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Not Antiaromaticity Gain, but Increased Asynchronicity Enhances the Diels-Alder Reactivity of Tropone

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1. Computational Details

All calculations in this study were performed utilizing the Amsterdam Modeling Suite (AMS2021.104).[1] The stationary points were attained using density functional theory at ZORA-BP86-D3(BJ)/TZ2P. This approach comprises the generalized gradient approximation (GGA) functional BP86[2] augmented by Grimme's D3 dispersion correction[3] using the damping function proposed by Becke and Johnson[4]. The TZ2P basis set is of triple ζ-quality augmented with polarization functions.[5] The zeroth-order regular approximation (ZORA) was used to account for scalar relativistic effects.[6] This level of theory has been proven to be accurate in computing relative trends in activation barriers and energies.[7] The accuracies of the fit scheme (Zlm fit)[8a] and the integration grid (Becke grid)[8b] were set to VERYGOOD. Vibrational analyses[9] were conducted on the stationary points to assess the nature of all structures: for equilibrium geometries no imaginary frequencies were found, whereas transition states contain one imaginary frequency. The potential energy surfaces of the studied Diels-Alder reactions were computed using the intrinsic reaction coordinate (IRC) method,[10] and further analyzed by the PyFrag 2019 program[11] by means of the activation strain and energy decomposition analyses at ZORA-ωB97X-D/TZ2P[12] level of theory on the geometries optimized by ZORA-BP86-D3(BJ)/TZ2P. All structures were visualized using CYLview.[13]

Voronoi Deformation Density Analysis

Atomic charges were computed using the Voronoi deformation density (VDD)[14] method. The VDD atomic charge on atom *A* (Q_A^{VDD}) is computed as given in Equation S1.

$$Q_{\mathrm{A}}^{\mathrm{VDD}} = -\int_{\text{Voronoi cell of A}} \left[\rho(\boldsymbol{r}) - \sum\nolimits_{B} \rho_{\mathrm{B}}(\boldsymbol{r})\right] d\boldsymbol{r} \tag{S1}$$

Herein, the (numerical) integral is taken of the deformation density in the volume of the Voronoi cell of atom *A*. The deformation density is the density change from a superposition of atomic densities $\sum_B \rho_B(\mathbf{r})$ of a fictitious promolecule (that is associated with the ground-state atomic densities) to the density in the final molecular system $\rho(\mathbf{r})$. The Voronoi cell of atom *A* is defined as the space bounded by the bond midplanes on and perpendicular to all bond axes between nucleus *A* and its neighboring nuclei.

Activation Strain Model and Energy Decomposition Analysis

Quantitative analyses of the potential energy surfaces associated with the studied reactions were obtained by applying the activation strain model (ASM) of chemical reactivity.[15] The ASM is a fragment-based approach built upon the concept that the energy of a reacting system (*i.e.* the potential energy surface) can be described with respect to, and understood in terms of the characteristics of the original reactants. It considers the rigidity of the original reactants, the extent of their deformation during the reaction, and their capability to interact. In this model, the potential energy surface $\Delta E(\zeta)$ is decomposed into the total strain energy, $\Delta E_{\mathrm{strain}}(\zeta)$, and interaction energy, $\Delta E_{\mathrm{int}}(\zeta)$ in which these values are projected onto a reaction coordinate ζ that is critically involved in the transformation:

$$\Delta E(\zeta) = \Delta E_{\mathrm{strain}}(\zeta) + \Delta E_{\mathrm{int}}(\zeta) \tag{S2}$$

In this equation, the total strain energy, $\Delta E_{\mathrm{strain}}(\zeta)$, is associated with the rigidity and structural deformation of the reactants from their equilibrium structure to the geometry they adopt at the reaction coordinate ζ. On the other hand, the interaction energy, $\Delta E_{\mathrm{int}}(\zeta)$, is related to the electronic structure and spatial orientation of the reactants.

It accounts for all mutual chemical interactions between the deformed reactants. The total strain energy can be further decomposed into the strain energies corresponding to the deformation of maleimide $\Delta E_{\text{strain,}\mathbf{M}}(\zeta)$ and the deformation of the diene $\Delta E_{\text{strain,diene}}(\zeta)$:

$$\Delta E_{\text{strain}}(\zeta) = \Delta E_{\text{strain,}\mathbf{M}}(\zeta) + \Delta E_{\text{strain,diene}}(\zeta) \tag{S3}$$

To obtain more insights into the physical mechanism behind $\Delta E_{\text{int}}(\zeta)$, we utilized our canonical energy decomposition analysis (EDA).[16] In the EDA, the $\Delta E_{\text{int}}(\zeta)$ is decomposed, within the framework of Kohn-Sham DFT, into four physically meaningful energy terms:

$$\Delta E_{\text{int}}(\zeta) = \Delta V_{\text{elstat}}(\zeta) + \Delta E_{\text{Pauli}}(\zeta) + \Delta E_{\text{oi}}(\zeta) + \Delta E_{\text{disp}}(\zeta) \tag{S4}$$

Herein, the electrostatic interaction, $\Delta V_{\text{elstat}}(\zeta)$, corresponds to classical electrostatic interaction between the unperturbed charge distributions of the deformed reactants and is usually attractive. The Pauli repulsion, $\Delta E_{\text{Pauli}}(\zeta)$, compromises for the destabilizing interaction between occupied closed-shell orbitals of both deformed reactants due to the Pauli principle. The orbital interaction, $\Delta E_{\text{oi}}(\zeta)$, accounts for polarization and charge transfer between the fragments. The dispersion term ΔE_{disp} corresponds to the dispersion corrections as introduced by Grimme *et al*.[3]

2. Electronic and Gibbs free reaction barriers and C···C distances for the Diels-Alder reactions

Table S1 Electronic ($\Delta E^{\ddagger}$) and Gibbs free reaction barriers ($\Delta G^{\ddagger}$) (in kcal mol^{-1}) and C···C distances (in Å) for the Diels-Alder reactions between **M** and **1**, **2-prot**, **3-prot**, **2**, and **3**.[a]

diene	$\Delta G^{\ddagger}$(TS1)[a]	$\Delta E^{\ddagger}$(TS1)[a]	r(C···C$_{\alpha}$)[a]	r(C···C$_{\alpha'}$)[a]	$\Delta G^{\ddagger}$(TS1)[b]	r(C···C$_{\alpha}$)[b]	r(C···C$_{\alpha'}$)[
1	38.3	24.3	2.16	2.32	30.2	2.18	2.31
2-prot	39.6	25.1	2.23	2.25	30.7	2.20	2.29
3-prot	44.6	28.7	2.23	2.24	31.9	2.21	2.27
2	9.8	–4.8	3.22	2.00	3.0	3.25	2.17
3	23.9	9.4	3.01	1.97	16.2	3.04	2.01

[a] Computed at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P. [b] Data taken from previous work of Karas *et al.*, computed at ωB97X-D/6-311+G(d,p).[17]

