Electronic Supporting Information (ESI)

Conformational Switch In the Crystal States of A Calix[4]arene

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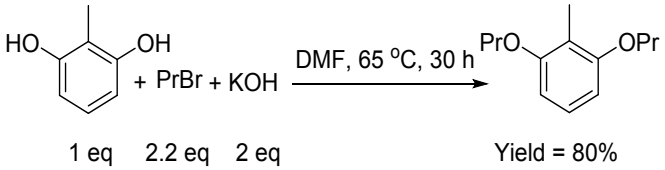
S1. General Methods and Synthesis

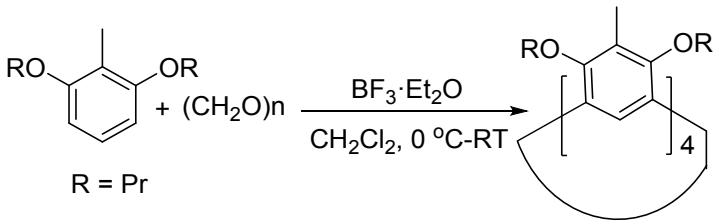
All reactions were performed under nitrogen atmosphere unless otherwise noted. NMR spectra were recorded on Varian 400 MHz NMR spectrometer. Mass spectra were recorded on Bruker Daltonics MALDI-TOF mass spectrometer and Dithranol has been used as the matrix. All solvents and starting materials are used without further purification.

Synthesis of 2-methyl-1,3-dipropoxybenzene:



The mixture of 2-methyresorcinol (6.2 g, 50 mmol, 1.0 eq), 1-bromopropane (2.2 eq) (13.53 g, 110 mmol, 2.2 eq) and KOH (6.16 g, 110 mmol, 2.2 eq) as the base in the N,N-dimethylformamide (DMF, 100 mL) stirred for 30 h at 65 °C. After cooled down to room temperature, water (100 mL) was added to the mixture and organic product extracted with dichloromethane (DCM, 3×100 mL). The collected DCM dried with $MgSO_4$ and evaporated under reduced pressure to obtain a brownish oil, which was further purified by flash column (silica gel and hexanes as eluent). The pure product was obtained as colorless oil with 80% yield (8.32 g), ^{1}H-NMR ($CDCl_3$ at 20 °C) δ: 1.06 (t, 6H), 1.81 (sext, 4H), 2.14 (s, 3H), 3.93 (t, 4H), 6.51 (d, 2H), 7.07 (t, 1H); ^{13}C-NMR ($CDCl_3$ at 20 °C) δ: 8.3, 10.8, 22.9, 69.9, 104.5, 115.2, 126.1, 158.0.

Synthesis of Calixarene:



To a solution of 2,6-dipropoxytoluene (1.04 g, 5 mmol, 1.0 eq) in anhydrous dichloromethane (30 ml), paraformaldehyde was added (0.30 g, 10 mmol, 2.0 eq) under the nitrogen atmosphere. The mixture was cooled down to 0 °C with ice bath, $BF_3 \cdot Et_2O$ (1 ml, 15 mmol, 3 eq) was added at one portion and the reaction was allowed to slowly warm up to room temperature and stirred for overnight. The reaction was quenched by adding saturated sodium bicarbonate solution (30 ml) to the mixture and keep stirring vigorously for 30 min. The organic layer was separated using the separation funnel, dried with $MgSO_4$ and evaporated to give crude product. The pure product (white solid) was obtained by further purification with flash column (silica gel and Hexane/Ethyl acetate = 10/3 as eluent). (yield = 85%, 0.936 g). The MALDI-TOF spectrum is collected by dissolving the pure product in potassium acetate solution in DCM. MALDI Mass (calculated: 880.59; experimental: 880.76); ^{1}H-NMR ($CDCl_3$ at 20 °C) δ: 0.99 (t, 24H), 1.72 (sext, 16H), 2.15 (s, 12H), 3.63 (t, 16H), 3.83 (s, 8H), 6.18 (s, 4H); ^{13}C-NMR ($CDCl_3$ at 20 °C) δ: 10.1, 10.7, 23.7, 29.5, 74.3, 123.7, 128.9, 154.9. m.p. (Closed-I): 241-243 °C. m.p. (Open): 254-255 °C.

Figure S1. ^{1}H and ^{13}C NMR spectra of 2,6-diproxytoluene ($CDCl_3$, 20 °C)

