heteroatom substitution (Fig. 1e). ²¹ One way to red-shift the absorption maxima is by tethering conjugated units to NBD, but this increases the molecular weight and reduces the energy storage per unit mass. ²⁰ It was found that bulky groups at the C7 bridge could introduce steric stress, improving the quantum yield and increasing the thermal life-time of QC, although storage energy decreases modestly. ²⁰ Enhanced storage enthalpies, $\Delta H_{\rm storage}$, ²² and red-shifted absorptions ¹⁷ often correlate with reduced thermal isomerization barriers, ΔH^{\ddagger} . Computational screening identified candidates with improved red-shift absorptions, storage capacity, and thermal half-lives. ^{23,24} Yet, strategies to maximize storage

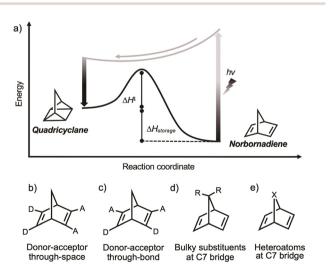


Fig. 1 (a) Schematic illustration of the photoisomerization of norbornadiene (NBD) and quadricyclane (QC). NBD motifs with donor (D) and acceptor (A) groups (b) through-space or (c) through-bond, and with modified C7 bridges by (d) alkyl (R) groups or (e) heteroatom (X = O or NH) substitution.

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Fig. 2 (a) NBD frameworks investigated. (b) Resonance forms of 15'-TS vs. 3S'-TS illustrate how non-cross-conjugative vs. cross-conjugative patterns affect delocalization of the unpaired electrons at the TS structure. (c) Resonance forms of 5p-TS vs. 5m-TS illustrate stabilization of unpaired electrons at the para-position. Thermal half-lives at 25 °C were taken from ref. 25.

enthalpies while targeting suitable storage half-lives remain elusive.

Here, we investigate the storage enthalpies ($\Delta H_{\text{storage}}$), thermal back reaction barriers (ΔH^{\ddagger}) , and computed absorption maxima (λ_{max}) for a series of NBD-QC frameworks containing through-bond donor-acceptor substituents (Fig. 2). Structures 1' and 3' were inspired by NBD-QC systems reported by Moth-Poulsen and co-workers, in which a π -accepting CN group is placed at C2 and a (hetero)arene is attached to C3; increasing donor strength and extending conjugation across the double bonds of NBD was found to increase storage half-lives from hours to days at room temperature. 22,25 Although the original work focused on the effects of para-substitution on ΔH^{\ddagger} , the authors reported rather different thermal half-lives for 1S' $(t_{1/2} = 0.22 \text{ days}) \text{ vs. } 3S' (22.7 \text{ days}) \text{ and for } 5p (7.74 \text{ days}) \text{ vs. } 5m$ (108.7 days), at room temperature, which caught our attention.

We wondered whether the contrasting thermal stability of 1S'-QC vs. 3S'-QC might be explained by differences in their conjugation patterns. We noted that, in 1S', the two double bonds in the thiophene ring are non-cross-conjugated with the NBD double bond. Therefore, the transition state (TS) structure for the QC → NBD isomerization can be stabilized by delocalization of the unpaired electrons to the heteroarene, resulting in a lower ΔH^{\ddagger} and shorter thermal half-life (Fig. 2b, top, in purple). In 3S', the two double bonds of the thiophene ring are cross-conjugated with the NBD double bond. Thus, the QC \rightarrow NBD TS structure is less stabilized by delocalization of the unpaired electrons, giving rise to a higher ΔH^{\ddagger} and longer thermal half-life (Fig. 2b, bottom, in orange). A similar explanation was put forth by Adrion and Lopez to rationalize the thermal half-lives of azoarenes.²⁶

We expect that non-cross-conjugative vs. cross-conjugative patterns may provide a means to modulate ΔH^{\ddagger} barriers and tested our hypothesis by investigating a series of heteroarenes tethered to the double bond(s) of CN-substituted NBD frameworks, 1' and 3'; CN group placed at the C2 position, and an heteroarene (X = NH, O, S) attached to the C3 position. We also investigated NBD frameworks containing two sets of throughbond donor-acceptor pairs; two CN groups placed at the C2 and C6 positions of NBD, and two heteroarenes (X = NH, O, S) placed at C3 and C5. In structure 1, the heteroarene double bonds are non-cross-conjugated to the NBD double bonds. In structure 2, a mixed set of non-cross-conjugated and crossconjugated heteroarenes are tethered to the NBD double bonds. In structure 3, the heteroarene double bonds are crossconjugated to the NBD double bonds.