3. Transition state structures

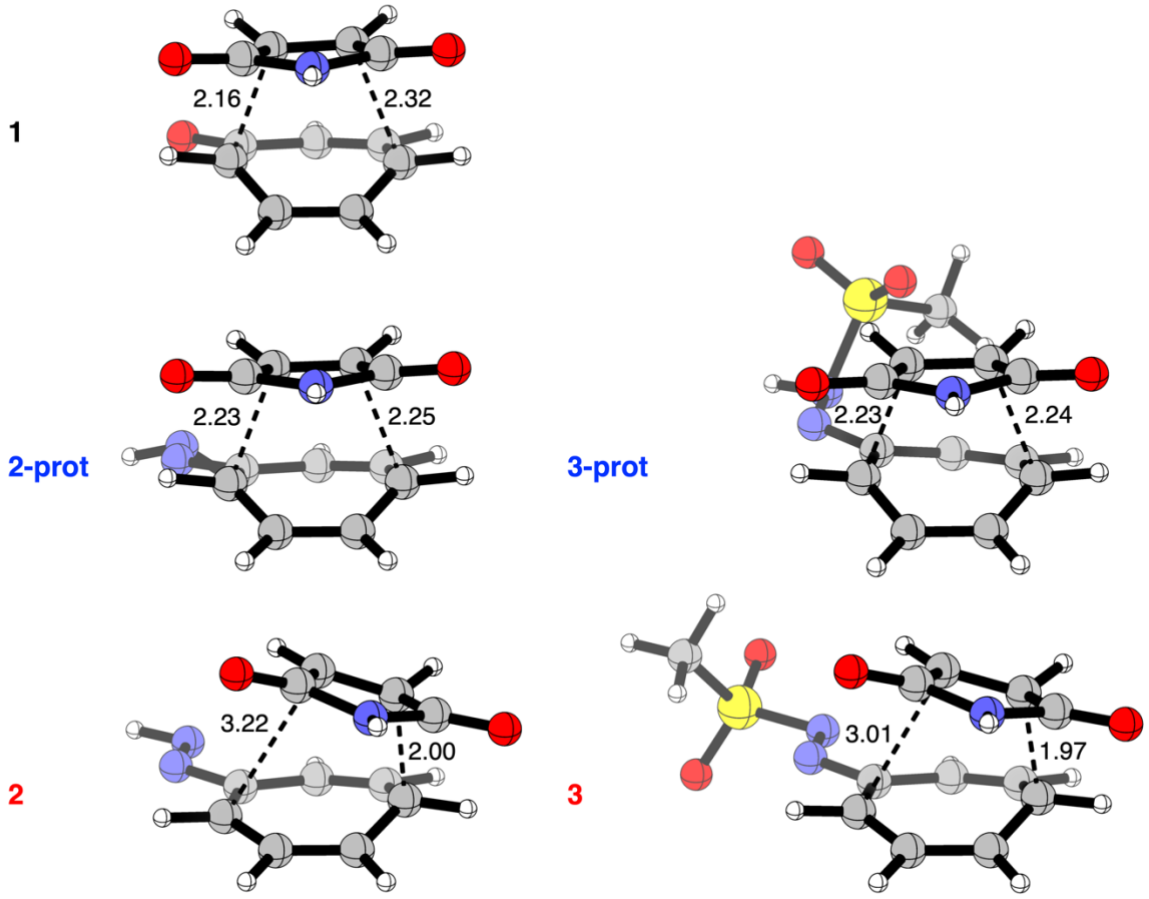


Fig. S1 Transition state structures (TS1) with key structural information (in Å) for the Diels-Alder reactions between **M** and **1**, **2-prot**, **3-prot**, **2**, and **3**, computed at ZORA-BP86-D3(BJ)/TZ2P.

4. Activation strain analyses and energy decomposition analyses along the IRC

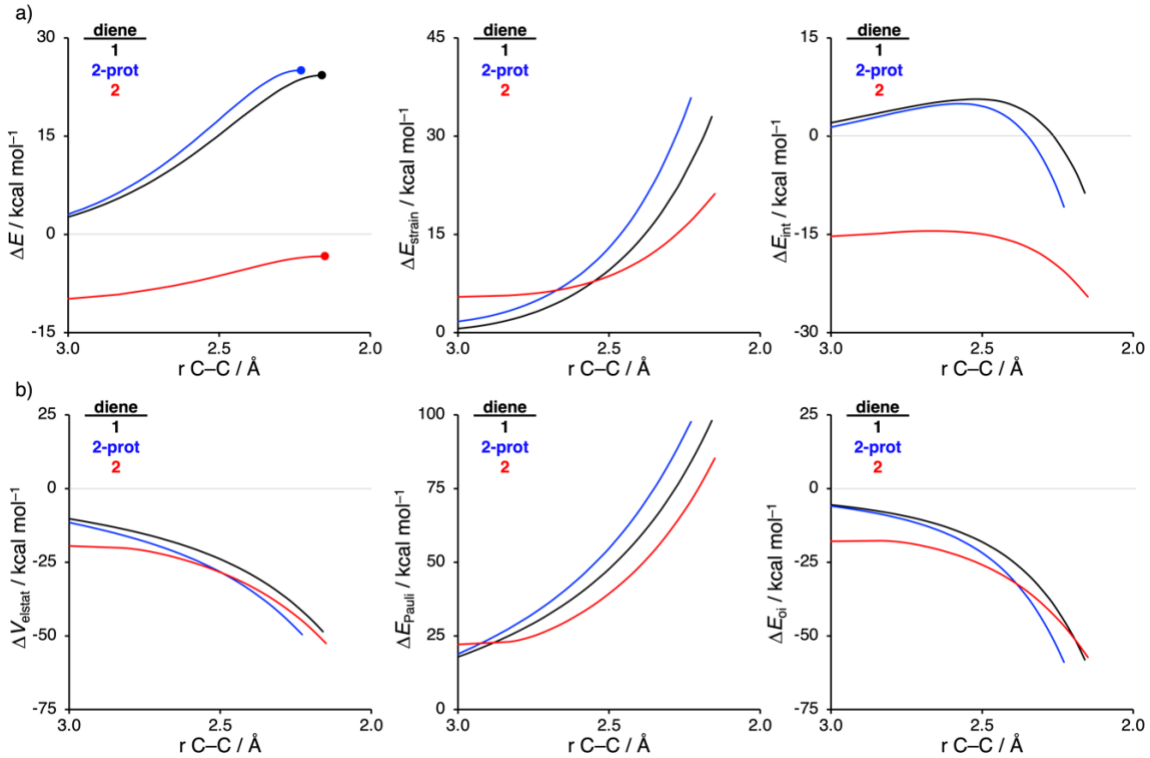


Fig. S2 (a) Activation strain analyses and (b) energy decomposition analyses of the Diels-Alder reactions between **M** and diene **1**, **2**, and **2-prot**, where the reaction barriers are indicated with a dot and the energy terms along the IRC are projected on the shorter of the two newly forming C–C bonds between **M** and the diene, Computed at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P.

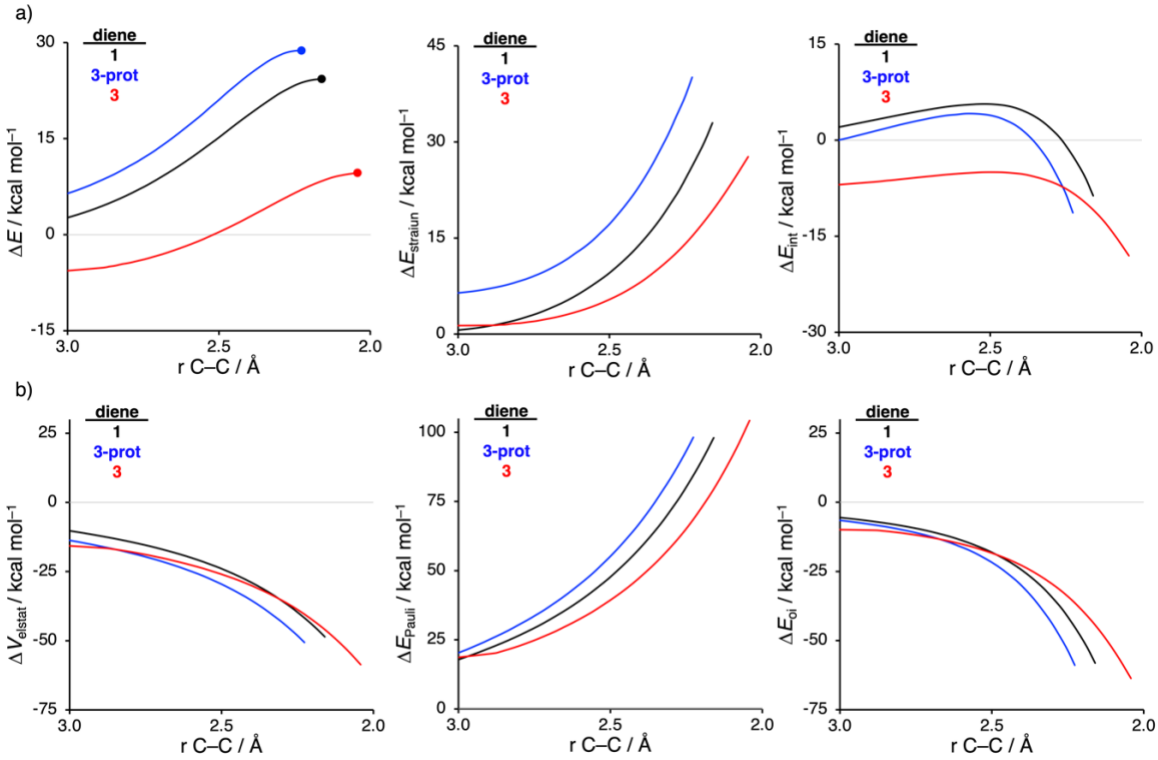
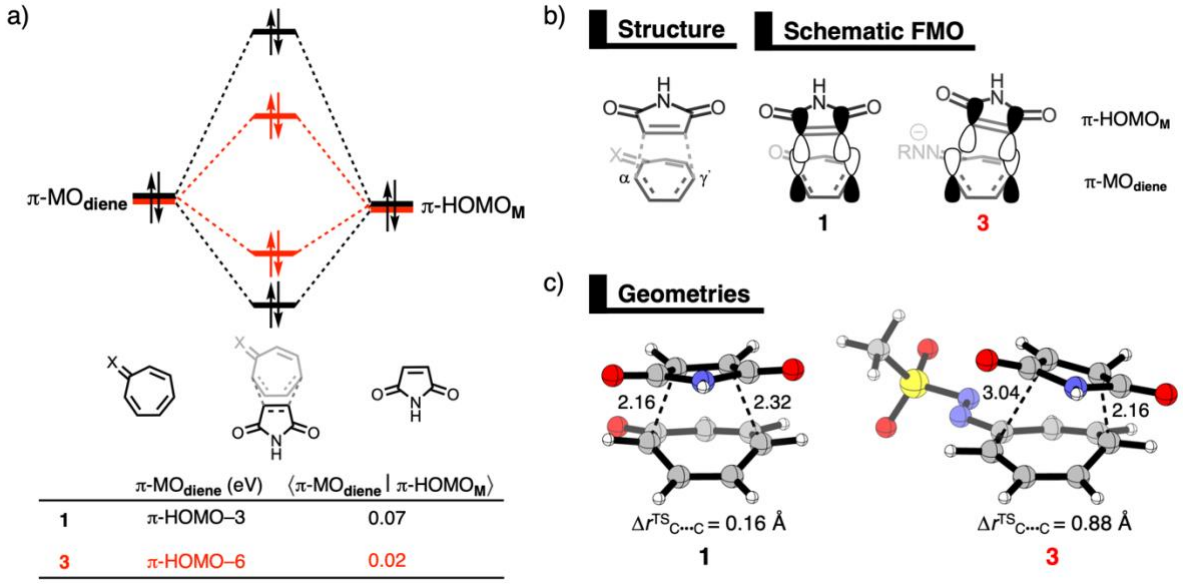