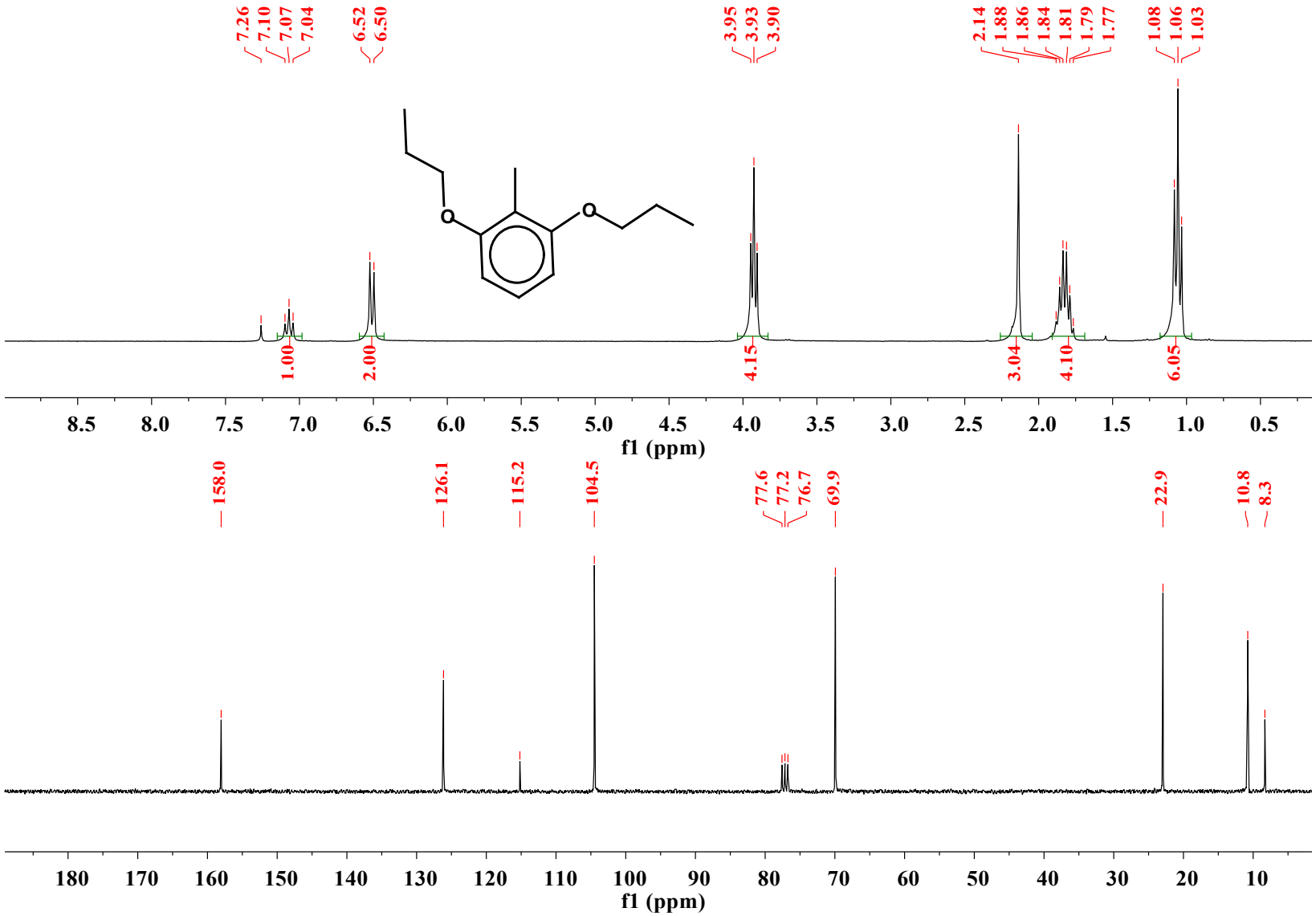


Figure S2. ^{1}H and ^{13}C NMR spectra of calixarene ($CDCl_3$, 20 °C)

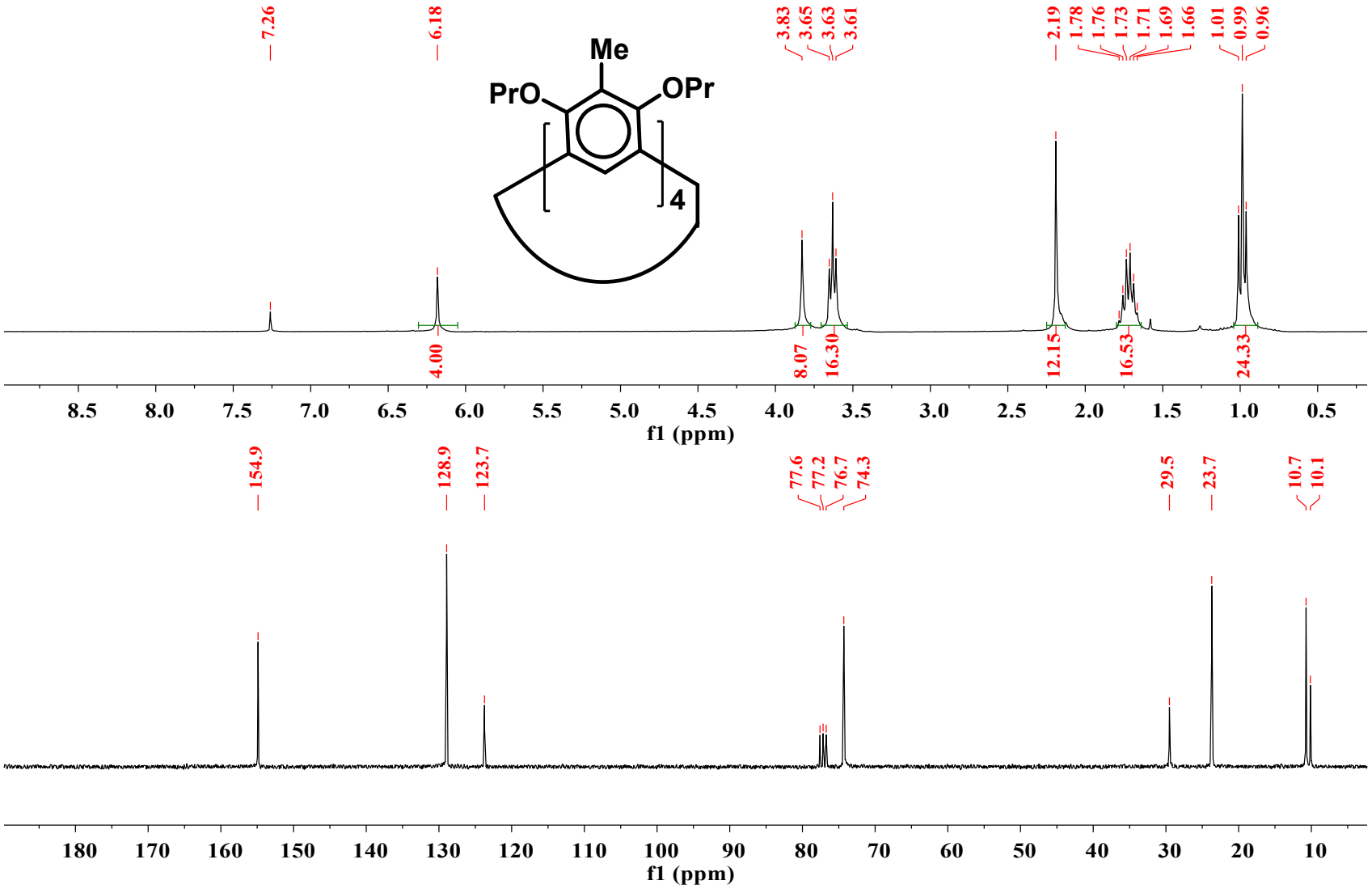


Figure S3. Variable temperature ^{1}H NMR spectra of calixarene (CD_2Cl_2, 20 °C to -70 °C)

