Electronic Supplementary Information for

Boron-Nitride and Aluminum-Nitride "Pringles" and Flapping Motion

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I. Computational Details

Geometry optimizations: In this study, all the nanoplate structures are fully optimized using the density-functional theory (DFT) calculations at the B3LYP/6-31G(d) level without imposing any symmetry constraints.[1] Harmonic vibrational frequency analyses are performed at the same level of theory to assure that the optimized structures give no imaginary frequencies and that the transition states possess one imaginary frequency.[2] Zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm are estimated. Intrinsic reaction coordinate (IRC) calculations are also performed to survey all possible pathways connecting reactant to product via a transition state.[3] UV-vis absorption spectra are computed using the time-dependent DFT (TD-DFT) method at the level of B3LYP/6-31G(d), for which 20 singlet excited states are predicted. All calculations are carried out using the GAUSSIAN 09 program package.[4] Optical absorption spectra are simulated by using a Lorentzian convolution with 500 cm^{-1} half-width in the GaussSum software.[5]

To validate the computational scheme selected, benchmark calculations using the corannulene and warped $C_{80}H_{30}$ as two model systems are performed. For the corannulene, its bowl-to-bowl inversion barrier has been measured in the experiment and computed theoretically.[6-8] The best estimate from experiments is about 11.5 kcal/mol.[8] We have computed the bowl inversion barrier of corannulene using two DFT methods: B3LYP and M06-2X[9] and a more computationally demanding level of theory, MP2,[10] all with the same 6-31G(d) basis set for comparisons. As shown in **Table S1**, the bowl-to-bowl inversion barrier of corannulene follows the order 10.4 kcal/mol (B3LYP) < 10.9 kcal/mol (M06-2X) < 11.4 kcal/mol (MP2). From the Cartesian coordinates given in **Table S2**, one can find that the bowl depth computed is 0.87 Å (B3LYP), 0.88 Å (M06-2X), and 0.90 Å (MP2), respectively. All the computed activation energies are in good agreement with the experimental value (11.5 kcal/mol) and previous MP2/cc-pVDZ (sp) calculation (11.0 kcal/mol).[8] Thus, we can conclude all three levels of theory selected (B3LYP, M06-2X, and MP2) can give reliable value of bowl inversion barrier of corannulene.

Since the M06-2X functional has been proven reliable for studying main-group thermochemistry, reaction energies, kinetics, and even excited states, we have compared B3LYP data with M06-2X data for the warped $C_{80}H_{30}$. As shown in **Table S1**, the bowl-to-bowl inversion and racemization barriers of $C_{80}H_{30}$ from the M06-2X are 1.4 and 19.1 kcal/mol, respectively, in good agreement with the corresponding data of 1.7 and 18.9 kcal/mol from the B3LYP. For the racemization barrier, both 18.9 kcal/mol (B3LYP) and 19.1 kcal/mol (M06-2X) are higher than the experimental activation enthalpy (13.6± 1.5 kcal/mol) for $(t\text{-Bu})_{10}C_{80}H_{20}$[11]. The same barrier for the unsubstituted corannulene is 11.5 kcal/mol, which is extrapolated from the bowl-to-bowl inversion barriers of two bis(bromomethyl)corannulenes (10.4-10.5 kcal/mol) and mono(bromomethyl)corannulene (11.0 kcal/mol).[8] To summarize, the B3LYP/6-31G(d) level of theory can give reasonable description of racemization pathway.

Table S1. Reaction barriers of bowl-to-bowl inversion (ΔE_{flip}) of corannulene and ΔE_{flip} and racemization (ΔE_{rac}) of the warped $C_{80}H_{30}$, computed based on the B3LYP, M06-2X, and MP2 levels of theory, respectively, all with the same basis set of 6-31G(d). All data listed are in units of kcal/mol.

Method	ΔE_{flip} of corannulene	ΔE_{flip} of $C_{80}H_{30}$	ΔE_{rac} of $C_{80}H_{30}$
B3LYPP	10.4	1.7	18.9
M06-2X	10.9	1.4	19.1
MP2	11.4	-	-
experiment	~11.5 (Ref. 8)	-	-

Table S2. Cartesian coordinates of the optimized ground-state and transition-state corannulene, based on the B3LYP, M06-2X, and MP2 levels of theory, respectively.

Corannulene-GS-B3LYP

C	1.5981270	1.9090887	0.0931902	C	2.2836596	-2.3364564	-0.2506411	H	-3.3341066	2.6479332	-0.6053898
C	-1.3216474	2.1094067	0.0926587	C	3.2654493	0.1019446	-0.2505752	H	-4.2391595	0.4016723	-0.6049614
C	-2.4149440	-0.6050549	0.0928876	C	2.9278742	1.4499465	-0.2502295	H	-3.5484140	-2.3526316	-0.6059193
C	-0.1707476	-2.4835959	0.0931027	C	0.9121728	3.1371532	-0.2507345	H	-1.6913337	-3.9069436	-0.6058926
C	2.3092015	-0.9298818	0.0926087	C	-0.4741882	3.2322080	-0.2509873	H	1.1411470	-4.1020721	-0.6049637
C	-2.7018022	1.8368783	-0.2507604	C	1.1177498	-0.4500496	0.6099632	H	3.1931782	-2.8164507	-0.6052238
C	-3.2211514	0.5479202	-0.2505293	C	-0.0826300	-1.2020808	0.6101858	H	4.2538850	-0.1823448	-0.6049058
C	-2.5818928	-2.0018192	-0.2507645	C	-1.1689607	-0.2928322	0.6101450	H	3.6656469	2.1666012	-0.6044245
C	-1.5162680	-2.8937379	-0.2507586	C	-0.6397428	1.0211273	0.6102913	H	1.4877993	3.9891953	-0.6057323
C	1.1060753	-3.0742112	-0.2504945	C	0.7735638	0.9240805	0.6103774	H	-0.9280330	4.1548349	-0.6062005

Corannulene-TS-B3LYP

C	2.4311073	0.7899148	0.0000000	C	-1.3669496	3.0752514	0.0000000	H	1.1956311	-4.2607373	0.0000000
C	1.5025070	-2.0680233	0.0000000	C	1.3669495	3.0752515	0.0000000	H	-1.1956309	-4.2607374	0.0000000
C	-1.5025069	-2.0680233	0.0000000	C	2.5023271	2.2503513	0.0000000	H	-3.6827318	-2.4537529	0.0000000
C	-2.4311073	0.7899147	0.0000000	C	3.3471485	-0.3497412	0.0000000	H	-4.4216724	-0.1795277	0.0000000
C	-0.0000001	2.5562176	0.0000000	C	2.9134728	-1.6844576	0.0000000	H	-3.4716845	2.7442348	0.0000000
C	0.7017021	-3.2914033	0.0000000	C	0.0000000	1.1888431	0.0000000	H	-1.5371130	4.1497833	0.0000000
C	-0.7017019	-3.2914033	0.0000000	C	-1.1306569	0.3673728	0.0000000	H	1.5371127	4.1497834	0.0000000
C	-2.9134727	-1.6844578	0.0000000	C	-0.6987844	-0.9617941	0.0000000	H	3.4716844	2.7442349	0.0000000
C	-3.3471484	-0.3497413	0.0000000	C	0.6987844	-0.9617941	0.0000000	H	4.4216724	-0.1795274	0.0000000
C	-2.5023272	2.2503512	0.0000000	C	1.1306569	0.3673728	0.0000000	H	3.6827319	-2.4537527	0.0000000