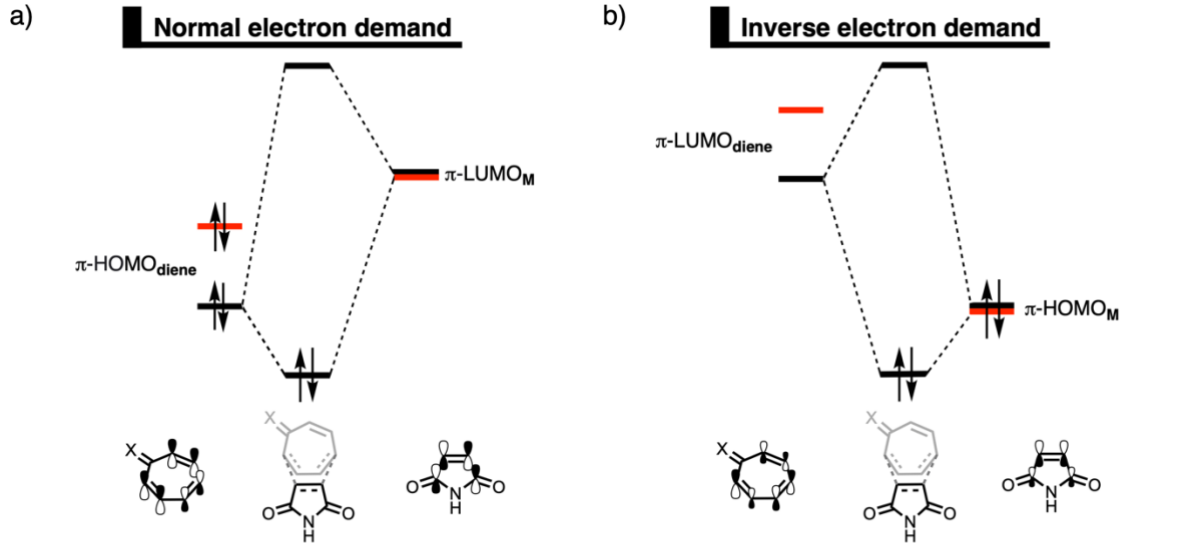
Fig. S3 (a) Activation strain analyses and (b) energy decomposition analyses of the Diels-Alder reactions between **M** and diene **1**, **3**, and **3-prot**, where the reaction barriers are indicated with a dot and the energy terms along the IRC are projected on the shorter of the two newly forming C–C bonds between **M** and the diene. Computed at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P.

5. Molecular orbital diagrams explaining the Pauli repulsion and orbital interaction



	π-MO$_{diene}$ (eV)	⟨π-MO$_{diene}$ | π-HOMO$_M$⟩
1	π-HOMO–3	0.07
3	π-HOMO–6	0.02

Fig. S4 (a) Molecular orbital diagram with the most significant occupied orbital overlaps; (b) key occupied orbitals (isovalue = 0.03 au); and (c) the structures with key structural information (in Å) of the Diels-Alder reactions between **M** and diene **1** and **3**, computed at consistent TS-like geometries ($C_M\cdots C_{diene}$ = 2.160 Å) at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P.



	ε π-HOMO$_{diene}$ (eV)	⟨π-HOMO$_{diene}$ | π-LUMO$_M$⟩
1	–8.3	0.15
3	–2.4	0.08

	ε π-LUMO$_{diene}$ (eV)	⟨π-LUMO$_{diene}$ | π-HOMO$_M$⟩
1	–1.2	0.13
3	3.0	0.06

Fig. S5 Kohn-Sham molecular orbital diagrams with orbital energy levels and overlaps for (a) the normal electron demand π-HOMO$_{diene}$–π-LUMO$_M$; and (b) the inverse electron demand π-LUMO$_{diene}$–π-HOMO$_M$ of the Diels-Alder reactions between **M** and diene **1** and **3**, computed at consistent TS-like geometries ($C_M\cdots C_{diene}$ = 2.160 Å) at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P.

6. Orbital interaction terms

Table S2 Orbital interaction ΔE_{oi} (in kcal mol^{-1}) computed for the Diels-Alder reactions of **1**, **2** and **3** with **M** without and with virtual orbital deletion. [a]

diene	ΔE_{oi} all virtuals	ΔE_{oi} no virtuals on the **diene** (NED)	ΔE_{oi} no virtuals on **M** (IED)
1	–58.1	–29.3	–23.0
2	–55.9	–42.6	–8.4
3	–44.4	–31.5	–9.4

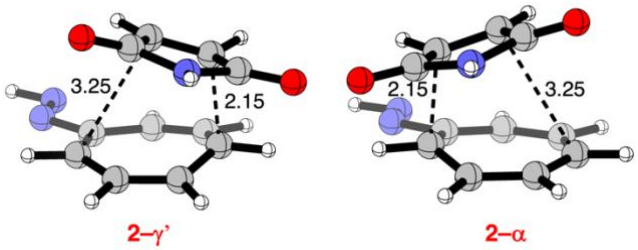
[a] Computed on consistent TS-like geometries with a $C_{\mathbf{M}}\cdots C_{\mathbf{diene}}$ bond length of 2.160 Å, at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P.

7. Understanding the asynchronicity difference

During the Diels-Alder (DA) reaction between **1** and **M**, the C···C_α bond is formed ahead of the C···$C_{\gamma'}$ bond (Fig. S1). The DA reaction of **2**, on the other hand, follows an opposite order of bond formation, namely the C···$C_{\gamma'}$ bond is formed ahead of the C···C_α bond. In addition, the degree of asynchronicity, that is, the difference in bond length of the newly formed C···C bonds, is higher for the DA reaction of **2** compared to **1**. Following a more asynchronous reaction mode relieves destabilizing Pauli repulsion, despite the loss of favorable orbital and electrostatic interactions as explained in the work of Ref. [18].

In this section, we study the difference in the order of C···C bond formations. Therefore, we compare the TS structure of the DA reaction of **2** (**2–γ'**) with an artificially constrained structure in which the C···C_α bond is shorter than the C···$C_{\gamma'}$ bond (**2–α**). To acquire this structure, a geometry optimization was performed while artificially constraining the C···C_α bond length to resemble the C···$C_{\gamma'}$ bond length in the **2–γ'** structure, and *vice versa*. In addition, the CCNN dihedral angle was constrained to gain a structure comparable to the TS **2–γ'** structure but with opposite C···C bond lengths. (See molecular structures in Table S3.) The energy of **2–γ'** is –3.3 kcal mol^{-1} and the energy increases to 7.7 kcal mol^{-1} when the formation of the C···C_α bond would be ahead of C···$C_{\gamma'}$ bond formation (**2–α**). The strength and nature of the interaction between **2** and **M** in both, **2–γ'** and **2–α**, was further analyzed by applying the activation strain model (ASM)[15] of reactivity with a matching canonical energy decomposition analysis (EDA).[16] Table S3 shows that the increase of energy from –3.3 kcal mol^{-1} to 7.7 kcal mol^{-1} arises from a more destabilizing strain energy ($\Delta\Delta E_{strain}$ = 4.5 kcal mol^{-1}) and a less stabilizing interaction energy ($\Delta\Delta E_{int}$ = 6.5 kcal mol^{-1}). The strain energy emerges from pyramidalization of the carbon atoms of **2**, which is required to form the two C···C bonds with **M**. Pyramidalization of the α-carbon requires more energy than pyramidalization of the γ'-carbon and therefore the strain energy is more destabilizing for **2–α** than for **2–γ'**. An EDA[16] was performed to find out that the less stabilizing interaction energy of **2–α** arises from less stabilizing electrostatic ($\Delta\Delta V_{elstat}$ = 7.1 kcal mol^{-1}) and orbital interactions ($\Delta\Delta E_{oi}$ = 8.3 kcal mol^{-1}), see Table S3.