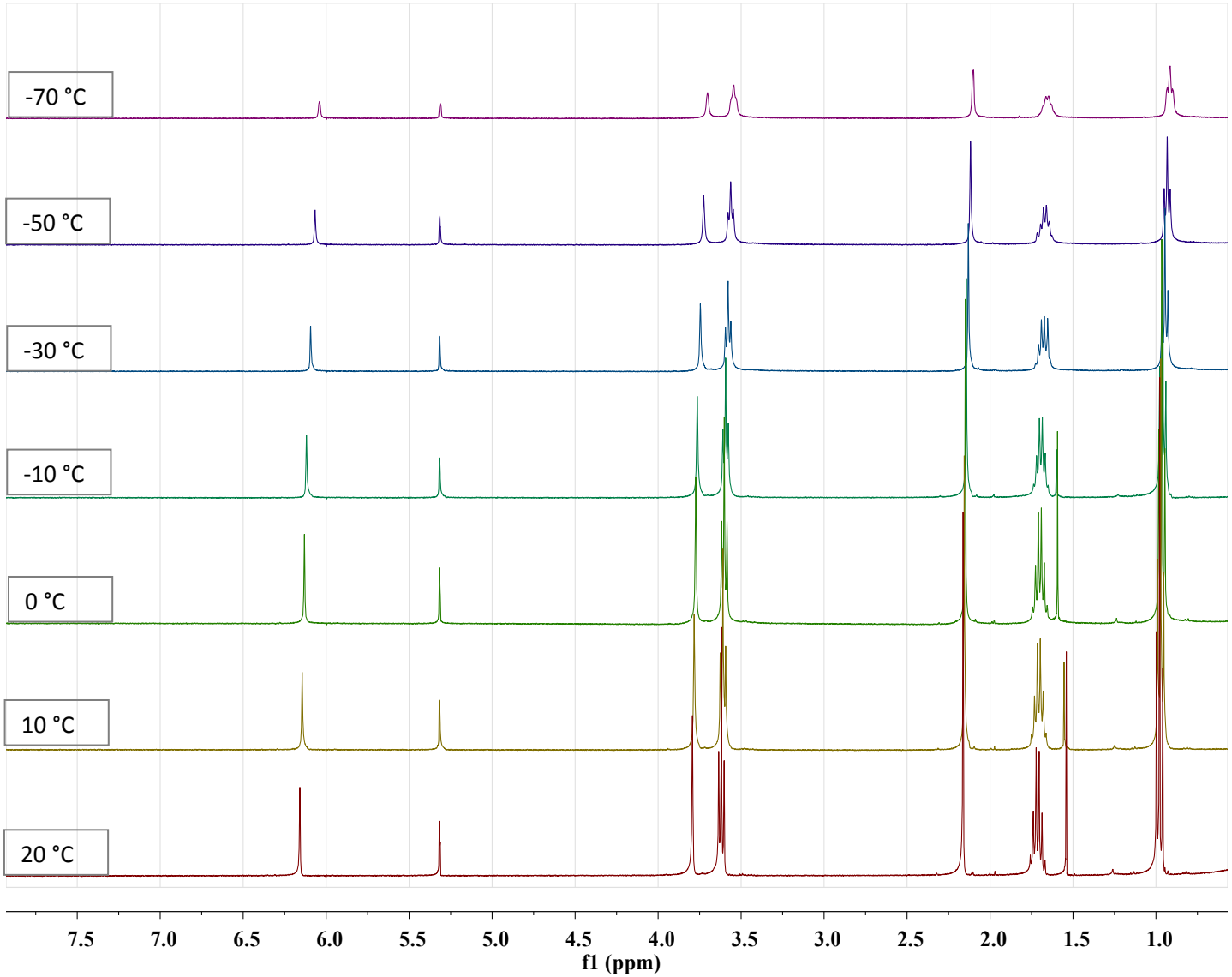
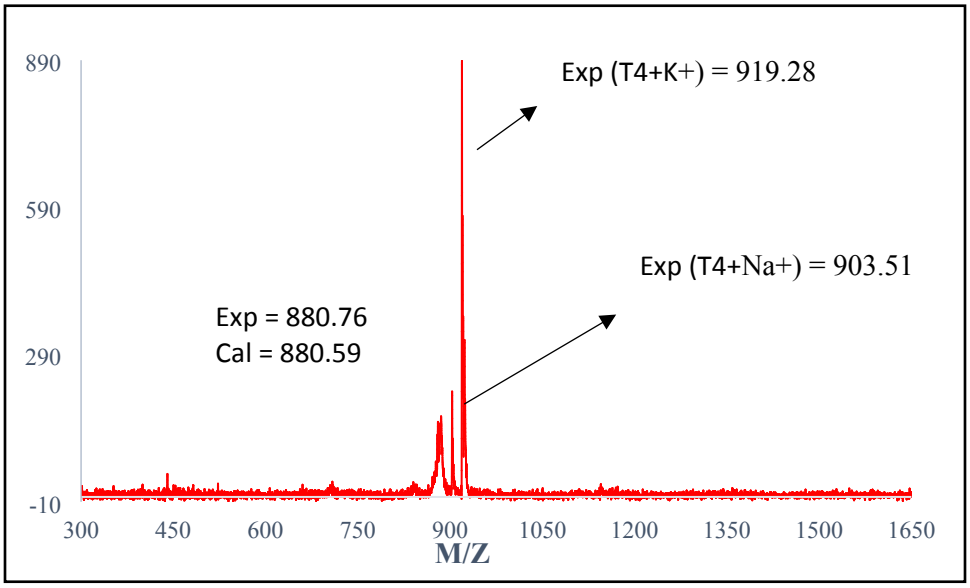


Figure S4. MALDI-TOF data of calixarene product.



S2. X-Ray Crystallography Data

Table S1. X-ray crystallographic data collection of **Closed-I**, **Intermediate**, **Closed-II** and **Open** conformations.

Identification code	Closed-I (kad1j)	Intermediate (kad1i)	Closed-II (kad1ix)	Open (kad1r)
Empirical formula	$C_{56}H_{80}O_8$	$C_{56}H_{80}O_8$	$C_{56}H_{80}O_8$	$C_{56}H_{80}O_8$
Formula weight	881.20	881.20	881.20	881.20
Temperature/K	250.00(14)	210.05(10)	99.8(4)	100.05(10)
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1	P-1
a/Å	12.6612(4)	13.0566(3)	12.9716(3)	6.8417(3)
b/Å	14.1198(3)	13.1211(3)	13.0379(3)	12.7268(6)
c/Å	15.7544(4)	15.1852(3)	14.9706(3)	15.2879(6)
α/°	104.714(2)	92.7541(18)	95.6026(16)	104.555(4)
β/°	96.728(2)	96.9186(18)	92.8626(16)	99.233(3)
γ/°	99.499(2)	94.0236(18)	94.0129(16)	98.058(4)
Volume/Å^3	2649.12(12)	2571.97(10)	2509.49(9)	1248.84(9)
Z	2	2	2	1
ρ_{calc}g1.47/cm^3	1.105	1.138	1.166	1.172
μ/mm^{-1}	0.568	0.585	0.599	0.602
F(000)	960.0	960.0	960.0	480.0
Crystal size/mm^3	0.463 × 0.398 × 0.177	0.372 × 0.238 × 0.093	0.332 × 0.233 × 0.093	0.384 × 0.03 × 0.014
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.18 to 141.192	6.84 to 141.194	6.832 to 141.226	7.308 to 141.264
Index ranges	-15 ≤ h ≤ 15, -17 ≤ k ≤ 17, -19 ≤ l ≤ 17	-15 ≤ h ≤ 15, -16 ≤ k ≤ 15, -18 ≤ l ≤ 18	-15 ≤ h ≤ 15, -15 ≤ k ≤ 15, -18 ≤ l ≤ 18	-8 ≤ h ≤ 7, -15 ≤ k ≤ 15, -18 ≤ l ≤ 18
Reflections collected	48412	46925	45942	19839
Independent reflections	10031 [R_{int} = 0.0194, R_{sigma} = 0.0116]	9768 [R_{int} = 0.0241, R_{sigma} = 0.0143]	9537 [R_{int} = 0.0262, R_{sigma} = 0.0171]	4745 [R_{int} = 0.0347, R_{sigma} = 0.0272]
Data/restraints/parameters	10031/6/636	9768/139/692	9537/0/589	4745/0/297
Goodness-of-fit on F^2	1.065	1.044	1.037	1.018
Final R indexes [I>=2σ (I)]	R_1 = 0.0748, wR_2 = 0.2460	R_1 = 0.0581, wR_2 = 0.1717	R_1 = 0.0359, wR_2 = 0.0935	R_1 = 0.0363, wR_2 = 0.0895
Final R indexes [all data]	R_1 = 0.0844, wR_2 = 0.2636	R_1 = 0.0666, wR_2 = 0.1837	R_1 = 0.0411, wR_2 = 0.0981	R_1 = 0.0463, wR_2 = 0.0973
Largest diff. peak/hole / e Å^{-3}	0.40/-0.22	0.57/-0.35	0.45/-0.24	0.20/-0.19

Single crystals X-ray diffraction data were collected using an Oxford SuperNova diffractometer with Cu(Kα) (λ = 1.54184) radiation. Using Olex2[1], the structure was solved with the ShelXS structure solution program[2] using Direct Methods and refined with the ShelXL refinement package[3] using Least Squares minimization.