Following the suggestion of one reviewer, we further examined a series of para- and meta-phenyl substituted 2-cyano-3-phenyl-NBD derivatives (4–8). Replacing the five-membered heterocycles by a phenyl group increases the thermodynamic penalty for dearomatization, resulting in modestly higher activation enthalpies for the thermal back reaction (Table 1). As shown in Fig. 2c, the TS structure for the QC → NBD isomerization can be further stabilized by π -donating or π -accepting substituents at the paraposition, but not at the meta-position. As a result, 2-cyano-3phenyl-NBD frameworks with para-substituted phenyl groups exhibit lower ΔH^{\ddagger} and shorter thermal half-lives compared to their meta-substituted counterparts (see Y = NO2 example in Fig. 2c).

Computations for ΔH^{\ddagger} and $\Delta H_{\text{storage}}$ values were carried out at the CAM-B3LYP-D3(BJ)/6-311+G(d,p)//(U)PBE0-D3(BJ)/def2-TZVPP level, following the protocols of previous benchmarking studies.²⁰ Jorner *et al.* reported that computed ΔH^{\ddagger} and $\Delta H_{\text{storage}}$ values for the parent NBD-QC pair, based on single-point CAM-B3LYP energies and PBE0 geometries, agreed satisfactorily with CASPT2 energies and with experimental data. 15,20 The computed ΔH^{\ddagger} values for 1S', 3S', 5p, 5m, 8p, and 9 correlate satisfactorily with experimental values measured in toluene at 25 $^{\circ}$ C (R^2 = 0.754), displaying a standard error of \pm 0.63 (see Table 1 footnote and correlation plot in Fig. S4). However, direct comparisons of the computed and experimental ΔH^{\ddagger} indicate that the computed values are systematically underestimated, as found previously.²⁵ Absolute values for spin densities at the C3 and C5 positions were computed for the QC → NBD TS using the Natural Bond Orbital (NBO) program²⁷ at (U)PBE0-D3(BJ)/def2-TZVPP. Averaged absolute spin density values at the C3 and C5 positions, $|\delta_{avg}| = (|\delta_{C3}| +$ $|\delta_{C5}|$)/2, indicate the extent of delocalization of the unpaired electrons. Absorption maxima (λ_{max}) for all substituted NBD and QC derivatives were computed at TD-PBE0-D3(BJ)/def2-TZVPP.

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Table 1 Computed activation enthalpies (ΔH^{\ddagger}) , storage enthalpies $(\Delta H_{\text{storage}})$, averaged absolute spin density values at the C3/C5 positions $(|\delta_{
m avq}|)$ of the TS structure, absorption maxima ($\lambda_{
m max}$, nm), and absorption intensity at λ_{max} (f). All energies are in kcal mol⁻¹

	$ \delta_{\mathrm{avg}} $	ΔH^{\ddagger}	$\Delta H_{\mathrm{storage}}$	$QC \; \lambda_{max}$	NBD λ_{max}	NBD $f_{ m max}$
Parent	0.84	31.1	-20.9	185.7	246.5	0.000
1NH'	0.67	19.4	-28.7	248.8	333.5	0.272
10'	0.65	19.2	-25.7	241.3	334.4	0.254
1S'	0.65	20.1^{a}	-25.0	253.1	337.5	0.245
3NH'	0.71	22.6	-26.8	236.2	321.3	0.144
3O'	0.70	22.8	-24.9	226.6	317.9	0.103
3S'	0.70	22.5^{a}	-24.6	238.4	325.2	0.151
1NH	0.52	9.7	-34.6	307.1	409.1	0.040
10	0.49	7.1	-33.3	287.6	394.4	0.041
1S	0.50	8.2	-31.7	294.9	402.4	0.035
2NH	0.56	11.0	-35.8	292.9	386.3	0.042
20	0.54	10.9	-32.3	283.5	381.8	0.040
2S	0.54	12.7	-30.9	272.6	385.6	0.031
3NH	0.60	14.0	-34.1	284.3	372.1	0.023
3O	0.59	14.7	-31.2	264.4	359.5	0.012
3S	0.58	14.9	-30.2	369.6	369.6	0.025
4p	0.68	22.4	-23.1	335.5	335.5	0.214
4m	0.70	23.3	-23.2	324.7	324.7	0.120
5 p	0.67	22.3^{a}	-22.8	352.3	352.3	0.218
5m	0.70	23.2^{a}	-23.2	346.3	346.3	0.030
6р	0.70	23.0	-25.0	325.2	325.2	0.273
6m	0.70	23.4	-23.6	323.9	323.9	0.146
7 p	0.69	22.3	-25.5	337.8	337.8	0.378
7 m	0.70	23.2	-24.1	353.0	353.0	0.067
8p	0.68	22.2^{a}	-25.8	354.0	354.0	0.499
8m	0.70	23.5	-24.2	395.1	395.1	0.036
9	0.70	23.2^{a}	-23.9	241.7	317.3	0.171