Table S3 Energy decomposition analysis terms (in kcal mol^{-1}) computed on the Diels-Alder TS structure **2–γ'** and its artificially constrained analog **2–α**.[a]



structure	ΔE	ΔE_{strain}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	$\Delta E_{strain,\ 2}$	$\Delta E_{strain,\ M}$
2–γ'	–3.3	21.2	–24.5	–52.5	85.3	–57.3	9.4	11.8
2–α	7.7	25.7	–18.0	–45.4	76.4	–49.0	14.7	11.0

[a] Computed at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P.

Now, we look into the orbital interactions by studying the normal electron demand (NED) and inverse electron demand (IED) interactions between **2** and **M** in the **2–α** and **2–γ'** molecular structures. A weakening of

NED interactions from –43.6 kcal mol^{-1} in **2–γ'** to –31.7 kcal mol^{-1} in **2–α** leads to the less stabilizing orbital interactions in **2–α** (Table S4). The weakening of the NED interactions is primarily caused by a reduction in orbital overlap between the HOMO of **2** and the LUMO of **M**, going from 0.09 in **2–γ'** to 0.05 in **2–α** (Fig. S6). The amplitude of the HOMO of **2** is smaller at the α-carbon than at the γ'-carbon and therefore the HOMO has less orbital overlap with the LUMO of **M** when **2** is orientated closer to the α-carbon than the γ'-carbon as in **2–α** (Fig. S7a). However, this is not observed for tropone (**1**) because the HOMO of **1** is differently shaped than the HOMOs of **2** and **3** (Fig. S7b). Therefore, the NED interactions, and thus the total orbital interactions, are not weaker when the C···C_α bond formation is ahead of the C···$C_{\gamma'}$ formation in the DA reaction of **1**.

Table S4 Orbital interaction ΔE_{oi} (in kcal mol^{-1}) computed for the Diels-Alder TS structure **2–γ'** and its artificially constrained analog **2–α** without and with virtual orbital deletion.[a]

structure	ΔE_{oi}	NED (no virtuals on **2**)	IED (no virtuals on **M**)
2–γ'	–57.3	–43.6	–8.7
2–α	–49.0	–31.7	–9.3

[a] Computed at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P.

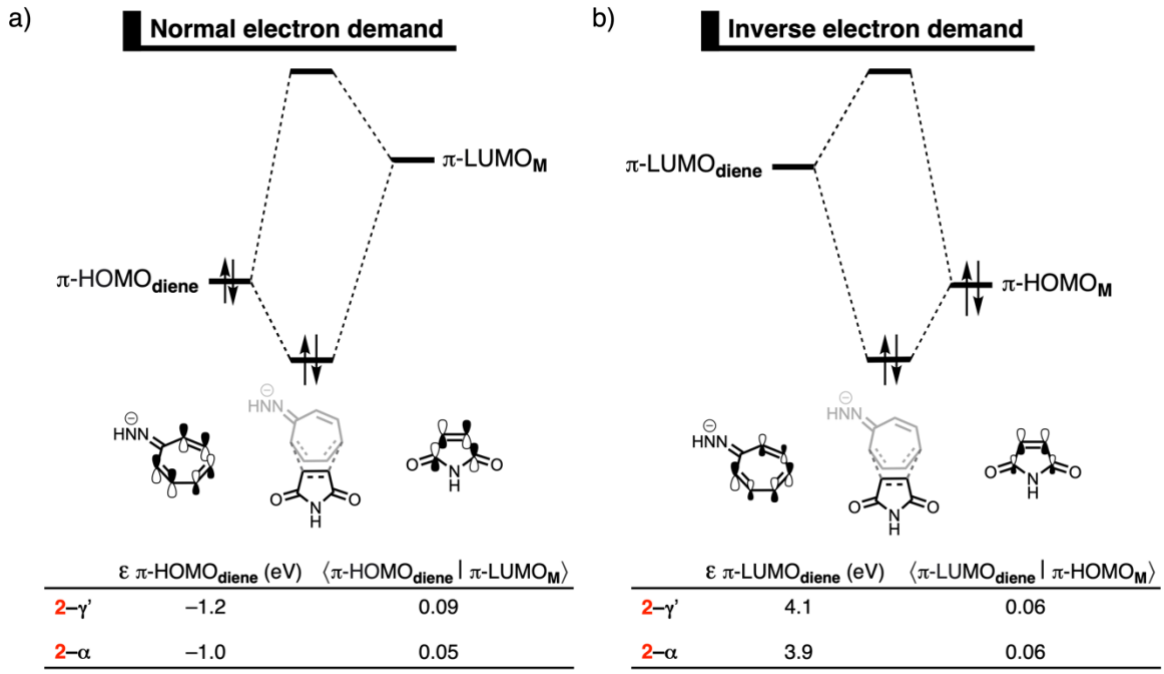


Fig. S6 Molecular orbital diagrams with orbital energy levels and overlaps for (a) the normal electron demand π-HOMO$_{diene}$–π-LUMO$_M$; and (b) the inverse electron demand π-LUMO$_{diene}$–π-HOMO$_M$ of **2–γ'**and **2–α** computed at ZORA-ωB97X-D/TZ2P//ZORA-BP86-D3(BJ)/TZ2P.

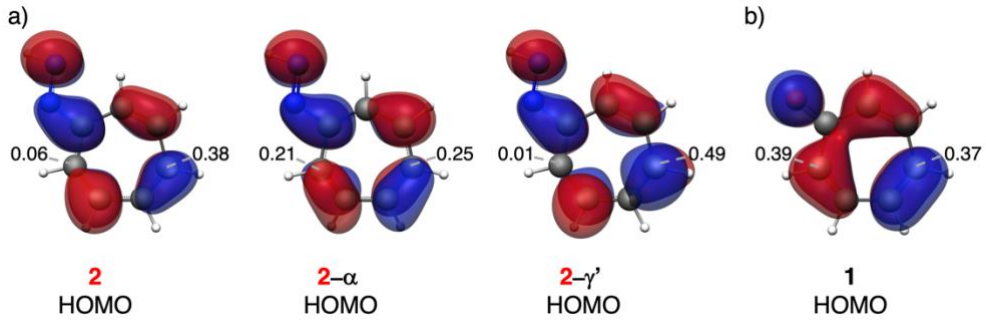


Fig. S7 The highest occupied molecular orbitals (HOMOs) of (a) **2** in its optimized geometry, in **2**–α and in **2**–γ'; and of (b) **1** with the $2p_z$ AO coefficients of the reactive carbon atoms.

The Voronoi deformation density (VDD)[14] charges of **2** were computed to understand the less stabilizing electrostatic interaction term of **2**–α compared to **2**–γ' (Fig. S8). The α-carbon of **2** is less negatively charged than the γ'-carbon, and thereby **2**–α will have less favorable electrostatic interactions than **2**–γ'. Besides that, we computed the VDD charges of **1** and observed that the α-carbon of **1** is slightly more negatively charged than the γ'-carbon atom. Hence, the electrostatic interactions would not be favored when forming the C···$C_{\gamma'}$ bond between **1** and **M** first.

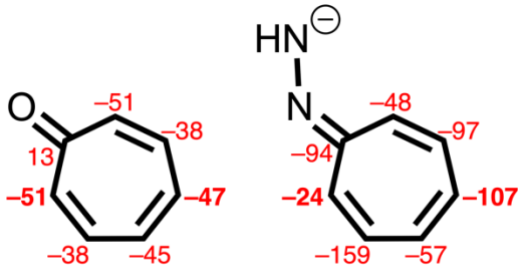


Fig. S8 The VDD charges (in milli-electrons) of the α and γ' carbon atoms of **1** and **2**.