Figure S5. The structure superimposition of Closed-I (grey) and Closed-II (blue) conformation; hydrogen atoms are omitted for clarity.

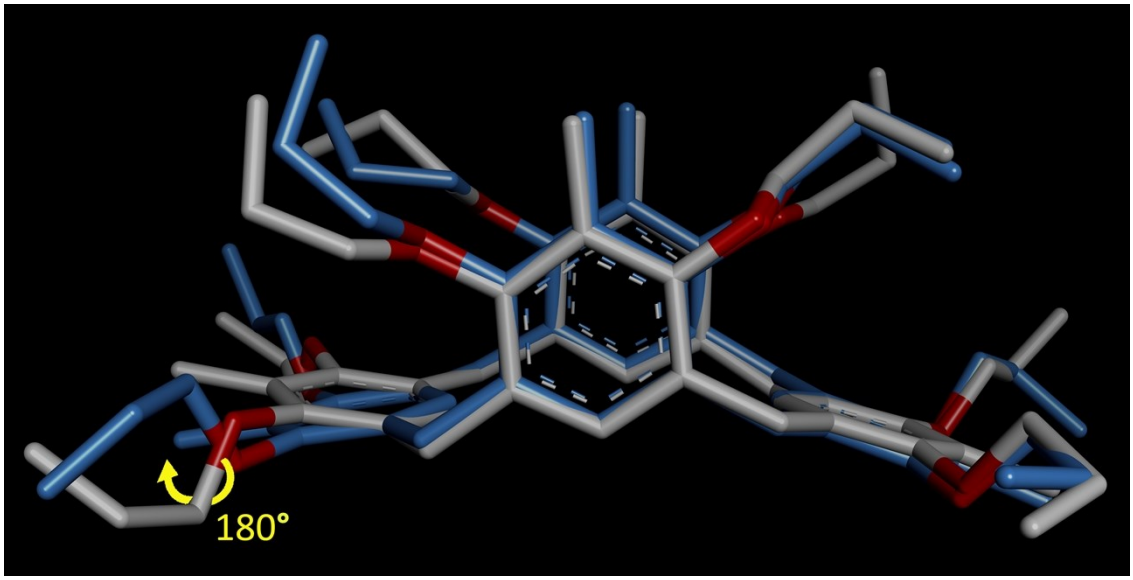


Figure S6. The structure superimposition of Closed-I (grey) and Closed-II (blue) of tetracyclic backbones; hydrogen atoms and OPr groups are omitted for clarity.

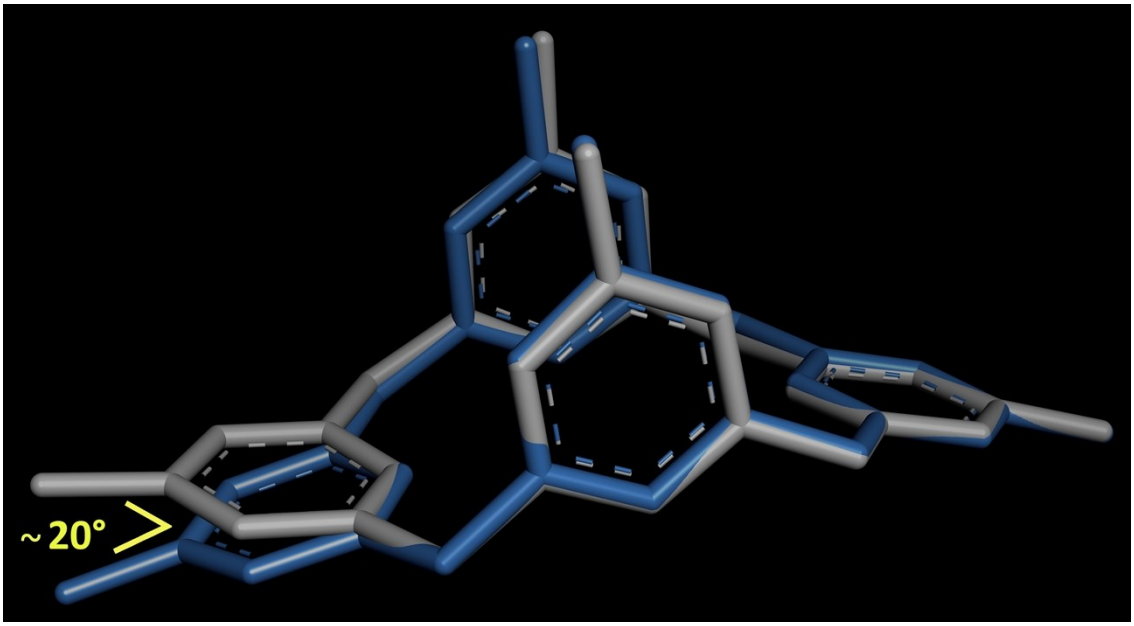
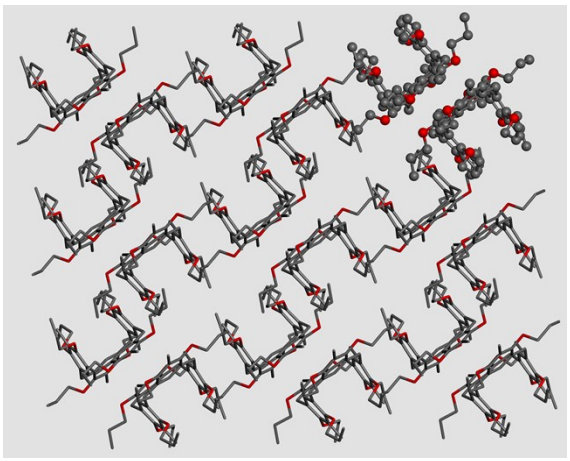
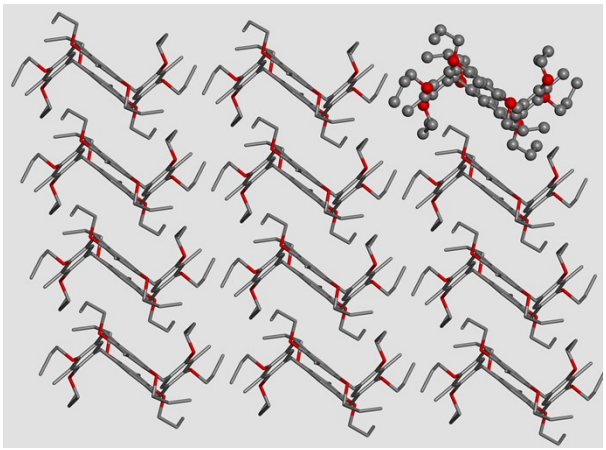


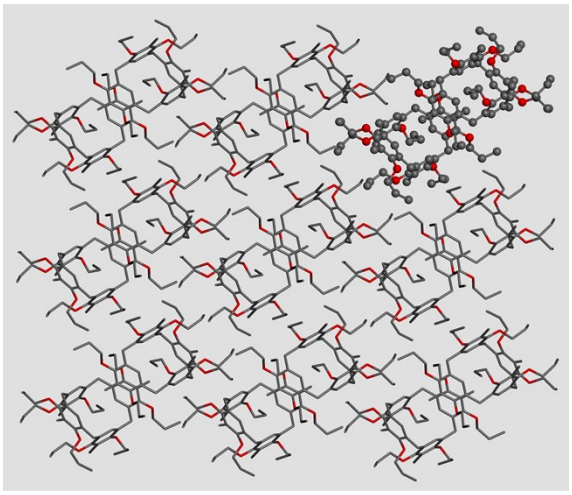
Figure S7. Packing order of Closed-I and Open forms along various planes.