Corannulene-GS-M06-2X

C	-0.5919092	-2.4066460	0.0963371	C	-3.0672003	1.0898452	-0.2556208	H	4.1421057	-0.9100086	-0.6187324
C	2.1059738	-1.3066385	0.0962782	C	-2.8760718	-1.5244993	-0.2556008	H	3.9660786	1.5028234	-0.6179011
C	1.8935574	1.5990291	0.0959386	C	-1.9842754	-2.5802821	-0.2557515	H	2.1452459	3.6580719	-0.6193734
C	-0.9357510	2.2951007	0.0963881	C	0.5610499	-3.2061737	-0.2560055	H	-0.2038628	4.2360805	-0.6183228

C	-2.4718200	-0.1807824	0.0963879	C	1.8407479	-2.6844250	-0.2559341	H	-2.8162004	3.1708939	-0.6184084
C	3.2227699	-0.4573151	-0.2559169	C	-1.2014934	-0.0879085	0.6217236	H	-4.0916571	1.1151615	-0.6182953
C	3.1220666	0.9210266	-0.2559682	C	-0.4548403	1.1155684	0.6215569	H	-3.8862140	-1.6985489	-0.6177251
C	1.4307735	2.9236651	-0.2562180	C	0.9203926	0.7772754	0.6213651	H	-2.3250298	-3.5467400	-0.6184345
C	0.0887467	3.2538201	-0.2559525	C	1.0236332	-0.6350740	0.6216368	H	0.4146315	-4.2204062	-0.6188434
C	-2.3385926	2.2642316	-0.2556705	C	-0.2876982	-1.1698279	0.6217996	H	2.6545471	-3.3072670	-0.6186022

Corannulene-TS-M06-2X

C	2.4249931	0.7879282	0.0000000	C	-1.3662109	3.0675037	0.0000000	H	1.1923231	-4.2525771	0.0000000
C	1.4987282	-2.0628222	0.0000000	C	1.3662108	3.0675038	0.0000000	H	-1.1923229	-4.2525772	0.0000000
C	-1.4987281	-2.0628223	0.0000000	C	2.4951869	2.2472547	0.0000000	H	-3.6759932	-2.4480852	0.0000000
C	-2.4249931	0.7879281	0.0000000	C	3.3395517	-0.3514328	0.0000000	H	-4.4128893	-0.1801521	0.0000000
C	-0.0000001	2.5497888	0.0000000	C	2.9083213	-1.6786238	0.0000000	H	-3.4642118	2.7395774	0.0000000
C	0.6977457	-3.2847011	0.0000000	C	0.0000000	1.1884886	0.0000000	H	-1.5349927	4.1412372	0.0000000
C	-0.6977455	-3.2847011	0.0000000	C	-1.1303198	0.3672632	0.0000000	H	1.5349925	4.1412372	0.0000000
C	-2.9083212	-1.6786240	0.0000000	C	-0.6985760	-0.9615074	0.0000000	H	3.4642117	2.7395776	0.0000000
C	-3.3395517	-0.3514330	0.0000000	C	0.6985761	-0.9615073	0.0000000	H	4.4128894	-0.1801519	0.0000000
C	-2.4951870	2.2472545	0.0000000	C	1.1303198	0.3672633	0.0000000	H	3.6759933	-2.4480850	0.0000000

Corannulene-GS-MP2

C	2.3570455	-0.7760335	0.0949939	C	-1.3154171	-2.9755027	-0.2638225	H	1.2287475	4.0588627	-0.6339681
C	1.4664171	2.0018671	0.0947676	C	1.2921427	-2.9856833	-0.2638080	H	-1.1969989	4.0683378	-0.6339830
C	-1.4507423	2.0132633	0.0947518	C	2.4233772	-2.1705274	-0.2638256	H	-3.4805571	2.4228341	-0.6338545
C	-2.3630327	-0.7576002	0.0949450	C	3.2388504	0.3062585	-0.2639300	H	-4.2391648	0.1187404	-0.6336927
C	-0.0096908	-2.4814665	0.0950149	C	2.8131586	1.6340220	-0.2640282	H	-3.3798421	-2.5615288	-0.6335495
C	0.7095742	3.1749369	-0.2641975	C	-0.0047065	-1.2037066	0.6443647	H	-1.4229333	-3.9950045	-0.6334878
C	-0.6847514	3.1803806	-0.2642127	C	-1.1462853	-0.3674663	0.6443051	H	1.3916963	-4.0059926	-0.6334764
C	-2.8003043	1.6559426	-0.2640850	C	-0.7037456	0.9766513	0.6442159	H	3.3597470	-2.5878454	-0.6334907
C	-3.2363545	0.3315449	-0.2639887	C	0.7113400	0.9711275	0.6442338	H	4.2399782	0.0856301	-0.6336065
C	-2.4402512	-2.1515364	-0.2638602	C	1.1433664	-0.3764070	0.6443162	H	3.4993827	2.3955772	-0.6337935

Corannulene-TS-MP2

C	-0.7678705	-2.4393893	-0.0084722	C	3.2926178	-0.6744028	0.0085701	H	-4.1622949	1.4983890	0.0133908
C	-2.5558247	-0.0235247	0.0194328	C	1.7138479	-2.8913904	0.0039561	H	-2.7757526	3.4447540	-0.0055092
C	-0.8125123	2.4235829	-0.0206475	C	0.3758450	-3.3401381	-0.0015626	H	0.1385266	4.4217262	-0.0043001
C	2.0537428	1.5215892	0.0190515	C	-2.2211806	-2.5226409	0.0083730	H	2.4182460	3.7044145	0.0113912
C	2.0825619	-1.4832493	-0.0161565	C	-3.0607544	-1.3884656	-0.0074018	H	4.2481929	1.2350044	0.0113443
C	-3.0854199	1.3320621	-0.0067571	C	0.9655149	-0.6874854	0.0241038	H	4.2708790	-1.1544093	-0.0096577
C	-2.2666420	2.4812693	0.0100842	C	0.9520047	0.7051980	-0.0299656	H	2.4873301	-3.6591357	0.0009036
C	0.3131030	3.3460313	0.0095015	C	-0.3765717	1.1232518	0.0186337	H	0.2214928	-4.4189616	0.0058244
C	1.6592039	2.9225252	-0.0062399	C	-1.1847780	-0.0109569	-0.0322952	H	-2.7125833	-3.4952363	-0.0081491
C	3.2791824	0.7366195	-0.0079658	C	-0.3560139	-1.1307745	0.0114916	H	-4.1343747	-1.5748129	0.0103569

To validate the TD-DFT method for computing the UV-vis absorption spectra of the warped $C_{80}H_{30}$ (see Fig.S1), we compare the simulated UV-vis spectra of the warped $C_{80}H_{30}$ with the

experimental spectra (inset in Fig. S1). One can see that both spectra exhibit some significant absorption peaks in the visible and near-UV range, where the theoretical peaks located at 424, 433, and 483 nm are in good agreement with the experimental data, for which the β band and the longest wavelength absorption maximum are located at 418 and 491 nm, respectively.[11]