8. Cartesian coordinates

Table S5. Cartesian coordinates (in Å), ADF total energies (in kcal mol^{-1}), and number of imaginary frequencies (NIMAG) of all stationary points, computed at ZORA-BP86-D3(BJ)/TZ2P when not otherwise stated.

maleimide (M)

E = -1568.04
H = -1522.60
G = -1545.12
E*(ZORA-ωB97X-D)* = -2434.43
N_{imag} = 0

O	-2.17459810	-2.30679541	0.19519550
O	-2.19714183	2.28142667	-0.24624280
N	-2.43467922	0.01340452	0.25833758
H	-3.09912891	0.08360492	1.02197780
C	-1.92528478	1.11267261	-0.44293083
C	-0.99075170	0.52710395	-1.46573253
H	-0.44360385	1.15495888	-2.16306311
C	-1.91408819	-1.19438515	-0.22105851
C	-0.98437422	-0.80547007	-1.33768370
H	-0.43062121	-1.54941191	-1.90315538

Tropone (1)

E = -2070.58
H = -1999.60
G = -2022.45
E*(ZORA-ωB97X-D)* = -3095.76
N_{imag} = 0

O	1.23769148	0.04409980	0.15264949
C	-0.00272472	-0.00012329	0.10316866
C	-0.76406577	1.25615180	0.07396343
C	-2.10679145	1.48991896	0.02755490
C	-0.67266779	-1.30742501	0.07448421
C	-3.19948296	0.57003702	-0.00976705
C	-1.99532162	-1.63623532	0.02776562
C	-3.15071050	-0.79648756	-0.00971553
H	-4.10827513	-1.31924415	-0.04291396
H	-0.10335453	2.12572047	0.09644858
H	-2.40024345	2.54251808	0.01698991
H	-4.19185208	1.02324192	-0.04295170
H	-2.21311151	-2.70705182	0.01737763
H	0.04829556	-2.12772772	0.09730829

Tropone hydrazone(2-prot)

E = -2443.32
H = -2353.25
G = -2379.10
E*(ZORA-ωB97X-D)* = -3667.90
N_{imag} = 0

N	-2.05298706	-0.69547738	0.06090583
C	-0.80187921	-0.33425537	-0.09762939
C	-0.38852224	1.05769314	-0.28886964
C	0.13953347	-1.43502334	-0.18983109
C	0.83923164	1.62104048	-0.15190063
H	-1.18883848	1.72446811	-0.62016574
C	1.49261767	-1.43301087	-0.04714497
H	-0.34999898	-2.39770391	-0.35474709
C	2.09136809	1.00299280	0.20617899
H	0.89629954	2.69531291	-0.34515308
C	2.37320448	-0.32882382	0.23359056
H	1.98047923	-2.40708620	-0.11519431

H	2.91387449	1.68922609	0.41532183
H	3.40435570	-0.60451823	0.46508458
N	-3.00291846	0.30146515	0.12321920
H	-3.86014507	-0.08379122	0.51108002
H	-2.72103480	1.14850966	0.62848193

Methylsulfonyl tropone hydrazone (3-prot)

E = -3205.32
H = -3089.47
G = -3123.30
E*(ZORA-ωB97X-D)* = -4931.21
N_{imag} = 0

N	0.10306836	-0.68334825	0.03584276
C	-1.04541440	-0.17711904	-0.34555907
C	-2.13883080	-1.13215787	-0.35874140
C	-1.20312501	1.19792112	-0.81461801
C	-3.48057037	-0.91844853	-0.42708249
H	-1.79790860	-2.16370688	-0.24850134
C	-2.33484928	1.93446681	-0.97189421
H	-0.27387079	1.69393382	-1.10373050
C	-4.20256112	0.32088883	-0.51793017
H	-4.10460451	-1.81208123	-0.36995718
C	-3.70646448	1.56981791	-0.74258876
H	-2.18678783	2.95665307	-1.32813603
H	-5.28685446	0.23549929	-0.42312787
H	-4.42811121	2.38520965	-0.81213381
N	1.19609110	0.15513160	0.06053566
S	2.49248495	-0.42415509	1.02163951
O	2.03484687	-1.00586166	2.26888423
O	3.42841488	0.68813142	1.01553077
C	3.07565400	-1.74562777	-0.02605747
H	3.87633557	-2.24666679	0.52685839
H	2.23410375	-2.42485798	-0.19439361
H	3.44232209	-1.31535428	-0.96155352
H	1.04450830	1.14317986	0.30981215

Tropone hydrazone anion (2)

E = -2371.58
H = -2291.09
G = -2316.99
E*(ZORA-ωB97X-D)* = -3550.88
N_{imag} = 0

N	-2.18141082	0.58368006	0.03663895
C	-0.85600031	0.28785010	0.02071181
C	-0.39984820	-1.11849818	0.01849952
C	0.01406563	1.40071497	0.00714760
C	0.85159286	-1.62966606	0.00368487
H	-1.24130542	-1.81583838	0.03123954
C	1.39757981	1.49489894	-0.01073479
H	-0.53926606	2.34752991	0.01203822
C	2.14408927	-0.93105597	-0.01499219
H	0.92791717	-2.72333390	0.00565847
C	2.35331950	0.41580411	-0.02074912
H	1.81900242	2.50242743	-0.01834599
H	3.02901249	-1.57336047	-0.02512711
H	3.40310074	0.73279317	-0.03519831
N	-3.03198629	-0.42462023	0.04947918
H	-3.95840780	0.03239152	0.06005636

Methylsulfonyl tropone hydrazone anion (3)

E = -3158.12

H = -3051.19
G = -3085.18
E*(ZORA-ωB97X-D)* = -4840.53
N_{imag} = 0

N	0.23816745	-0.60682991	0.00009882
C	-1.05522023	-0.28138551	0.00011706
C	-1.95386552	-1.39868929	0.00011262
C	-1.49509093	1.12043629	0.00022799
C	-3.32335014	-1.45912841	0.00000460
H	-1.41486356	-2.35091524	0.00018434
C	-2.74300942	1.64742262	0.00012680
H	-0.65296693	1.81578678	0.00043218
C	-4.27195876	-0.36834933	-0.00018283
H	-3.76265914	-2.45889977	0.00001168
C	-4.03483158	0.97062494	-0.00014845
H	-2.80359198	2.74040097	0.00027734
H	-5.32391146	-0.67123548	-0.00037317
H	-4.90854973	1.62752279	-0.00030993
N	1.11169712	0.40723289	0.00016275
S	2.67206437	-0.15011819	0.00009336
O	3.07785194	-0.81948817	-1.24825058
O	3.07787512	-0.81974395	1.24829243
C	3.46390951	1.47104766	0.00024832
H	4.54216162	1.27903623	0.00015698
H	3.16183112	2.01200567	-0.90111156
H	3.16194415	2.01178240	0.90178024

RC: 1-M
E = -3646.20
H = -3528.55
G = -3563.36
E*(ZORA-ωB97X-D)* = -5530.85
N_{imag} = 0

O	2.62047555	-0.70191678	-1.81595230
C	2.26407391	-0.34253746	-0.68099746
C	1.76119056	-1.34275780	0.26627807
C	2.37780646	1.06952928	-0.30531506
C	0.97538320	-1.18461671	1.37136458
H	1.99809063	-2.36231982	-0.04499096
C	1.70334869	1.77034727	0.65097270
H	3.02840598	1.62673944	-0.98291085
C	0.47599149	0.01252939	1.96460754
H	0.64855705	-2.10772897	1.85484999
C	0.78293731	1.30675562	1.63979396
H	1.87353960	2.84953011	0.65907223
H	-0.22028512	-0.12878998	2.79257301
H	0.29662302	2.08536184	2.22887150
C	-2.09387487	0.84870665	-0.08786998
C	-1.09759454	0.72091720	-1.20248225
H	-0.64988645	1.59049229	-1.67303448
C	-1.73239876	-1.39878544	-0.52596537
C	-0.88634356	-0.57741281	-1.45671778
H	-0.21808963	-1.03302747	-2.18154672
O	-1.81726990	-2.60910354	-0.43931965
O	-2.53522085	1.85836429	0.42939515
N	-2.42504605	-0.46700304	0.25833130
H	-3.09517373	-0.71518955	0.97816683

RC: 2prot-M
E = -4019.01
H = -3882.78

G = -3919.21
E*(ZORA-ωB97X-D)* = -6101.97
N_{imag} = 0

N	3.24920983	-0.79585594	-0.89528200
C	2.24524086	-0.38604798	-0.15192088
C	1.27465800	-1.42036473	0.14433404
C	2.07583547	1.00420528	0.27053129
C	0.24920547	-1.43875363	1.04218664
H	1.44760644	-2.33136886	-0.43260454
C	1.20993733	1.54064654	1.16846331
H	2.71131281	1.72131160	-0.25352658
C	-0.20455848	-0.40035213	1.92322462
H	-0.30903977	-2.37395021	1.10062482
C	0.20216983	0.89947303	1.97526498
H	1.27019431	2.62430283	1.29563282
H	-1.01003414	-0.68371607	2.60307270
H	-0.31142830	1.54755705	2.68648567
C	-2.66221837	0.67012295	0.04936254
C	-1.50432322	1.13778061	-0.77707392
H	-1.14128526	2.15886254	-0.72491895
C	-1.89014207	-1.09654202	-1.24262274
C	-1.05012416	0.11573691	-1.51772662
H	-0.22634975	0.09099782	-2.22393349
O	-1.82956036	-2.20253227	-1.74773740
O	-3.35237435	1.30251116	0.82925804
N	-2.81073347	-0.68684011	-0.26778769
H	-3.55636558	-1.27439486	0.08949894
N	4.21430171	0.11870850	-1.24002248
H	5.03605892	-0.37453894	-1.57883891
H	4.46467630	0.80334491	-0.51892920

RC: 3prot–M
E = -4781.45
H = -4618.60
G = -4663.93
E*(ZORA-ωB97X-D)* = -7363.01
N_{imag} = 0