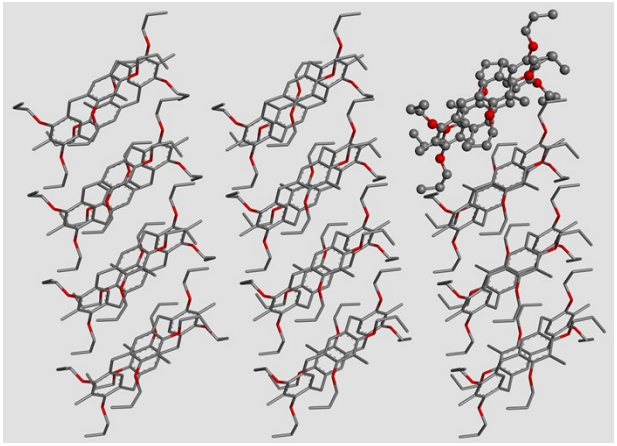
Closed, ab



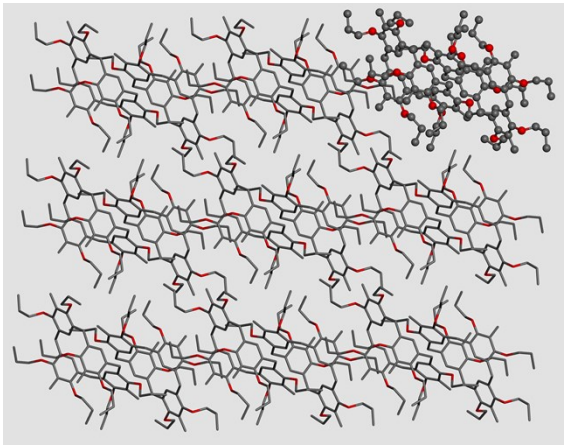
Open, ab



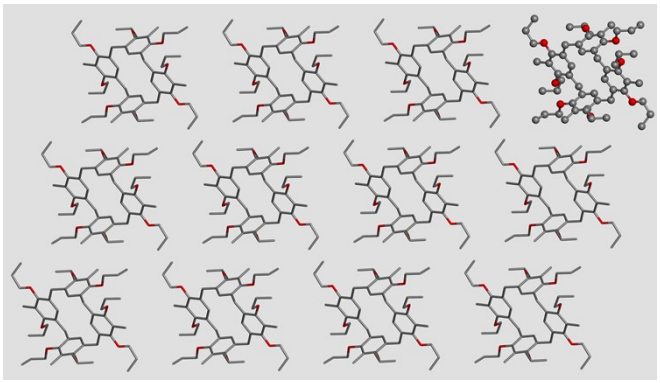
Closed, ac



Open, ac



Closed, bc



Open, bc

S3. PXRD Data

Figure S8. Schematic representation of enantiotropic polymorphism where T_0 denotes the transition temperature from closed-I to Closed-II.

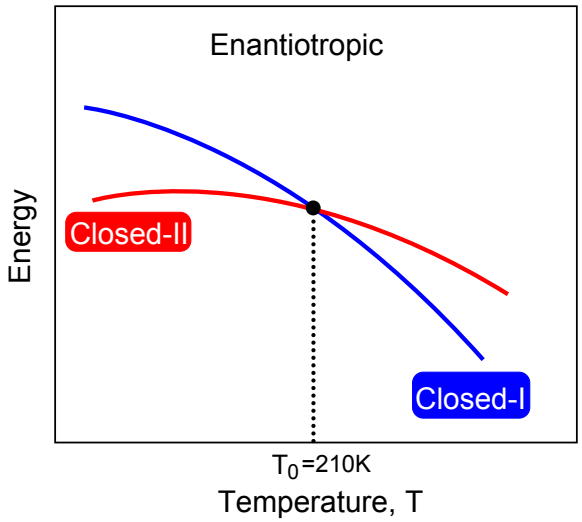


Figure S9. PXRD results of heating process (from 100K to 250 K) which corresponding to Closed-II to Closed-I transition.

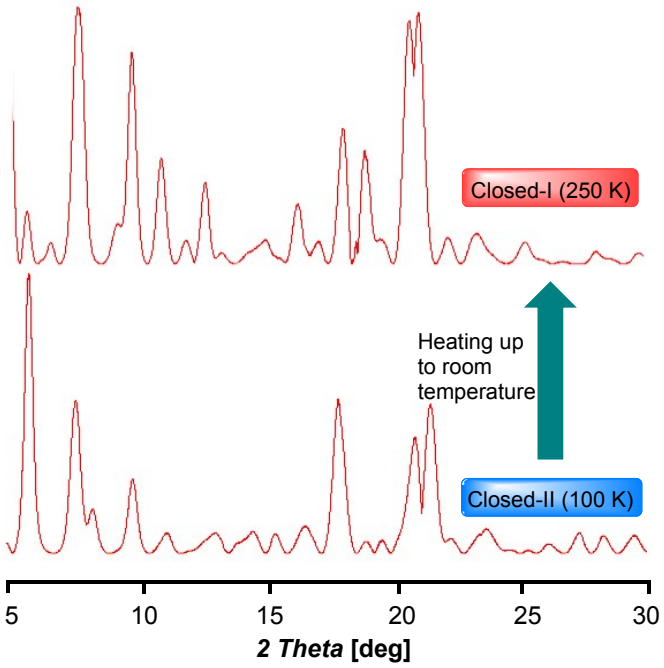


Figure S10. PXRD results of cooling process (from 270K to 100 K) which corresponding to Closed-I to Closed-II transition. The simulated results are also included.