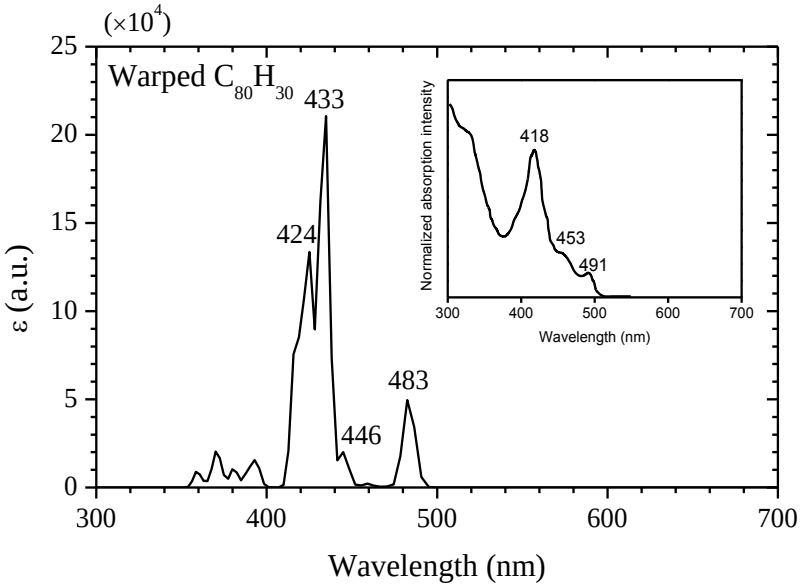

Figure S1 Simulated UV-vis spectra of the warped $C_{80}H_{30}$ with a full width at half maximum being 350 cm^{-1}. The inset is the experimental UV-vis absorption spectra in CH_2Cl_2, taken from Fig. 4 of *Nat. Chem*., 2013, **5**, 739.

Born-Oppenheimer molecular dynamics simulations: To simulate the racemization process of the $B_{40}N_{40}H_{30}$ nanoplate, a Born-Oppenheimer molecular dynamics (BOMD) simulation within the framework of Kohn-Sham formulation of DFT and the Gaussian plane-wave (GPW) method[12] is performed using the QUICKSTEP program implemented in the CP2K software package.[13] The Perdew-Burke-Ernzenhof (PBE)[14] functional within the generalized gradient approximation (GGA) is employed for the BOMD. Furthermore, the core electrons are described by the Goedecker-Teter-Hutter (GTH) norm-conserving pseudopotential,[15,16] and the wave functions of valence electrons are expressed through a combination of the polarized double-ξ quality Gaussian basis[17] and a plane-wave basis set (with an energy cutoff of 280 Ry). To overcome the racemization barrier (4.3 kcal/mol) and to accelerate the barrier-crossing process, the $B_{40}N_{40}H_{30}$ nanoplate with the *MPMPM* geometry is placed in a periodic box of 50 Å × 50 Å × 50 Å, and the subsequent BOMD simulation in the constant-volume and constant-temperature (*NVT*) ensemble is performed with the temperature controlled at 1200 K. The time step is 1.0 fs. The first 4-ps runs are long enough to see the iterative racemization transition between the *MPMPM* and *PMPMP* geometries as shown in Movie S1.

II. Examination of various low-energy nanoplate isomers

The initial structures are constructed based on the 26-ring $C_{80}H_{30}$ as a template, which contains one pentagon, five heptagons, and twenty hexagons. Previous computational studies of BN clusters have shown that the *homonuclear* B-B and N-N bonds should be avoided as much as possible since these *homonuclear* bonds would result in much less stable isomers.[19] So, we firstly consider the configurations with only six homonuclear bonds in the odd-membered-ring sites. The central pentagon in the warped nanoplate can be occupied by two boron and three nitrogen atoms with at least one homonuclear N-N bond, which possesses five possible core arrangements in the template as illustrated in Fig. S2. To maximize the BNBN alternation, only two possible isomers are allowed for the five possible core*i* (*i*=1-5) configurations. Using core1 as an example, two possible isomers would be resulted by letting either position 1 or 2 (see the red labels in Fig. S2) occupied by a nitrogen atom. Hence, group I has 10 possible initial configurations whose 19 out of 20 hexagons in each configuration exhibit BNBN alternation and each configuration has only six homonuclear bonds when the central pentagon is occupied by 2 boron and 3 nitrogen atoms. On the other hand, by exchanging the B and N atoms in the above-mentioned isomers, group II is obtained, which has ten possible initial configurations as well, each containing six homonuclear bonds. In the group II, the central pentagon is occupied by 3 boron and 2 nitrogen atoms. After optimizing these 20 isomers at the B3LYP/6-31G(d) level, we find that the configurations in the group I are energetically more favorable than those in the group II. For clarity, only the first five isomers for group I (isomer A-E) and group II (isomer F-J) are shown in Fig. S3. Compared to the lowest-energy isomer, i.e., isomer A, all other isomers in the group I are within energy difference of 0.35 eV. For example, the isomer C, which has the core1 structure but with the position 2 being occupied by a nitrogen atom, is only 88 meV higher in energy than the isomer A. The lowest-energy isomer F and highest-energy isomer in the group II are 0.853 eV and 1.664 eV, respectively, higher in energy than the isomer A.

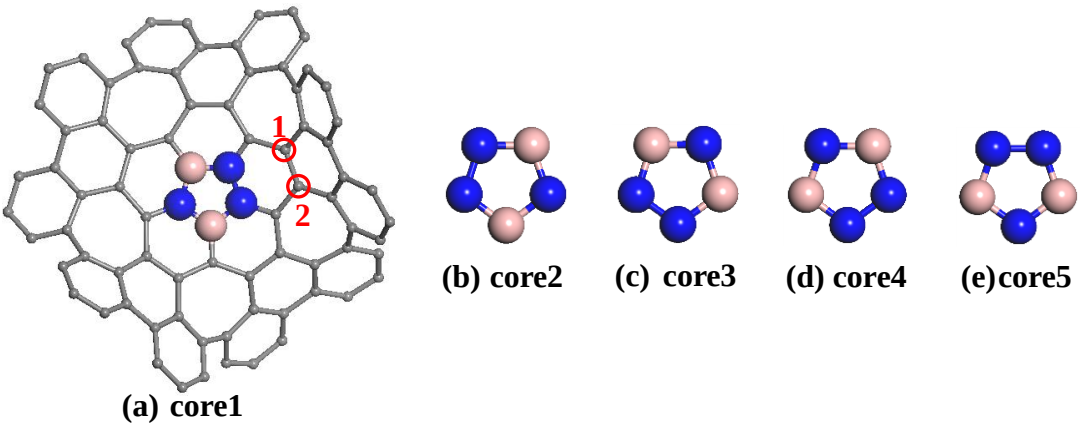

Figure S2 Schematic diagrams of possible atomic arrangements in the central pentagon with 2 boron and 3 nitrogen atoms.