N	1.61585521	0.84165423	1.56431043
C	0.64864747	1.33947694	0.82382888
C	-0.57866835	1.57656653	1.56184771
C	0.80679903	1.74140259	-0.56179409
C	-1.83116029	1.85497657	1.10425654
H	-0.44912400	1.47049349	2.64083271
C	-0.13513832	2.01304533	-1.50251421
H	1.85046312	1.84478055	-0.86140118
C	-2.30314798	1.96504769	-0.24363401
H	-2.59910660	1.95336074	1.87310935
C	-1.56568134	2.00117517	-1.39075042
H	0.24331223	2.27854179	-2.49256229
H	-3.38561863	2.03978930	-0.35659177
H	-2.11495167	2.09207009	-2.32847203
C	-2.86526412	-1.12038883	-1.10641475
C	-1.41574853	-1.31058358	-0.77899762
H	-0.64076600	-1.33479012	-1.53723271
C	-2.62654736	-1.31538045	1.19221270
C	-1.27646954	-1.42454403	0.54908720
H	-0.36349229	-1.56091532	1.11916117
O	-2.92193794	-1.37029668	2.37195119
O	-3.39515460	-0.98518436	-2.19516941
N	-3.52346547	-1.12226154	0.13110631
H	-4.52939093	-1.05410712	0.24159461

N	2.85105120	0.60698096	0.92712108
H	3.51560072	0.37994370	1.67206488
S	3.01149784	-0.75578754	-0.14715330
O	1.68853597	-1.26719502	-0.46324732
O	4.04860746	-1.59636644	0.43083675
C	3.70245332	-0.04311102	-1.63945171
H	3.94869352	-0.89401170	-2.28394145
H	2.95708633	0.59580570	-2.11893384
H	4.60545154	0.51356336	-1.37409637

RC: 2-M

E = -3967.00
H = -3839.41
G = -3876.68
E*(ZORA-ωB97X-D)* = -5995.35
N_{imag} = 0

N	3.53560262	-1.10433522	-0.12923601
C	2.47215082	-0.29477513	0.19964942
C	1.48048998	-0.92723092	0.96367852
C	2.41496736	1.08909899	-0.26801047
C	0.28513199	-0.44805823	1.49560470
H	1.70967617	-1.98008225	1.15533040
C	1.46765969	2.03453309	-0.05270916
H	3.27582428	1.35559165	-0.88488908
C	-0.22239835	0.88529367	1.44276297
H	-0.29973122	-1.15859187	2.07809754
C	0.24430520	1.95244728	0.72769542
H	1.63761188	3.00456430	-0.52987316
H	-1.15643893	1.04775157	1.98522015
H	-0.35044965	2.86635282	0.77112600
C	-2.64878847	0.77425888	-0.57208774
C	-1.42726390	0.38481917	-1.28806710
H	-0.88463653	1.07026846	-1.92944653
C	-2.13747081	-1.45015342	-0.06493607
C	-1.11684997	-0.91197283	-0.97996757
H	-0.28440286	-1.50785582	-1.33686751
O	-2.31394622	-2.59195190	0.37175244
O	-3.30914583	1.81879400	-0.60383292
N	-2.98453980	-0.35491430	0.20543205
H	-3.86704131	-0.44674069	0.69478352
N	4.48603030	-0.56405063	-0.83461530
H	5.16961951	-1.32723569	-0.97182251

RC: 3-M

E = -4747.32
H = -4594.17
G = -4637.48
E*(ZORA-ωB97X-D)* = -7280.86
N_{imag} = 0

N	-1.92308993	-0.11496960	0.51986287
C	-0.68981846	-0.65299524	0.59603550
C	0.21372584	0.07448404	1.41815059
C	-0.34917687	-1.86946890	-0.13753001
C	1.53721941	-0.15225736	1.73217511
H	-0.24867231	0.96115303	1.86025065
C	0.83342037	-2.52765878	-0.22004752
H	-1.19605625	-2.27203233	-0.69654822
C	2.38469327	-1.22134367	1.29454234
H	1.99763536	0.56844542	2.40783297
C	2.10280655	-2.22232497	0.41113700
H	0.84363479	-3.41898860	-0.85316327

H	3.40670085	-1.19238878	1.67791727
H	2.92179988	-2.90247220	0.17037300
N	-2.78987858	-0.72873396	-0.26782221
S	-4.28424230	0.03025443	-0.19600394
O	-4.90449999	-0.06877725	1.12862178
O	-5.03610226	-0.46150007	-1.35001952
C	-3.93665402	1.78441889	-0.46649685
H	-4.89221600	2.31063134	-0.37572044
H	-3.22690396	2.10496517	0.30183691
H	-3.51333771	1.90370138	-1.46846793
C	4.14455028	0.10575129	-0.94618109
C	2.75174085	0.14093482	-1.44282476
H	2.36521661	-0.59647147	-2.13756139
C	3.03467463	1.91873320	0.01246208
C	2.10139780	1.19087437	-0.87829695
H	1.07225662	1.50309355	-1.01773777
O	2.88772437	2.96883309	0.63362555
O	5.07875703	-0.63568134	-1.24709662
N	4.22448895	1.16605431	-0.02454542
H	5.09273818	1.47498216	0.39691827

TS: 1-M

E = -3632.67
H = -3515.22
G = -3547.57
E*(ZORA-ωB97X-D)* = -5505.89
N_{imag} = 1, -356.903i cm^{-1}

O	-3.15808322	1.37839223	-0.45595779
C	-2.32681426	0.52792576	-0.12172430
C	-1.12648039	0.97297175	0.65274531
C	-2.49090263	-0.87425705	-0.49460326
C	-0.50885759	0.25275023	1.70100340
H	-1.12702748	2.06090778	0.75181960
C	-1.60008099	-1.87638245	-0.29461751
H	-3.39115741	-1.07323986	-1.07744054
C	-0.12601728	-1.06859612	1.60260625
H	-0.11790376	0.83495386	2.53670597
C	-0.37344180	-1.86885686	0.47011843
H	-1.82239256	-2.83357720	-0.77360047
H	0.56094449	-1.46267548	2.35209539
H	0.20789691	-2.78961674	0.40447489
C	2.08109385	-0.73365269	-0.44948389
C	0.74893185	-0.56899560	-1.09541191
H	0.43547631	-1.24418434	-1.88346394
C	1.42291428	1.49612988	-0.21036888
C	0.32478272	0.75752592	-0.93274850
H	-0.30760667	1.30007427	-1.63017090
O	1.51461692	2.68263121	0.03920061
O	2.81111617	-1.70870496	-0.41164641
N	2.35609091	0.51294080	0.13791524
H	3.21379362	0.71432267	0.64370721

TS: 2prot-M

E = -4005.58
H = -3869.57
G = -3903.85
E*(ZORA-ωB97X-D)* = -6077.28
N_{imag} = 1, -386.344i cm^{-1}

N	-3.03861295	0.99593305	-0.06148414
C	-2.06392329	0.15080619	0.16190175
C	-0.91129320	0.75518241	0.84352580

C	-2.05745039	-1.23909650	-0.26175575
C	-0.05489274	0.13078734	1.77412533
H	-1.05005266	1.83093095	0.96997678
C	-1.01639823	-2.09903775	-0.18220544
H	-2.93038812	-1.59499630	-0.80959900
C	0.50965538	-1.11899091	1.60055126
H	0.36991074	0.77302385	2.54660790
C	0.27913313	-1.91437751	0.46246574
H	-1.13667991	-3.06680763	-0.67456253
H	1.33813995	-1.40206160	2.25053710
H	0.96940535	-2.74721878	0.32064551
C	2.46297083	-0.48792945	-0.58564192
C	1.06273074	-0.49511150	-1.10009761
H	0.77863868	-1.17934330	-1.89230714
C	1.53555607	1.63129528	-0.23103008
C	0.49910729	0.77532213	-0.88219150
H	-0.27735300	1.23116198	-1.48804323
O	1.50344268	2.81761067	0.04868199
O	3.31808861	-1.35693443	-0.64396592
N	2.61713726	0.76855633	0.01818133
H	3.48362622	1.07633027	0.44956272
N	-4.16604115	0.55667056	-0.70605368
H	-4.92215860	1.21783562	-0.55104741
H	-4.46404873	-0.40322198	-0.50821888