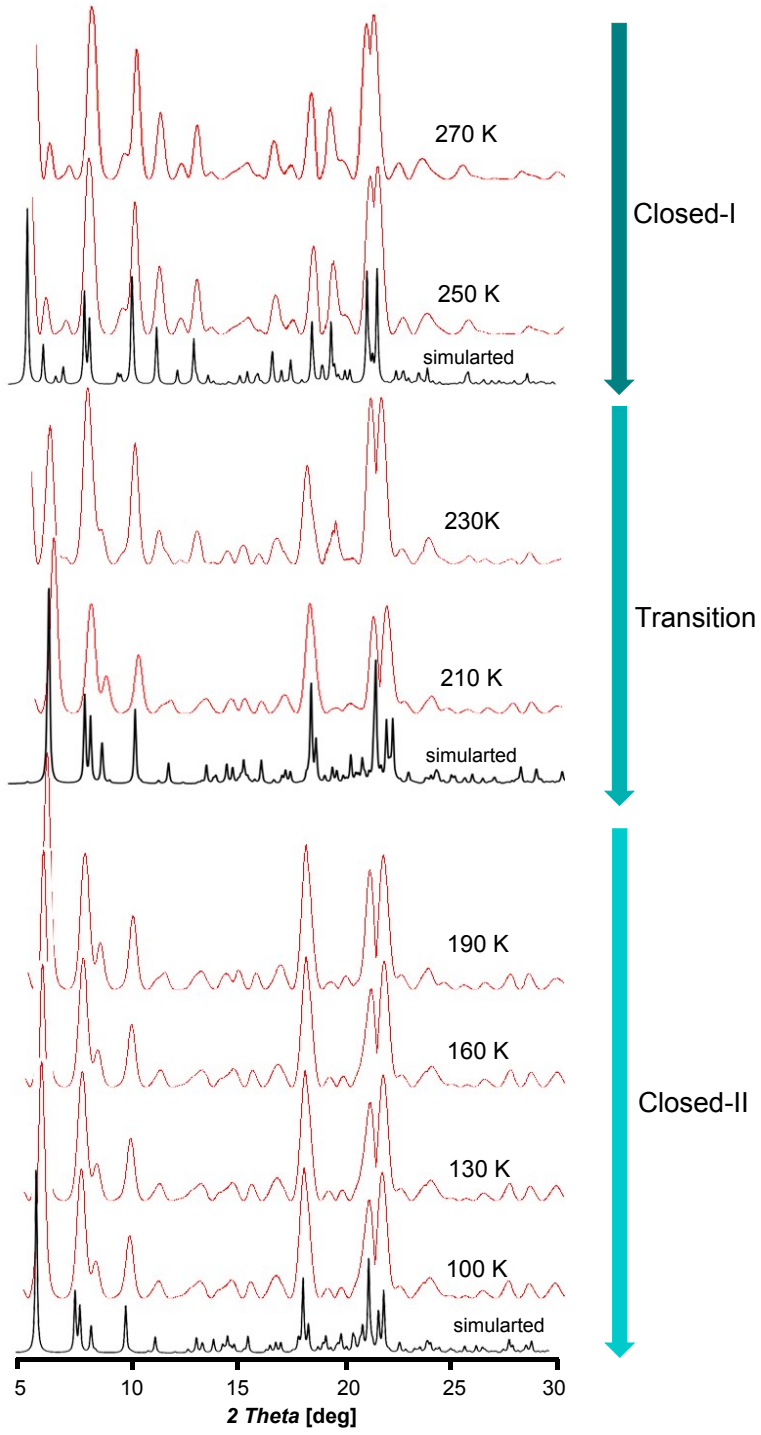
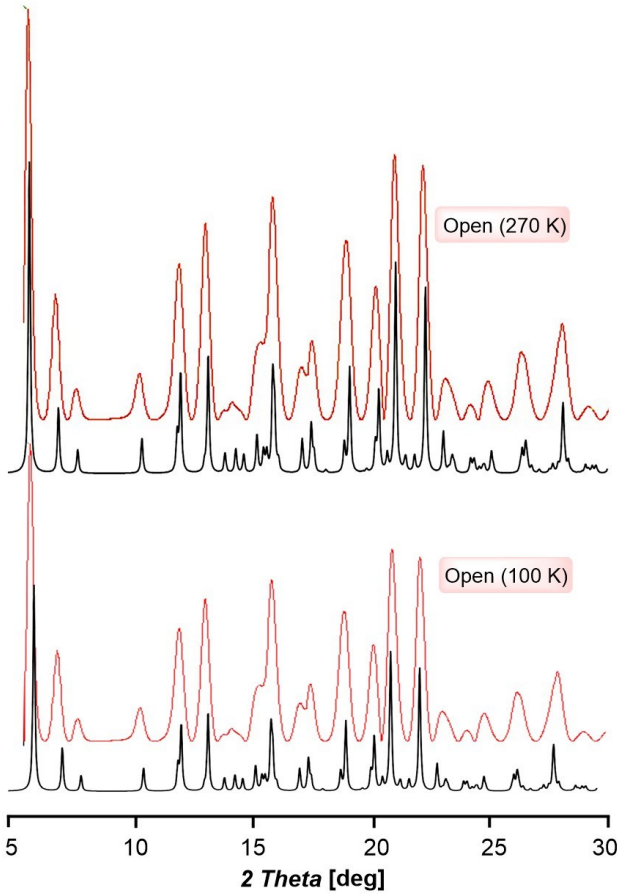


Figure S11. PXRD results of cooling process (from 270K to 100 K) of open conformer. The simulated result are also included.



S4. Computational Data

All investigated molecules were fully optimized using Gaussian 16 software package[4] with the dispersion corrected hybrid meta-GGA density functional (M062X)[5] and double-zeta quality basis set 6-31G(d). The crystal structures are used as the starting geometries. Also, the frequency calculations were performed for all of the optimized conformers to verify the lack of any imaginary normal modes. For the sake of accuracy, the bigger basis set (6-311++G(2d,2p)) is used for calculating the single point energies. In both optimization and energy calculation, solvent effect (dichloromethane, CH_2Cl_2) is considered by employing SMD solvation model.[6] The intermolecular non-covalent interaction plots obtained by fragmentation and subsequent calculation of reduced density gradient with increment value 0.2 in all directions using NCIplot software.[7] Snapshots were generated with the Visual Molecular Dynamics (VMD) package and rendered with Tachyon ray-tracer.[8]

These calculations assist us to have better insights about the dynamic behavior of these polymorphs. We build up both monomer and dimer models to study the intramolecular and intermolecular interaction, respectively. The relative energies of monomers (intramolecular interactions) indicated that closed conformers have a small energy difference (3 kJ mol^{-1}); however, the open conformer is ~14 kJ mol^{-1} less stable than closed conformers (Table S2). To the contrary of monomers, the relative energies of dimers showed higher preference for open conformer over the closed forms (~8 kJ mol^{-1}). This significant value can justify the spontaneous transformation from closed to open conformer. Also, the small energy difference between closed-I and closed-II dimers (less than 1 kJ mol^{-1}) and relatively low rotational transition barrier around single bond (ΔH = 31.4 kJ mol^{-1}) can rationalize the reversible conversion between these two conformers. However, the computational results cannot justify the temperature effects; the ΔH values at 298 K vs. 100 K indicate that the relative stabilities is not temperature dependent.

Moreover, Table S2 listed the average distance between optimal atomized molecules superimposed on the X-ray structure (RMSD) for both monomers and dimers. The low RMSD values also verify the reliability of selected method. These results can suggest that the observed transition from Closed to Open is following the Ostwald rule[9] (i.e. molecules in the crystallization process may not adopt their most stable forms at first and instead grow in a metastable form)[10, 11] Therefore, we believe that Closed-I polymorph is a free energy minimum but not necessarily the global minimum for crystallization. On the other hand, Open polymorph is the global minimum in the crystal state (based on the experimental results and DFT calculation of dimer energies).