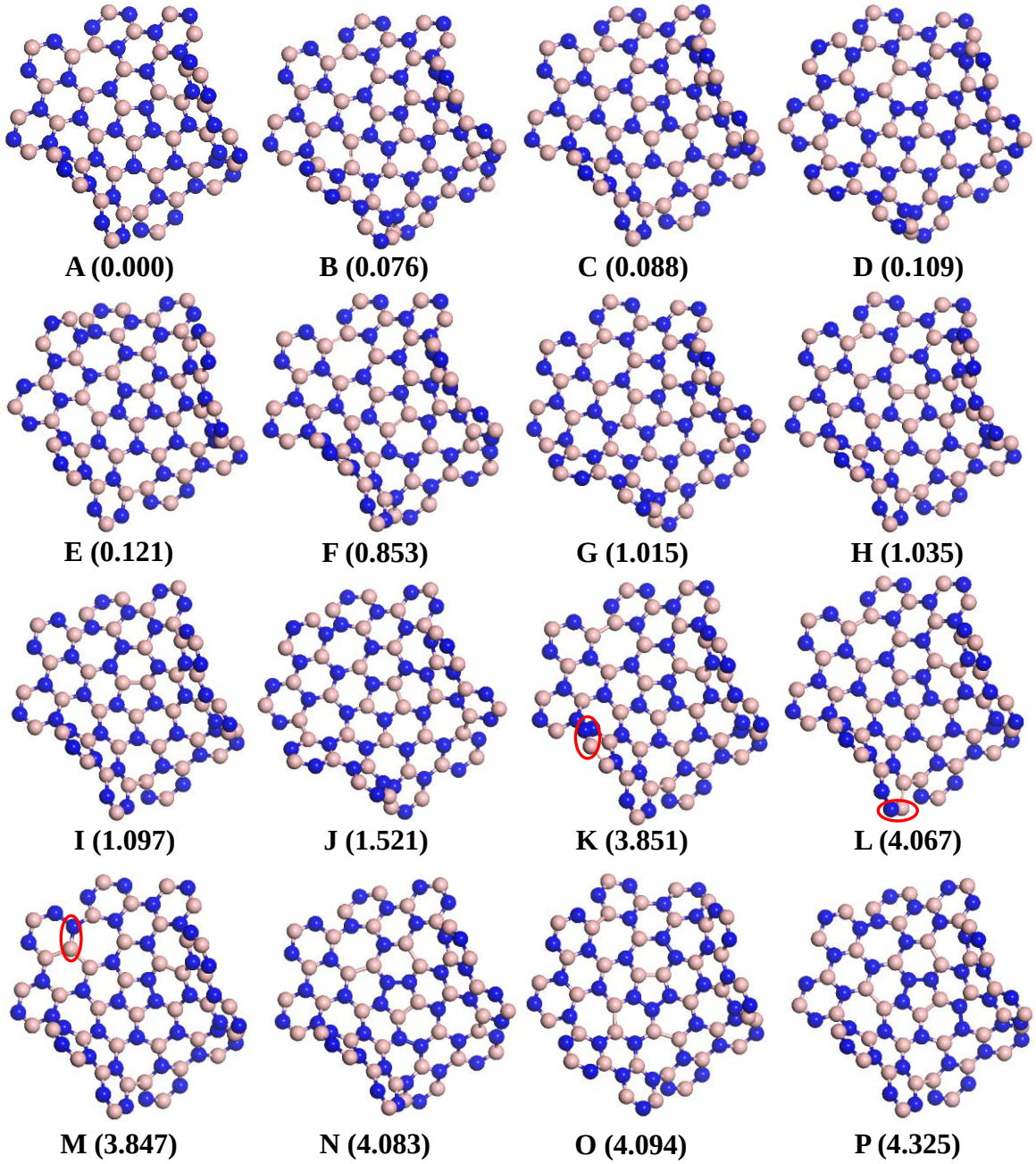

Figure S3 Selected sixteen geometrical structures of the warped $B_{40}N_{40}H_{30}$ isomers.[18] The values in the parentheses are the relative energies (in units of eV) with respect to the lowest-energy structure, i.e., isomer A. Boron and nitrogen atoms are shown by the light pink and navy blue balls, respectively. All hydrogen atoms on the perimeter are omitted for clarity. Isomers A-E belong to group I and isomers F-J belong to group II, all have 19 hexagons with BNBN alternation.

Next, we consider isomers with less number of hexagons that exhibit BNBN alternation. The nanoplates with 18 hexagons having BNBN alternation can be obtained by exchanging a pair of B and N atoms at the edge of the above 20 isomers in the group I and group II. Furthermore, there are many possible arrangements for the warped nanoplates with 17 hexagons having BNBN alternation. These isomers can be constructed from different methods, e.g., by assigning three

consecutive atoms the same in the central pentagon, or by exchanging a pair of B and N atoms located at the common edge of two adjacent hexagons. More than 30 additional isomers with 17 hexagons having BNBN alternation are constructed. However, as pointed out by previous theoretical predictions that the B-B and N-N bonds should be avoided as much as possible in BN clusters. These isomers with less number of hexagons having BNBN alternation indeed have large energy differences from the ground-state isomer A. For example, isomer K and L, both containing 18 hexagons having BNBN alternation, can be obtained from the isomer A by only exchanging a pair of B and N atoms circled by a red oval as illustrated in Fig. S3, respectively. Both isomers K and L have much higher in energy than the ground state isomer A. The lowest-energy isomer with 17 hexagons with BNBN alternation is 3.847 eV higher in energy than the isomer A, which can be obtained from the isomer A by exchanging a pair of B and N atoms in the red oval. All other isomers with less than 17 hexagons having BNBN alternation have considerably higher energy than the isomer A.