TS: 3prot-M

E = -4766.64

H = -4604.62

G = -4645.87

E*(ZORA-ωB97X-D)* = -7336.90

N_{imag} = 1, -384.812i cm^{-1}

N	-1.57201583	0.50382508	1.63246163
C	-0.58664437	-0.30596234	1.32084183
C	0.72945103	0.20852563	1.71287008
C	-0.73988720	-1.58092855	0.65448854
C	1.91387561	-0.52337259	1.93939113
H	0.63898572	1.15715654	2.24728579
C	0.23540385	-2.27834602	0.03216055
H	-1.75737575	-1.96683494	0.62323197
C	2.37902903	-1.53020787	1.11709913
H	2.61519914	-0.09197827	2.65448811
C	1.66290900	-1.99810327	-0.00436054
H	-0.06171881	-3.17864664	-0.51182127
H	3.42030166	-1.83793537	1.21628558
H	2.22743354	-2.61238557	-0.70719215
C	3.04308981	-0.01274972	-1.38678695
C	1.56536441	-0.08943828	-1.18011560
H	0.92480977	-0.54453674	-1.92787491
C	2.40917858	1.73040945	0.03876353
C	1.17813245	0.96189885	-0.33417648
H	0.20654589	1.44590544	-0.36217443
O	2.51864250	2.74982736	0.69548350
O	3.76232006	-0.68193561	-2.10898951
N	3.47309332	1.01874040	-0.53871299
H	4.44263255	1.31337808	-0.46715291
N	-2.85181932	0.11509386	1.17084624
H	-3.51898205	0.74067834	1.63149526
S	-3.19152949	0.37392243	-0.52159897
O	-1.93574606	0.59239036	-1.22070178
O	-4.28543969	1.33076170	-0.57633252
C	-3.85788511	-1.20189170	-1.05380864

H	-4.20847753	-1.04291176	-2.07935489
H	-3.06830760	-1.95676226	-1.03149023
H	-4.69176512	-1.46700704	-0.39787210

TS1: 2-M

E = -3959.94
H = -3832.85
G = -3867.78
E*(ZORA-ωB97X-D)* = -5990.11
N_{imag} = 1, -415.118i cm^{-1}

N	-3.46311408	0.92714324	-0.18396613
C	-2.35732946	0.18519862	0.20411138
C	-1.51346390	0.85034981	1.07654682
C	-2.16388146	-1.18439694	-0.26899085
C	-0.36552965	0.38898847	1.77303021
H	-1.84716822	1.86491366	1.30942637
C	-1.06061016	-1.95107730	-0.16254158
H	-3.03360283	-1.59412916	-0.78458984
C	0.34287386	-0.78057982	1.58457784
H	-0.00574743	1.05243935	2.56189045
C	0.25536632	-1.63342115	0.44369157
H	-1.12366471	-2.95796120	-0.58838152
H	1.18777584	-0.95563008	2.25414413
H	0.91456226	-2.50398328	0.49429738
C	2.59123981	-0.64350737	-0.36255362
C	1.22324725	-0.64250106	-0.99194220
H	1.01666396	-1.39870262	-1.75036547
C	1.76323617	1.55733907	-0.44491893
C	0.83194428	0.71663744	-1.12687182
H	-0.05376221	1.09267884	-1.62458839
O	1.86101054	2.78345626	-0.28921286
O	3.37797932	-1.58456756	-0.21602085
N	2.77105645	0.64845847	0.07922116
H	3.63388584	0.98106414	0.49604647
N	-4.30899438	0.32582574	-0.95363808
H	-5.04473141	1.03129643	-1.13313463

INT: 2-M

E = -3964.97
H = -3836.88
G = -3871.67
E*(ZORA-ωB97X-D)* = -6000.41
N_{imag} = 0

N	-3.29170976	1.00048362	0.06755706
C	-2.23885254	0.11637534	0.27695470
C	-1.30674138	0.55631836	1.20927083
C	-2.16435904	-1.15203028	-0.42081753
C	-0.28814289	-0.20542888	1.86613343
H	-1.52830974	1.54237965	1.62351541
C	-1.07564499	-1.93430550	-0.56324130
H	-3.09978214	-1.46327952	-0.88965455
C	0.35834012	-1.29788158	1.38176525
H	-0.01202553	0.14793527	2.86408658
C	0.32532442	-1.65735288	-0.06149892
H	-1.20447297	-2.88724505	-1.08594435
H	1.08106766	-1.81215892	2.01680702
H	0.93053735	-2.56106756	-0.21673880
C	2.53893184	-0.51645968	-0.43016182
C	1.07341630	-0.53604775	-0.91717246
H	1.04827798	-0.92401072	-1.95153259
C	1.66454718	1.68391714	-0.28648049

C	0.63327913	0.88064970	-0.80557042
H	-0.27534989	1.28690710	-1.22945064
O	1.80572453	2.89965544	-0.06029674
O	3.32488289	-1.46917263	-0.40184941
N	2.76975508	0.75441418	-0.00692645
H	3.66670980	1.07701279	0.34230837
N	-4.20915717	0.61188127	-0.74885992
H	-4.88989524	1.39165110	-0.76747127

TS2: 2-M

E = -3964.80
H = -3837.28
G = -3870.56
E*(ZORA-ωB97X-D)* = -5998.66
N_{imag} = 1, -112.505i cm^{-1}

N	-3.19444072	1.02872250	0.01313425
C	-2.17989678	0.11743526	0.23705494
C	-1.15589483	0.58322990	1.07660372
C	-2.16650141	-1.18406800	-0.39316497
C	-0.24228675	-0.23214916	1.83654334
H	-1.30956025	1.60515548	1.42950965
C	-1.09192834	-1.98823172	-0.54062277
H	-3.12397977	-1.49661805	-0.81455784
C	0.36067683	-1.35538321	1.38556244
H	-0.00711862	0.12371124	2.84410798
C	0.31929733	-1.69297094	-0.07005513
H	-1.24062777	-2.96493361	-1.01068170
H	1.02716247	-1.92067019	2.03819892
H	0.93961289	-2.58060954	-0.25270634
C	2.49387067	-0.48771501	-0.42052889
C	1.02397071	-0.53311925	-0.88873143
H	0.99882493	-0.86172339	-1.94283876
C	1.59378253	1.69524804	-0.23618265
C	0.54185324	0.87675497	-0.71484734
H	-0.30250605	1.29585160	-1.24631835
O	1.71557973	2.91256577	-0.01931973
O	3.30118683	-1.42059957	-0.40835780
N	2.70831196	0.78580589	0.01512919
H	3.60347866	1.11618547	0.36214126
N	-4.16997909	0.63917620	-0.74079112
H	-4.81265541	1.44954633	-0.77178285

TS2: 2-M

E = -3964.80
H = -3837.28
G = -3870.56
E*(ZORA-ωB97X-D)* = -5998.66
N_{imag} = 1, -112.505i cm^{-1}

N	-3.19444072	1.02872250	0.01313425
C	-2.17989678	0.11743526	0.23705494
C	-1.15589483	0.58322990	1.07660372
C	-2.16650141	-1.18406800	-0.39316497
C	-0.24228675	-0.23214916	1.83654334
H	-1.30956025	1.60515548	1.42950965
C	-1.09192834	-1.98823172	-0.54062277
H	-3.12397977	-1.49661805	-0.81455784
C	0.36067683	-1.35538321	1.38556244
H	-0.00711862	0.12371124	2.84410798
C	0.31929733	-1.69297094	-0.07005513
H	-1.24062777	-2.96493361	-1.01068170
H	1.02716247	-1.92067019	2.03819892

H	0.93961289	-2.58060954	-0.25270634
C	2.49387067	-0.48771501	-0.42052889
C	1.02397071	-0.53311925	-0.88873143
H	0.99882493	-0.86172339	-1.94283876
C	1.59378253	1.69524804	-0.23618265
C	0.54185324	0.87675497	-0.71484734
H	-0.30250605	1.29585160	-1.24631835
O	1.71557973	2.91256577	-0.01931973
O	3.30118683	-1.42059957	-0.40835780
N	2.70831196	0.78580589	0.01512919
H	3.60347866	1.11618547	0.36214126
N	-4.16997909	0.63917620	-0.74079112
H	-4.81265541	1.44954633	-0.77178285

TS: 3–M

E = -4737.35
H = -4584.26
G = -4626.97
E*(ZORA-ωB97X-D)* = -7265.56
$\boldsymbol{N}_{\mathbf{imag}}$ = 1, -438.318i cm^{-1}

N	-1.84948452	-0.08664673	0.49622166
C	-0.60691286	-0.63088633	0.57570024
C	0.24996690	0.03516756	1.46121267
C	-0.24141057	-1.81832624	-0.19304064
C	1.53877019	-0.31124640	1.91677338
H	-0.22096005	0.89333065	1.94629419
C	0.99690279	-2.29380680	-0.42088374
H	-1.08951646	-2.33489423	-0.64373299
C	2.43102003	-1.20532015	1.35334206
H	1.88537382	0.23688561	2.79473541
C	2.30244662	-1.76106179	0.04698129
H	1.07516766	-3.19597331	-1.03460571
H	3.40092706	-1.31536487	1.84176825
H	3.14078861	-2.40106112	-0.23966643
C	4.07555410	0.05597912	-0.73048249
C	2.66426507	-0.25782385	-1.16544122
H	2.53763167	-0.85491184	-2.06907035
C	2.66913397	1.85240043	-0.16528270
C	1.88787286	0.90098578	-0.90417345
H	0.87006159	1.09009073	-1.22120992
O	2.43684344	2.98723999	0.26328496
O	5.10282475	-0.59645774	-0.91671332
N	3.96698470	1.22998510	-0.01572327
H	4.76186274	1.72002544	0.38077517
N	-2.68945637	-0.68124737	-0.31209439
S	-4.20318650	0.08205611	-0.26080477
O	-4.88847360	-0.17615493	1.00725346
O	-4.87366266	-0.28989827	-1.50407494
C	-3.84795031	1.85109606	-0.32019167
H	-4.81478906	2.35823826	-0.24273746
H	-3.19523724	2.09332515	0.52285075
H	-3.35854738	2.07503399	-1.27261401