Table S2. The relative energies (ΔE+*ZPE*) and enthalpies (ΔH at 298 K and 100 K values in brackets and parenthesis, respectively).[a]

Compound	Monomer	Dimer	RMSD[b]
Closed-I	2.8[6.8](3.6)	8.1[9.1](8.5)	0.37(0.43)
Closed-II	0.0[0.0](0.0)	8.4[9.9](9.0)	0.31(0.36)
Chair	14.1[18.4](15.3)	0.0[0.0](0.0)	0.40(0.41)

[a] Studied at M062X/6-311++G(2d,2p)+SMD(CH_2Cl_2) // M062X/6-31G(d)+SMD(CH_2Cl_2) level of theory in kJ mol^{-1}. [b] Root Mean Square Deviation (RMSD) values in Å obtained by aligning the optimized monomers and dimers (in parenthesis) structures on the X-ray coordinates (just heavy-atoms).

Figure S12. Intermolecular non-covalent interaction between two pairs of Closed forms and their neighboring molecules and between pair molecules in the crystal structures (green surfaces). (Hydrogens in cyan, carbons in white and oxygens in red).

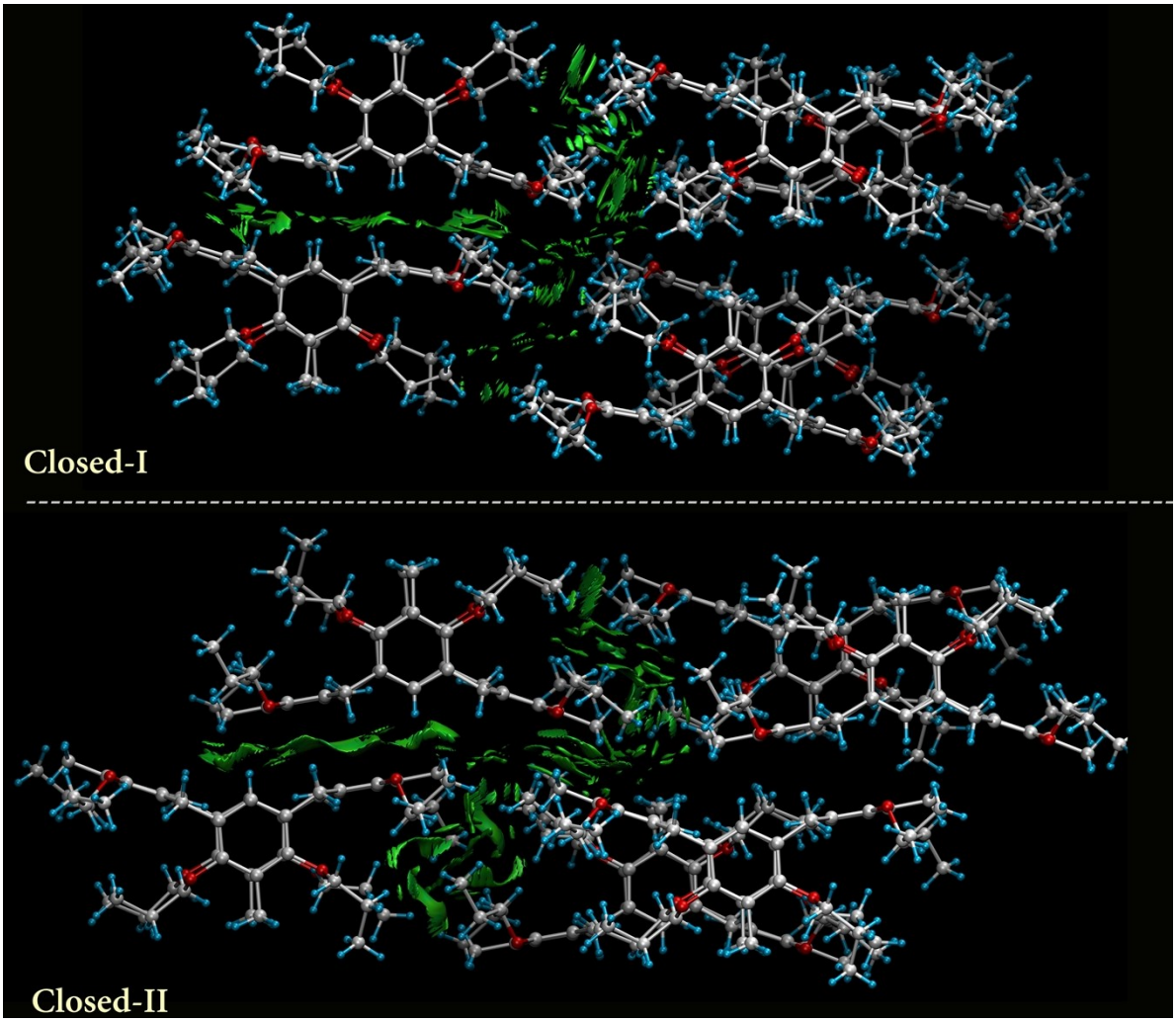


Table S3. Summary of DFT calculations (in a.u.).

			Closed-I	Closed-II	Open
SP energy 6-311++G(2d,2p)		Monomer	-2783.663271	-2783.665613	-2783.659340
		Dimer	-5567.351288	-5567.352263	-5567.355367
298.15 K	ZPE correction	Monomer	1.277731	1.278998	1.278084
		Dimer	2.556916	2.557987	2.557891
	Enthalpy correction	Monomer	1.348092	1.348782	1.348578
		Dimer	2.697835	2.699096	2.698429
	Free Energy correction	Monomer	1.170469	1.173499	1.168229
		Dimer	2.370740	2.369592	2.372967
100.00 K	ZPE correction	Monomer	1.277731	1.278994	1.278084
		Dimer	2.556900	2.557913	2.557896
	Enthalpy correction	Monomer	1.287839	1.288808	1.288365
		Dimer	2.576678	2.577832	2.577525
	Free Energy correction	Monomer	1.259223	1.260807	1.258819
		Dimer	2.529176	2.529473	2.530463

S5. References

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S6. Cartesian Coordinates of optimized molecules (M062X/6-31G*+SMD(CH_2Cl_2)