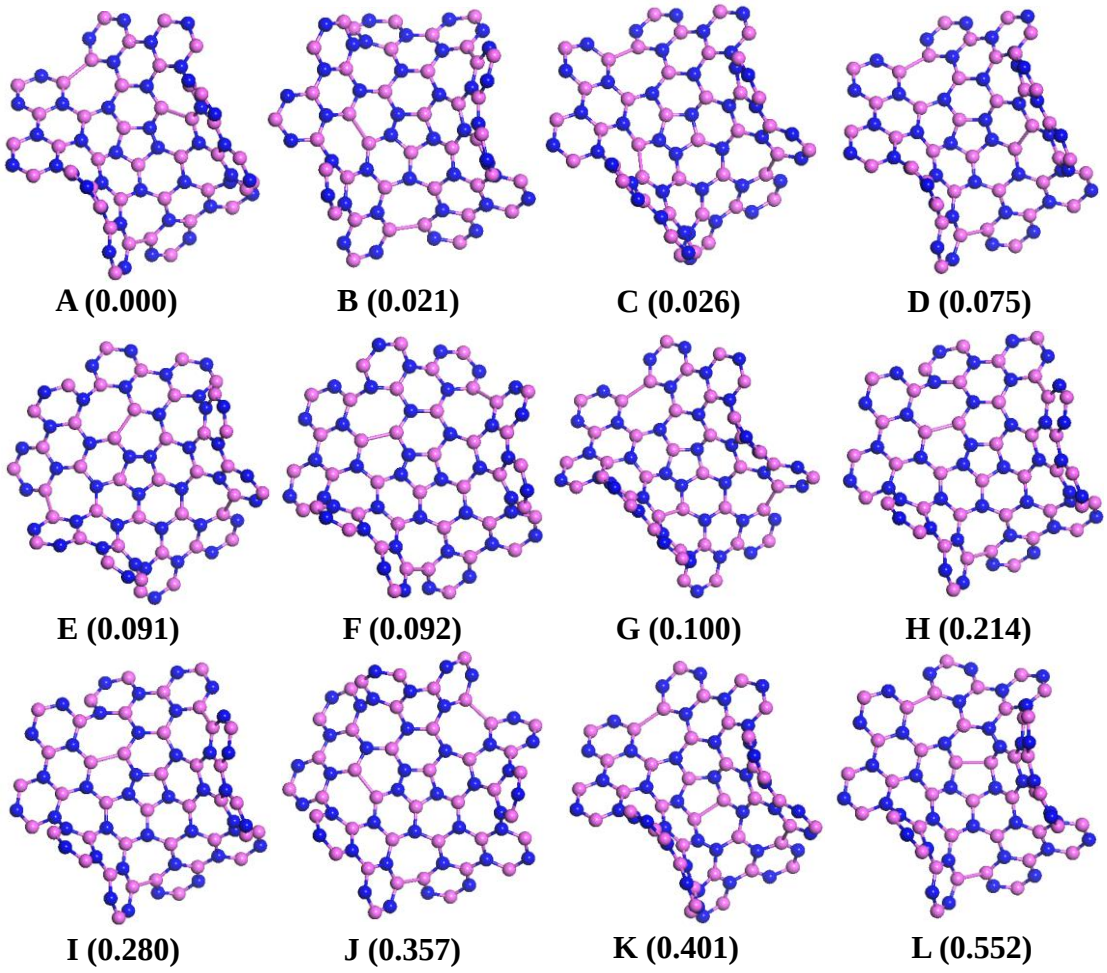

Figure S4 The first twelve low-lying warped $Al_{40}N_{40}H_{30}$ isomers.[18] The values in the parentheses are the relative energies (in units of eV) to the lowest-energy structure, i.e., isomer A. Aluminum and nitrogen atoms are shown by the pink and navy blue balls, respectively. All hydrogen atoms on the perimeter are omitted for clarity.

For the warped $Al_{40}N_{40}H_{30}$ structure, eleven low-lying isomers (B-L) are examined and shown in Fig. S4. The structural features of the warped $Al_{40}N_{40}H_{30}$ are very similar to those of the warped boron-nitride nanoplate, which favor the configurations with maximum 19 hexagons having AlNAlN alternation.

III. VDOS analysis of the optimized warped nanoplates

The vibration spectra of the optimized warped $C_{80}H_{30}$, $B_{40}N_{40}H_{30}$, and $Al_{40}N_{40}H_{30}$ are in the frequency range of (13.2 – 3242.3), (10.6 – 3622.2), and (3.5 – 3561.7) cm^{-1}, respectively. Since the high-frequency vibration modes stem from relative motion of the nearest neighbor atoms, they are correlated with the bond length and strength in systems. As illustrated in the vibrational density of states (VDOS) shown in Fig. S5, the highest vibration frequency of the warped $B_{40}N_{40}H_{30}$ is the higher than that of $C_{80}H_{30}$ and $Al_{40}N_{40}H_{30}$, reflecting a fact that the B-N bonds should be stronger than the C-C bonds or Al-N bonds.

The difference in the bowl-to-bowl inversion energy among the warped $C_{80}H_{30}$, $B_{40}N_{40}H_{30}$, and $Al_{40}N_{40}H_{30}$ is likely due to the difference in bowl depth and strength of chemical bonds. The bowl depth of the warped $C_{80}H_{30}$, $B_{40}N_{40}H_{30}$, and $Al_{40}N_{40}H_{30}$ is 0.37, 0.71, and 1.05 Å, respectively. Among them, the bowl inversion barrier of the warped $C_{80}H_{30}$ is only 1.7 kcal/mol, which is the lowest one due to the least bowl depth for $C_{80}H_{30}$ and relatively weak C-C bonds according to the frequency analysis. Although the bowl depth of the warped $B_{40}N_{40}H_{30}$ is smaller than that of the warped $Al_{40}N_{40}H_{30}$, the bowl inversion barrier of the $B_{40}N_{40}H_{30}$ (27.9 kcal/mol) is 4.7 kcal/mol higher than that of $Al_{40}N_{40}H_{30}$ (23.2 kcal/mol), due largely to the stronger B-N bonds than Al-N bonds.

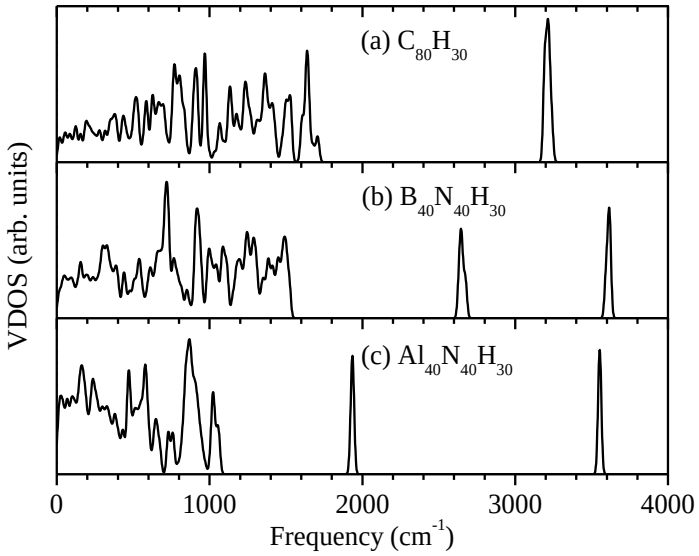

Figure S5 Vibrational densities of states (VDOS) of the optimized warped (a) $C_{80}H_{30}$, (b) $B_{40}N_{40}H_{30}$, and (c) $Al_{40}N_{40}H_{30}$. A broadening of the computed stick spectra with a Gaussian line shape function of 10 cm^{-1} full width at half-maximum.

IV. Flipping and racemization pathways of $B_{40}N_{40}H_{30}$ and associated coordinates

An enlarged view of Fig. 2. The corresponding Cartesian coordinates for the ground-state and transition-state structures are also given below.