^a Experimental ΔH^{\ddagger} values (in kcal mol⁻¹) for 1S' (22.8), 3S' (25.8), 5p (24.1), 5m (28.0), 8p (26.4), 9 (26.8) were derived from the Eyring equation, based on measurements at 25 °C in toluene. 22,25

Direct comparisons of pairs of cross-conjugated vs. non-crossconjugated species show that π -conjugation patterns can largely affect electron delocalization of the QC -> NBD TS structure (Table 1). Consistent with the schematic illustration shown in Fig. 2b, $|\delta_{avg}|$ values for the non-cross-conjugated TS structures, 1NH' (0.67), 1O' (0.65), 1S' (0.65), are smaller than those of the cross-conjugated isomers, 3NH' (0.71), 3O' (0.70), 3S' (0.70), indicating increased delocalization in 1NH', 10', 1S'. At the TS structure, non-cross-conjugated species exhibit more delocalization (i.e., less spin at C3 and C5, cf. Fig. 2b, top, in purple), while cross-conjugated species display less delocalization (i.e., more spin at C3 and C5, cf. Fig. 2b, bottom, in orange). Accordingly, computed ΔH^{\ddagger} barriers for the non-cross-conjugated, 1NH' $(19.4 \text{ kcal mol}^{-1})$, 10' (19. 2), 15' (20.1), are lower compared to those of their cross-conjugated isomers, 3NH' (22.6), 3O' (22.8), 3S' (22.5). Increased thermal stability of QC (i.e., a larger ΔH^{\ddagger}) correlates with a decreased storage enthalpy (i.e., a less negative $\Delta H_{\text{storage}}$). ^{20,28,29} Thus, the computed $\Delta H_{\text{storage}}$ values for **1NH** $(-28.7 \text{ kcal mol}^{-1})$, 10' (-25.7), and 15' (-25.0), are more exothermic than that of 3NH' (-26.8), 3O' (-24.9), and 3S'(-24.6). Nevertheless, we note that a meaningful increase in $\Delta\Delta H^{\ddagger}$ $(3.2, 3.6, 2.4 \text{ kcal mol}^{-1}, \text{ respectively, for 1NH' vs. 3NH', 10' vs. 30'},$ and 1S' vs. 3S') only is accompanied by a comparably small change in $\Delta\Delta H_{\text{storage}}$ (1.9, 0.8, 0.4 mol⁻¹, respectively, for 1NH' vs. 3NH', 10' vs. 30', and 15' vs. 35'). These results suggest that it is possible to modulate ΔH^{\ddagger} without significantly compromising $\Delta H_{\text{storage}}$.²⁰

NBD frameworks containing two sets of through-bond donor-acceptor pairs (1, 2, and 3, X = NH, O, S) display even more pronounced spin delocalization and barrier lowering effects. Isomers with two non-cross-conjugated heteroarenes tethered to the double bonds of NBD, 1 (X = NH, O, S), have largely delocalized unpaired electrons at the TS structure. This is followed by isomers with a mixed conjugative pattern, 2 (X = NH, O, S). Isomers with two cross-conjugated heteroarenes tethered to the double bonds of NBD, 3 (X = NH, O, S), display the least delocalized unpaired electrons at the TS structure. Indeed, computed $|\delta_{avg}|$ values for the non-cross-conjugated: **1NH** (0.52), **10** (0.49), 1S (0.50), are smaller than those computed for isomers of the mixed set: 2NH (0.56), 2O (0.54), 2S (0.54), while values for the cross-conjugated isomers: 3NH (0.60), 3O (0.59), 3S (0.58) are the highest, indicating decreased delocalization of the unpaired electrons (Table 1). Notably, computed ΔH^{\ddagger} barriers for **1NH** (9.7 kcal mol⁻¹), **10** (7.1), **1S** (8.2) are lower than that computed for the mixed set: 2NH (11.0), 2O (10.9), 2S (12.7), while the crossconjugated isomers, 3NH (14.0), 3O (14.7), 3S (14.9), display the highest ΔH^{\ddagger} barriers. By comparing examples from the two extreme cases, 1 vs. 3, we note again that a meaningful increase in $\Delta\Delta H^{\ddagger}$ (4.3, 7.6, and 6.7 kcal mol⁻¹, respectively, for **1NH** ν s. 3NH, 10 vs. 3O, and 1S vs. 3S) only is accompanied by a small decrease in $\Delta \Delta H_{\text{storage}}$ (0.5, 2.1, 1.5 kcal mol⁻¹, respectively, for 1NH vs. 3NH, 10 vs. 3O, and 1S vs. 3S).