P: 1–M

E = -3667.48
H = -3547.59
G = -3578.95
E*(ZORA-ωB97X-D)* = -5559.49
$\boldsymbol{N}_{\mathbf{imag}}$ = 0

O	-3.18675316	1.37117232	-0.35144136
C	-2.29295519	0.54841143	-0.18996714

C	-0.93814708	0.97725966	0.40222442
C	-2.48435802	-0.86353603	-0.58218859
C	-0.61358479	0.21289242	1.66338732
H	-1.01054986	2.05439290	0.58591490
C	-1.58200604	-1.85045626	-0.42898726
H	-3.46012546	-1.07497395	-1.02245068
C	-0.26500021	-1.07139285	1.56040185
H	-0.67176105	0.72767108	2.62124291
C	-0.20797642	-1.68475302	0.17298270
H	-1.84619855	-2.85294161	-0.77366200
H	-0.00541437	-1.68315014	2.42291855
H	0.30136439	-2.65413836	0.20258307
C	2.10193153	-0.75339290	-0.30540424
C	0.63356653	-0.73817076	-0.74183293
H	0.59145332	-1.11409273	-1.77250028
C	1.44771554	1.50087269	-0.22287903
C	0.19020862	0.73134605	-0.64917628
H	-0.13293741	1.13588095	-1.61724952
O	1.55620600	2.69395849	-0.03188614
O	2.82347595	-1.72200973	-0.17622579
N	2.47130650	0.56679663	-0.07261916
H	3.40394525	0.82745473	0.24231268

P: 2prot–M

E = -4043.47

H = -3904.95

G = -3938.23

E*(ZORA-ωB97X-D)* = -6134.42

N_{imag} = 0

N	-3.01861710	1.00722833	-0.02912230
C	-2.00429776	0.19121664	-0.01988404
C	-0.70146581	0.79356874	0.47812586
C	-2.03843401	-1.20113044	-0.44568919
C	-0.22477346	0.06523507	1.71686252
H	-0.89970271	1.85005658	0.68941352
C	-1.00671041	-2.06906045	-0.37707209
H	-2.96457663	-1.57070253	-0.88971726
C	0.28387453	-1.16130139	1.57221106
H	-0.32219640	0.54699163	2.68920037
C	0.36386483	-1.73807268	0.17132454
H	-1.14924086	-3.07982293	-0.76328501
H	0.63912133	-1.75450339	2.41416836
H	0.99103792	-2.63659885	0.16085031
C	2.51278202	-0.51217910	-0.39610423
C	1.03545970	-0.68246791	-0.75791493
H	0.98894116	-1.04463057	-1.79371273
C	1.57447470	1.63467502	-0.22320974
C	0.40963434	0.71930828	-0.61161513
H	-0.00592240	1.09231128	-1.55677584
O	1.53959896	2.82817160	-0.00065720
O	3.36324684	-1.37817144	-0.32557317
N	2.71859192	0.84093093	-0.14876691
H	3.62427347	1.21557990	0.12652002
N	-4.23470000	0.57926351	-0.47903851
H	-4.96536539	1.20803548	-0.16059237
H	-4.47309781	-0.40387631	-0.32657792

P: 3prot–M

E = -4803.12

H = -4638.57

G = -4678.89

E*(ZORA-ωB97X-D)* = -7392.12
N_{imag} = 0

N	-1.56291476	0.71620646	1.51377957
C	-0.59866128	-0.10506273	1.22240499
C	0.79153370	0.49250475	1.36549119
C	-0.76682126	-1.46493103	0.74098667
C	1.81610048	-0.40077097	2.02001096
C	0.21031576	-2.22589213	0.21087194
H	-1.75481203	-1.89566993	0.90431000
C	2.24812010	-1.47535989	1.35376092
H	2.20092579	-0.13226133	3.00285416
C	1.62964192	-1.75842544	-0.00499098
H	-0.01318062	-3.26272913	-0.04746509
H	2.99978309	-2.15477725	1.75369463
C	3.11079293	-0.20301962	-1.33166179
C	1.67397852	-0.45880957	-0.86973631
C	2.51975078	1.68324013	-0.06277672
C	1.26721737	0.80226112	-0.08785317
O	2.67550595	2.73862081	0.51577240
O	3.82054446	-0.94393631	-1.98362433
N	3.48323323	1.04490578	-0.84310818
H	4.41440217	1.43171044	-0.98399198
N	-2.86009458	0.29834150	1.13817415
H	-3.51146216	0.98283103	1.53276150
S	-3.24564535	0.34088321	-0.56304058
O	-2.02988164	0.58168648	-1.32041056
O	-4.40801030	1.20877429	-0.66308294
C	-3.80568384	-1.32158677	-0.92179553
H	-4.20492028	-1.28112296	-1.94108551
H	-2.95686974	-2.00696621	-0.86831597
H	-4.59203541	-1.58594142	-0.20937066
H	0.47048515	1.35852692	-0.59969951
H	1.04871221	-0.60903703	-1.75863555
H	2.19609214	-2.52965438	-0.53862750
H	0.68234749	1.44510821	1.89576277

P: 2-M
E = -3980.66
H = -3851.62
G = -3884.60
E*(ZORA-ωB97X-D)* = -6024.95
N_{imag} = 0

C	-2.03999912	0.16346566	-0.02968915
C	-0.75846061	0.78747127	0.48823286
C	-2.07973106	-1.21581200	-0.37567122
C	-0.31003856	0.04321147	1.72225845
H	-0.97903697	1.83930221	0.70891365
C	-1.04497942	-2.11121962	-0.31951692
H	-3.06250456	-1.56658860	-0.70181800
C	0.22521280	-1.18138445	1.57093480
H	-0.52781996	0.46343941	2.70581934
C	0.34099781	-1.73648786	0.16651341
H	-1.21564924	-3.15765995	-0.58105560
H	0.46893340	-1.82300035	2.42014623
H	0.99498240	-2.61833308	0.15144977
C	2.47553883	-0.50411239	-0.44449612
C	0.99611813	-0.66499778	-0.76240439
H	0.90659219	-1.02342787	-1.79697933
C	1.54451546	1.63994018	-0.18720597
C	0.37952854	0.74761060	-0.58456272
H	-0.04427509	1.13593117	-1.52023578

O	1.54921010	2.83808411	0.05236884
O	3.35320536	-1.35726044	-0.44725580
N	2.68210850	0.83033515	-0.11206107
H	3.59073053	1.19128730	0.16810340
N	-3.10113289	1.00573713	-0.10192471
N	-4.23690924	0.55430128	-0.56804666
H	-4.86835435	1.37106146	-0.52534630

P: 3-M

E = -4764.15

H = -4609.31

G = -4648.46

E*(ZORA-ωB97X-D)* = -7312.16

N_{imag} = 0

C	-0.44915863	-0.40198073	0.19240754
C	0.70750164	0.47602466	0.64295171
C	-0.21408394	-1.75774666	-0.22423179
C	1.43212397	-0.17204308	1.79942796
H	0.27967242	1.44436536	0.92653972
C	0.98804090	-2.38883210	-0.27919050
H	-1.11452842	-2.30831247	-0.50414112
C	2.20445665	-1.23882509	1.54887347
H	1.25898124	0.19573941	2.81140173
C	2.29565074	-1.73052307	0.11739719
H	1.03520428	-3.43208781	-0.59778916
H	2.70469475	-1.79929316	2.34014215
H	3.12019918	-2.44616931	0.00731670
C	4.04264173	-0.05136584	-0.62936106
C	2.60524787	-0.52214649	-0.81916834
H	2.49512903	-0.86190075	-1.85785114
C	2.70326200	1.82479208	-0.16670957
C	1.72081954	0.71316687	-0.51880252
H	1.14746711	1.03635568	-1.39808649
O	2.47016139	2.97690373	0.15250302
O	5.07190736	-0.69791765	-0.75332280
N	3.99123039	1.28712914	-0.26138737
H	4.82437959	1.82965147	-0.04611728
N	-1.64480944	0.17294296	0.23099370
N	-2.69150590	-0.53736736	-0.17239880
S	-4.09238183	0.36080931	-0.06793714
C	-5.20251148	-0.93586950	-0.64773255
H	-5.14538902	-1.78371380	0.04084390
H	-6.20528035	-0.49584606	-0.64706510
H	-4.90389811	-1.23034463	-1.65785446
O	-4.16893412	1.45718629	-1.04646693
O	-4.49501556	0.68557558	1.30940632

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