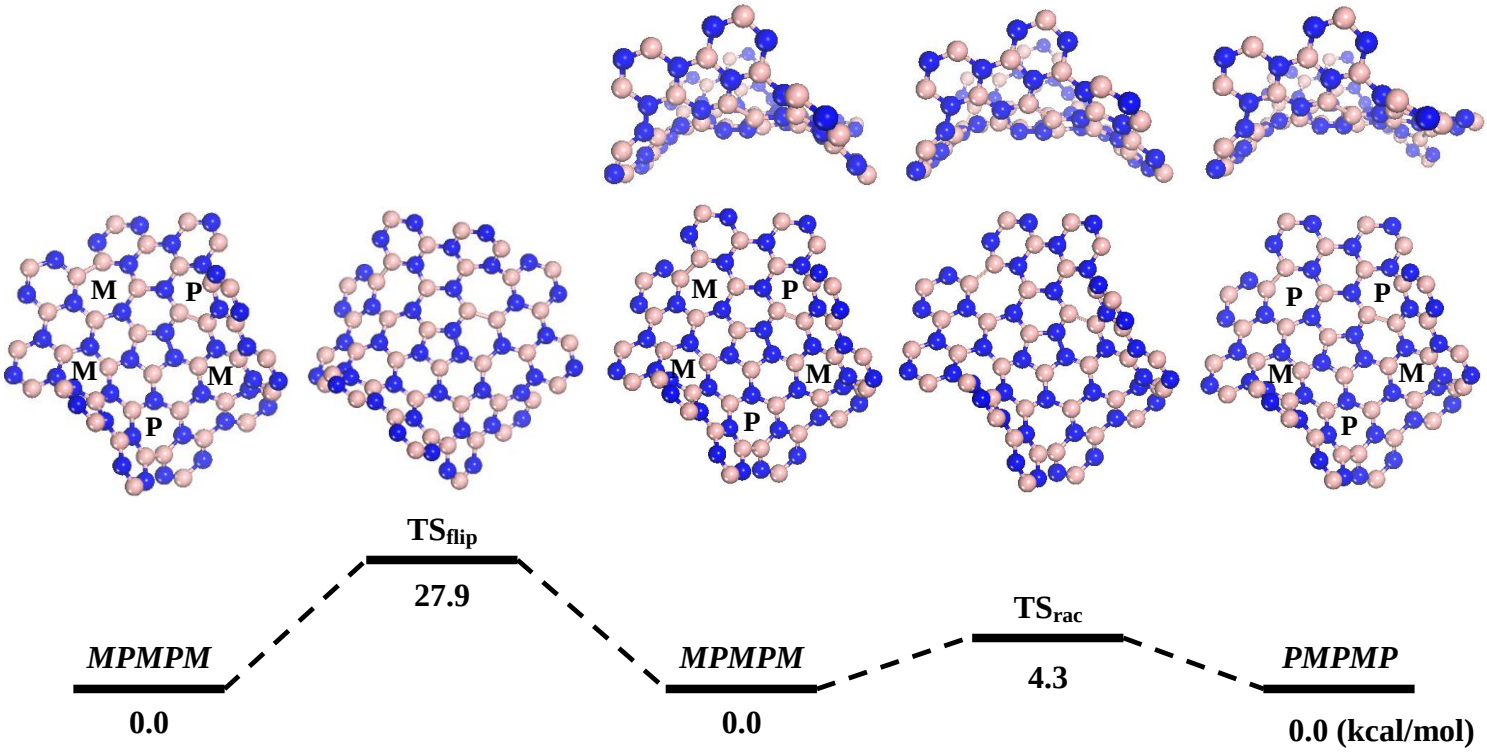

Figure S6 Bowl-to-Bowl inversion (left, *MPMPM*⇔TS$_{flip}$⇔*MPMPM*) and racemization (right, *MPMPM*⇔TS$_{rac}$⇔*PMPMP*) pathways of $B_{40}N_{40}H_{30}$, computed at the level of B3LYP/6-31G(d). All hydrogen atoms at the perimeter are omitted for clarity. Values (in unit of kcal/mol) are relative Gibbs free energies at 298.15 K and 1 atm. From the side view of nanoplates corresponding to the racemization pathway, the "flapping" between the *MPMPM* and *PMPMP* geometries can be seen.

$B_{40}N_{40}H_{30}$– GS- B3LYP

B	1.3301515	-0.0517758	-0.8068838	N	0.5322744	1.1317428	-0.8670765	H	1.7392782	-7.0889101	1.6019674
B	-0.8234064	0.6990888	-0.9211486	N	-0.8717431	-0.7324017	-1.0122685	H	3.6402041	-7.6996408	0.0936913
B	0.7891606	-2.3833902	-0.1904981	N	0.4572031	-1.1976382	-0.8820648	H	5.1484631	-6.2115427	-1.2302099
B	0.9314998	2.3026332	-0.1718929	N	2.7329703	-0.1042115	-0.5451745	H	5.7694550	-4.7817499	-2.4543760
B	-2.0297118	-1.4165818	-0.5500158	N	-1.9510652	1.5377311	-0.6946511	H	7.3249966	-3.2206690	-3.7165404
B	-0.5588819	-3.1640368	0.5111808	N	2.2325759	-2.5721238	-0.0737722	H	7.0191341	-0.8258024	-2.9105229
B	-1.6103777	2.7922152	-0.0324102	N	-1.9031275	-2.6756040	0.1678992	H	7.7483758	0.1246620	-1.0773075
B	-3.1989381	0.8132942	-1.0200061	N	-3.2571459	-0.6348270	-0.8122261	H	8.7796701	2.4208108	-0.6696285
B	3.2993862	1.2654942	-0.3945997	N	2.3962582	2.4029942	-0.0042088	H	6.9283905	4.1580211	-0.4283056
B	3.1830842	-1.5311893	-0.5179039	N	-0.1937338	3.1386066	0.3027282	H	5.7292556	5.6956054	-1.0325447
B	2.6737859	-3.9495973	0.1238742	N	3.8546534	-4.4042366	-0.5999187	H	4.0364008	7.4123860	-0.3395777
B	4.6565667	-3.4100609	-1.3013968	N	4.4550161	-1.9870093	-1.0400486	H	1.9527706	7.0553644	1.0879028
B	-3.0524288	-3.2454768	0.8591279	N	-2.8667193	-3.9018380	2.1465174	H	2.6344371	5.3704625	3.4557517
B	-1.5072766	-4.2190538	2.5788926	N	-0.4063993	-4.0611794	1.6363550	H	0.6153369	5.3510580	5.0150886
B	-5.1436719	0.6784554	-2.5876092	N	-4.3002086	1.4650963	-1.6999106	H	-1.8045453	5.0875126	4.3839687
B	-4.3700682	-1.3605250	-1.3880970	N	-5.1530507	-0.7770591	-2.4672062	H	-3.3818289	5.6565461	3.1094938
B	-0.0220722	4.0361273	1.4312987	N	-1.1397617	4.3953734	2.2924683	H	-5.6707763	5.9914176	2.0503952
B	-2.4582498	4.4127262	1.6753938	N	-2.6693353	3.6806937	0.4395523	H	-5.8340709	4.7194299	-0.1419254
B	5.2158501	2.9374110	-0.4904770	N	4.7189618	1.5643154	-0.5840274	H	-5.4165503	4.5355485	-2.5738701
B	2.9728028	3.7216976	0.1899911	N	4.2942030	4.0439849	-0.3089595	H	-6.7524574	3.3542008	-4.3811908
B	2.3293218	-6.2836959	0.9426040	N	1.9653006	-4.8901457	0.9798673	H	-6.5295763	0.8362123	-4.1751274
B	4.2040262	-5.7988266	-0.6209415	N	3.4046644	-6.7164458	0.1110844	H	-6.5413071	-1.2123447	-4.2572277
B	6.5231786	-2.8723173	-2.8985787	N	5.6679123	-3.7984849	-2.2437982	H	-6.5150857	-3.6359093	-3.6406291
B	5.4317770	-1.0361083	-1.5356079	N	6.3930056	-1.5068058	-2.5000629	H	-5.6315271	-4.7272463	-1.5186463
B	5.6896974	0.5391629	-0.9578495	N	7.0913779	0.8754382	-0.9088016	H	-6.6480176	-3.3190950	0.7249358
B	7.6059777	2.1872316	-0.6943052	N	6.6265001	3.2001204	-0.5411559	H	-6.1110704	-4.2748282	3.0125987
B	4.6800648	5.4127332	-0.5302274	N	3.7815982	6.4507049	-0.1595037	H	-3.8868168	-4.7985677	4.0138833
B	2.6155365	6.1800590	0.6194301	N	2.2671044	4.8092917	0.8335080	H	-1.9709356	-4.7661368	4.5674370
B	1.5359303	5.0210995	3.1446618	N	1.2644417	4.5665136	1.8165513	H	0.3167666	-5.4400830	5.4309811
B	-0.9006119	4.8627191	3.6304928	N	0.4426383	5.0497287	4.0654979	H	2.0446587	-5.3557229	3.5692058
B	-4.7913682	5.3279304	1.5810556	N	-3.5399066	5.1708929	2.2367407				
B	-3.9455259	3.7878188	-0.2502011	N	-4.9403400	4.6549369	0.3287886				
B	-4.4662105	2.9086509	-1.6156878	N	-5.3233088	3.5276382	-2.5904218				
B	-6.0639221	2.7980875	-3.5747203	N	-5.9704778	1.3780570	-3.5298186				
B	-5.9374391	-1.6362515	-3.3135496	N	-5.9848009	-3.0315461	-3.0272648				
B	-5.4476684	-3.5882004	-1.8236622	N	-4.6831350	-2.7162588	-0.9865078				
B	-5.5438313	-3.4900840	1.1428240	N	-4.4006719	-3.1530499	0.3462750				
B	-4.0059143	-4.2783827	2.9431671	N	-5.3126835	-4.0272573	2.4434895				
B	0.0938373	-5.0711342	4.3146702	N	-1.2149362	-4.6934236	3.9006576				
B	0.9012394	-4.6090179	1.9708865	N	1.1239588	-5.0131198	3.3271426				