Computed activation enthalpies (ΔH^{\ddagger}) , storage enthalpies $(\Delta H_{\text{storage}})$, and $|\delta_{\text{avg}}|$ values for the 2-cyano-3-phenyl-NBD derivatives support that stabilizing the unpaired electrons at the para-positions of the phenyl group lower ΔH^{\ddagger} . Parasubstituted analogs enable more efficient delocalization from the NBD core to the phenyl ring, and therefore display consistently lower $|\delta_{avg}|$ values than the parent 9 (0.70) and the metasubstituted analogs: 4p (0.68) < 4m (0.70), 5p (0.67) < 5m(0.70), **6p** $(0.70) \approx$ **6m** (0.70), **7p** (0.69) < **7m** (0.70), and **8p** (0.68) < 8m (0.70). Accordingly, the computed ΔH^{\ddagger} barriers are lower for the para-isomers than for 9 (23.2 kcal mol⁻¹) and the metaisomers: 4p (22.4) < 4m (23.3), 5p (22.3) < 5m (23.2), 6p (23.0) <6m (23.4), 7p (22.3) < 7m (23.2), and 8p (22.2) < 8m (23.5).

Finally, an effective MOST system also must absorb within the solar spectrum (i.e., between 300 to 700 nm). However, strategies that red-shift the absorption of NBD often also red-shift that of QC, which compromises the efficiency of photoconversion. As shown in Table 1, all of the NBD derivatives have absorption maxima at regions above 300 nm, while those the QC derivatives absorb at regions near or below 300 nm. We note that the noncross-conjugated species are modestly red-shifted compared to their cross-conjugated analogs, but the variations are small (less than 20 nm). This suggests that the choice of incorporating noncross-conjugated vs. cross-conjugated motifs has a minor effect on the absorption wavelength of NBD-QC systems. Interestingly, computed UV spectra indicate that NBD species with non-crossconjugated motifs generally exhibit stronger absorption intensities (f_{max}) than those with cross-conjugated motifs. Similarly, within the 2-cyano-3-phenyl-NBD framework, para-substituted phenyl groups with π -donating or π -accepting substituents have higher absorption intensities compared to the meta-substituted

derivatives. Plots of λ_{max} vs. ΔH^{\ddagger} ($R^2 = 0.691$) show some correlation between the maximum absorption wavelengths of the NDB structure and the activation enthalpies. Additional correlation plots are included to the SI Fig. S5.

An excellent correlation was found between computed $|\delta_{avg}|$ values for the QC \rightarrow NBD TS structures vs. the thermal back reaction barriers (ΔH^{\ddagger}) for all investigated compounds $(R^2 =$ 0.977, see data in SI). Yet, what do these calculations tell us about how to design effective MOST NBD-QC systems? The substituted NBD-QC systems investigated here meet several MOST criteria: they absorb within the solar window, exhibit high energy densities, and have meaningfully storage energies. A few structural features were identified as likely to prolong the thermal half-life of the QC → NBD transformation, including heteroarenes with cross-conjugative relationships to the NBD double bond and meta substituted phenyl groups. These insights offer practical chemical handles for the design of NBD-QC-based MOST systems and may be extend to other MOST frameworks with thermal back reactions that proceed through transition states with pronounced diradicaloid character.

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Conflicts of interest

There are no conflicts to declare.

Data availability

The data supporting this article have been included as part of the supplementary information (SI). Supplementary information is available. See DOI: https://doi.org/10.1039/d5cc05209b.

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