$B_{40}N_{40}H_{30}$ –TSflip- B3LYP

B	-0.2881349	1.2217511	0.0467628	N	0.9235058	-0.7227880	0.0933292	H	-2.9365919	-6.9639872	0.1783601
B	-0.4560952	-1.0428337	0.2313806	N	1.0293007	0.6755474	0.0706387	H	-2.0144313	-8.2726672	-1.7974976
B	1.9659720	-1.6478250	-0.1121398	N	-1.1949630	0.1610427	0.2197540	H	0.0323340	-7.1121851	-2.7580150
B	2.2075751	1.4126782	0.1561886	N	-1.0243417	-2.3392026	0.3206861	H	1.4049672	-6.1563815	-3.9606574
B	-2.5876084	0.2588876	0.1563591	N	-0.6268613	2.5807365	-0.1825038	H	3.7440714	-5.3644785	-4.4289983
B	-0.0428315	-3.3568080	-0.0933725	N	-3.2487082	-0.9967388	0.5455604	H	5.3189169	-4.1475107	-2.8413643
B	-2.4494715	-2.2374399	0.7601696	N	-3.0422118	1.5751570	-0.3069569	H	5.3213094	-5.4768717	-0.2236036
B	0.5619208	3.4469077	0.0273325	N	1.9205984	2.8653419	0.2567498	H	7.2881208	-4.4356126	1.0205516
B	-2.0586028	2.6629110	-0.6186334	N	3.3404600	-1.1023528	-0.1058251	H	7.9041625	-1.9939190	1.1241145
B	3.5642912	0.3566012	0.1477088	N	1.4016943	-3.0196571	-0.3237278	H	8.1456971	-0.1432887	-0.0243574
B	0.1608068	-5.4188912	-1.5016711	N	-0.4962714	-4.7024569	-0.4250905	H	8.6824971	2.3304909	-0.3337255
B	2.1194464	-3.9213005	-1.2123402	N	1.4130438	-4.9025354	-2.0294831	H	6.6303165	3.7465464	0.1299176
B	-4.5184087	-0.8507738	1.2293626	N	-4.8496295	-1.6931295	2.3660206	H	6.0597407	3.3828533	2.6682302
B	-4.1285125	-2.9558721	2.4963769	N	-3.0592311	-3.2863968	1.5604074	H	4.9227325	5.2509342	3.8614500
B	-3.6672035	3.4964503	-2.3792140	N	-2.5113110	3.7170038	-1.5135143	H	2.8754189	6.5341987	3.1631821
B	-4.3677038	1.6208874	-0.8993530	N	-4.6220140	2.4346805	-2.0758631	H	1.7529714	7.5262718	1.8032406
B	2.9180831	3.6675837	0.9565651	N	2.5129700	4.9557436	1.5225276	H	-0.1445940	8.9076068	0.8336171
B	1.3502089	5.6303099	0.9657640	N	0.4171345	4.8905994	0.1352839	H	-1.5895014	7.4816723	-0.7002431
B	4.5056914	-1.9738189	-0.0835433	N	5.8139053	-1.4797983	0.3148203	H	-1.4711987	6.6152535	-2.9277580
B	6.0514005	-0.0489694	0.2340164	N	4.9103450	0.8498071	0.2993965	H	-3.2397469	6.2072875	-4.7168374
B	-1.6513707	-5.2917515	0.2267416	N	-2.1205339	-6.5620031	-0.2653809	H	-4.6362176	4.1722742	-4.1247943
B	-1.5588565	-7.2431725	-1.3894440	N	-0.4200203	-6.6389084	-1.9876031	H	-6.0256420	2.8307991	-3.8686267
B	2.0054074	-5.4189390	-3.2323423	N	3.3320284	-5.0299893	-3.5684754	H	-7.5731199	1.0784037	-3.0078974
B	4.1566854	-4.3293969	-2.6375578	N	3.5478096	-3.8475262	-1.4340038	H	-7.4724057	-0.2015519	-0.8140816
B	5.4423643	-4.3111037	0.0038296	N	4.4501689	-3.3776125	-0.4332555	H	-7.1783122	1.5569568	1.5169210
B	6.8455723	-2.3927902	0.7317213	N	6.5819320	-3.7907651	0.6922175	H	-7.3311016	0.1974975	3.6626272
B	7.5949913	1.8924452	-0.0943317	N	7.3657397	0.4948612	0.0584940	H	-6.1464852	-1.9160135	4.2628556
B	5.1709175	2.2730156	0.4903825	N	6.4665639	2.7488390	0.0893468	H	-5.1819859	-3.6599421	4.1833904
B	4.9935114	3.8049577	2.3303029	N	4.2941054	3.2299808	1.2025559	H	-4.1884213	-5.9782274	4.4575667
B	3.2417549	5.5343962	2.6150732	N	4.4180304	4.8807475	3.0675299	H	-2.5547670	-6.4791511	2.5716964
B	0.0323675	7.7430336	0.6176436	N	1.1095913	7.0270333	1.2045305				
B	-0.6648253	5.5927410	-0.5274063	N	-0.8159368	7.0000359	-0.2597840				
B	-1.7481955	4.9503470	-1.6671584	N	-2.0364855	5.7848877	-2.8030888				
B	-3.0556885	5.5065130	-3.7638512	N	-3.8612946	4.3651695	-3.5054167				
B	-5.8080815	2.2188211	-2.8631971	N	-6.7505693	1.2405453	-2.4425324				
B	-6.6288399	0.5490619	-1.1998948	N	-5.4519322	0.7878752	-0.4204058				
B	-6.4718371	0.6340982	1.7878784	N	-5.4427812	0.2108126	0.8890992				
B	-5.8874069	-1.2871659	3.2773043	N	-6.6179685	-0.0954038	3.0082125				
B	-3.8875983	-5.2064633	3.5931637	N	-4.4693230	-3.9114520	3.5118897				
B	-2.5322146	-4.6450894	1.5301096	N	-2.9502730	-5.5473354	2.5691894				

$B_{40}N_{40}H_{30}$ –TSrac- B3LYP

B	-1.3441492	0.0449641	-0.9355268	N	-2.7414094	0.0987168	-0.6760476	H	-2.2340942	-6.5703130	2.3067195
B	0.8006171	-0.7116241	-1.0162974	N	-0.5527585	-1.1467707	-0.9586214	H	-4.3584554	-7.1781473	1.0531873
B	-0.9510683	-2.2420294	-0.1408371	N	1.9217542	-1.5411308	-0.7239529	H	-5.8036376	-5.7291288	-0.3585921
B	1.5772789	-2.7342971	0.0389691	N	-2.4059086	-2.3334970	0.0353301	H	-6.3233093	-4.5066035	-1.7394537
B	3.1757505	-0.8473702	-1.0832410	N	0.1616291	-3.0284092	0.4266399	H	-7.8213257	-3.0500787	-3.1944491
B	-3.2875703	-1.2712612	-0.5357222	N	-4.2702039	-4.0127556	-0.1303101	H	-7.1699274	-0.6601273	-2.9984238
B	-3.0097572	-3.5845855	0.4497035	N	-4.6095592	-1.6500056	-1.0111011	H	6.5264745	-1.0744949	-4.2085388
B	-4.9947561	-3.0648907	-0.9698797	N	2.6296628	-3.5976667	0.5643363	H	6.7611419	-3.5992575	-4.2391498
B	2.4202600	-4.2151724	1.8608165	N	1.1359405	-4.0444025	2.5276502	H	5.3970117	-4.6642626	-2.3842846
B	-0.0102379	-3.7304956	1.6859904	N	4.2770700	-1.5443778	-1.7161805	H	5.7569797	-4.7603429	0.0265278
B	5.1185299	-0.8150467	-2.6537510	N	-2.3808527	-4.4828141	1.3895609	H	5.5660859	-5.9110555	2.2801290
B	-2.8326421	-5.8274125	1.5902705	N	-4.0167646	-6.2372897	0.9107622	H	3.3147335	-5.4060550	3.3564860
B	-4.7706082	-5.3429540	0.1050966	N	-6.1015144	-3.5214659	-1.7574126	H	1.9018575	-4.4268373	4.6623485
B	-6.9028880	-2.6549772	-2.5359990	N	-6.5599751	-1.2724441	-2.4776923	H	-0.4753450	-4.2878110	5.4842894
B	-5.4648698	-0.7010410	-1.7359848	N	5.9625642	-1.5732795	-3.5332426	H	-2.6037868	-4.3967392	4.0872275
B	6.0598142	-2.9928396	-3.4814048	N	5.3054970	-3.6590892	-2.4628965	H	-1.8212213	6.7781098	2.1740587
B	4.4374821	-2.9805612	-1.5384307	N	4.8679592	-4.6418853	0.4957055	H	-3.9480951	7.4351772	1.0361067
B	3.8967620	-3.7785841	-0.1277317	N	3.4736033	-4.9928334	2.4472367	H	-5.5297782	6.0310954	-0.2760674
B	4.7073529	-5.2397662	1.7844593	N	-0.3516258	-4.1927440	4.4853104	H	-6.1384114	4.8621383	-1.6605386
B	0.9638606	-4.2418445	3.9405349	N	-1.3083398	-4.0705940	2.2369485	H	-7.6770033	3.4988797	-3.1586104
B	-1.5077393	-4.2275430	3.6446768	N	0.8505071	0.7178409	-1.1631024	H	-7.0961289	1.0864042	-3.0537182
B	-0.8101462	2.3475147	-0.2707664	N	-0.4790901	1.1937859	-1.0267714	H	6.4382502	0.9674749	-4.5033666
B	2.0127808	1.4024836	-0.7159974	N	-2.2541579	2.5188054	-0.0983739	H	6.3452831	3.4338791	-4.0956802
B	0.5627420	3.1044200	0.4287595	N	1.8998479	2.6633081	-0.0071887	H	5.4980311	4.6753577	-2.0425873
B	-3.2152718	1.4950700	-0.5791728	N	3.2373286	0.6080037	-0.9601218	H	6.6510448	3.4997959	0.2057885
B	-2.7409955	3.8153363	0.3547979	N	-4.0350508	4.2702954	-0.1389820	H	6.2341437	4.5382016	2.4783045
B	-4.8415492	3.3612562	-0.9482982	N	-4.5321505	1.9306502	-1.0100412	H	4.0654376	4.9170884	3.6621539
B	3.0811047	3.2598334	0.6029618	N	2.9671470	3.9064300	1.9020620	H	2.2507121	4.4770657	4.4575063
B	1.6353974	4.0794662	2.4758655	N	0.4642954	3.9166274	1.6219062	H	0.0091460	4.8462526	5.5927263
B	4.3284309	1.3015230	-1.6078272	N	5.1045440	0.6459670	-2.6493325	H	-1.8753174	4.8062592	3.8904475
B	-2.4445418	6.0273012	1.4825109	N	-1.9976342	4.6735066	1.2690228				
B	-4.4792520	5.6143823	0.1184982	N	-3.6473698	6.4842036	0.8702536				
B	-6.7779126	3.0528628	-2.5056334	N	-5.9541316	3.8698248	-1.6967947				
B	-5.4264465	1.0284448	-1.7391996	N	-6.4832622	1.6574004	-2.4908529				
B	5.8432223	1.4529121	-3.5838717	N	5.8510630	2.8688875	-3.4179717				
B	5.3344336	3.5111198	-2.2474251	N	4.6187073	2.6922598	-1.3191992				
B	5.5717915	3.6367099	0.6950162	N	4.3942011	3.2064032	-0.0020378				
B	4.1361532	4.3844135	2.5931911	N	5.4102370	4.2203012	1.9856461				
B	0.1518203	4.6163295	4.4271338	N	1.4399169	4.4057417	3.8583725				
B	-0.8359539	4.3408185	2.1218878	N	-0.9598081	4.5664594	3.5327328				

V. Movie S1: simulation of the iterative racemization transitions

Movie-S1.mpeg.

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