Monomer Closed-I

O	5.53165300	-1.64658900	-2.19682700
O	5.10438700	3.09444200	-1.63820200
O	2.14993300	2.01693500	2.01045900
O	-2.61204700	1.87037100	1.58659500
O	-5.30490400	2.19110300	-0.71893900
O	-5.00409800	-2.52196900	-1.43824500
O	-2.21285300	-2.52792300	0.95609100
O	2.56426000	-2.36385100	1.28937800
C	2.70417700	0.39373200	-1.12097600
H	1.66607500	0.26565500	-0.82469100
C	3.44890200	-0.72884300	-1.48427800
C	4.78780900	-0.54179800	-1.84130000
C	5.37913300	0.72586600	-1.88904500
C	4.58916100	1.82193000	-1.52509500
C	3.26173800	1.67208900	-1.10744600
C	2.49807300	2.90672300	-0.66203100
H	2.37722300	3.58012100	-1.51900800
H	3.11516100	3.44739300	0.06456500
C	-0.01445600	2.78478500	-0.82425900
H	0.08335600	3.08467100	-1.86616300
C	1.14275000	2.63507600	-0.06058900
C	1.00849500	2.20771800	1.26621600
C	-0.25558100	2.01818800	1.84554200
C	-1.38675000	2.16280000	1.03308500
C	-1.28671100	2.53341900	-0.31418900
C	-2.50201100	2.57967800	-1.21327200
H	-3.22591100	3.32210100	-0.86793700
H	-2.17571500	2.89949500	-2.21009500
C	-2.44793800	0.08491100	-1.59658400
H	-1.37182100	0.17633800	-1.73626200
C	-3.18668300	1.23215200	-1.31357200
C	-4.55584400	1.09000600	-1.07515300
C	-5.19273500	-0.15563600	-1.14573300
C	-4.40792200	-1.28123000	-1.42884800
C	-3.02887000	-1.17955800	-1.64834100
C	-2.17565600	-2.41476700	-1.85540600
H	-1.90268600	-2.51208900	-2.91317200
H	-2.77373800	-3.29177800	-1.59052300
C	0.34974900	-2.30987100	-1.62677400
H	0.41665300	-2.25436000	-2.71184200
C	-0.90771500	-2.38832100	-1.03209600
C	-0.97758200	-2.42649300	0.36725300
C	0.18025900	-2.44989000	1.15759600
C	1.42195100	-2.37818400	0.51242200
C	1.52867500	-2.29083000	-0.87880100
C	2.86900200	-2.13208700	-1.54961500
H	3.59575400	-2.82810400	-1.12131600
H	2.77287800	-2.41847500	-2.60423400
C	6.27587600	-2.18522200	-1.10244300
H	7.03463300	-1.45912200	-0.77591000
H	5.59846200	-2.36326100	-0.25246900
C	6.92195300	-3.48010900	-1.55136100
H	7.56864800	-3.27161600	-2.41133100
H	6.13510700	-4.16145300	-1.89589900
C	7.72400600	-4.12076700	-0.42287100
H	7.08191200	-4.34903800	0.43527300
H	8.18803200	-5.05481100	-0.75159400
H	8.52066100	-3.45346900	-0.07683300
C	6.79988500	0.90025300	-2.35274400
H	7.50994000	0.84246500	-1.51920900
H	7.06547100	0.11555200	-3.06561200
H	6.92691900	1.87678800	-2.82783700
C	5.94322200	3.51597100	-0.56067200
H	5.34224400	3.61833300	0.35385400
H	6.71968800	2.76239500	-0.37493900
C	6.55184800	4.85201700	-0.94029400
H	7.15746400	4.71901400	-1.84476200
H	7.23287600	5.15305200	-0.13606700
C	5.49129600	5.92551900	-1.16669100
H	4.82162100	5.64318500	-1.98390200
H	4.88324900	6.06610000	-0.26556900
H	5.94870100	6.88715900	-1.41787700
C	2.41060200	0.64237000	2.34173300
H	1.67532400	0.29191300	3.07628600
H	2.31616600	0.02885000	1.43987400
C	3.81277700	0.53669800	2.90860200
H	3.93388000	-0.48129000	3.29572300
H	3.90159200	1.21889400	3.76314100
C	4.89048900	0.83095200	1.87234400
H	4.81958400	0.12791900	1.03259200
H	4.76831800	1.84126800	1.47310300
H	5.89366200	0.75108800	2.30393900
C	-0.41805200	1.70720700	3.30964700
H	-1.27456400	2.24838300	3.72104700
H	-0.59667200	0.63951300	3.48823000
H	0.47746400	2.00036200	3.86311700
C	-3.41216700	2.99574800	1.96142900
H	-2.81526100	3.67709200	2.58559100
H	-3.73811200	3.54027600	1.06893700
C	-4.60816600	2.46345600	2.72656500
H	-5.32547500	3.28183900	2.85877300
H	-5.09510200	1.70634600	2.09860300
C	-4.21879300	1.87546900	4.07921200
H	-3.81159900	2.65202800	4.73721300
H	-5.07980400	1.42537100	4.58325600
H	-3.45291100	1.10318400	3.95817300
C	-5.85539900	2.89749900	-1.83287100
H	-5.03995200	3.27226800	-2.46737100
H	-6.46592500	2.21072300	-2.43678000
C	-6.70058900	4.03695900	-1.29832800
H	-7.07486000	4.60848200	-2.15533900
H	-6.05728700	4.71048000	-0.71884700
C	-7.86182600	3.54710100	-0.43849900
H	-8.48100900	4.38252500	-0.09814600
H	-8.50265300	2.86123900	-1.00472600
H	-7.49514600	3.01494700	0.44392000
C	-6.66927600	-0.27543100	-0.87813200
H	-6.95823500	0.34728100	-0.02648600
H	-7.26179200	0.05809900	-1.73897000
H	-6.93665200	-1.31342000	-0.66840800
C	-5.49642900	-2.91237300	-2.72043300
H	-6.22760600	-2.16918600	-3.07306300
H	-4.66554200	-2.93883000	-3.43958400

C	-6.14325600	-4.27655000	-2.58003400
H	-5.38207700	-4.99303100	-2.24896900
H	-6.47605000	-4.59582700	-3.57430300
C	-7.31673000	-4.26617800	-1.60486900
H	-8.08192100	-3.54925300	-1.92463400
H	-7.78589200	-5.25259000	-1.54082900
H	-6.98540200	-3.98232200	-0.60140600
C	-2.67486500	-1.36465700	1.66177200
H	-1.84150000	-0.90519200	2.20783900
H	-3.05157000	-0.62512700	0.94465600
C	-3.77046200	-1.81179600	2.61113100
H	-4.07779700	-0.94530800	3.20787700
H	-3.35324900	-2.55141200	3.30617600
C	-4.97511800	-2.39436200	1.87735700
H	-5.72391100	-2.77055000	2.58185700
H	-5.44891000	-1.62898300	1.25285400
H	-4.67233200	-3.21408800	1.22006100
C	0.10431300	-2.57068800	2.65539500
H	0.27490400	-1.60362100	3.14458000
H	-0.87839100	-2.93864100	2.95982000
H	0.86391300	-3.25985700	3.03310600
C	3.14800000	-3.65435300	1.50363000
H	2.36528200	-4.37046500	1.79097700
H	3.60363500	-4.01534400	0.57172200
C	4.18732400	-3.52377600	2.60124700
H	4.87980400	-2.71792000	2.32521700
H	4.77070500	-4.45125600	2.63180000
C	3.56781400	-3.24966700	3.96835100
H	2.92500400	-2.36455600	3.93601800
H	2.95403300	-4.09820900	4.29168100
H	4.33820100	-3.08362700	4.72767900

Monomer Closed-II

O	-4.69808600	-2.72643300	-2.39302300
O	-5.37741300	1.98640700	-1.92620000
O	-2.84504700	2.12475200	1.50334700
O	1.92576200	2.10640100	1.99642000
O	4.93608200	3.01965900	-1.69825800
O	5.59675100	-1.72911400	-1.83048000
O	2.40659900	-2.34806700	1.85293300
O	-2.31651600	-2.31487800	0.97971700
C	-2.35176300	-0.03364800	-1.61427400
H	-1.29835800	0.09225500	-1.37290200
C	-2.83605000	-1.31798800	-1.85757300
C	-4.19478300	-1.46520200	-2.15572000
C	-5.06558000	-0.37052000	-2.20087400
C	-4.53705800	0.89401100	-1.92094300
C	-3.18369500	1.08566800	-1.62231200
C	-2.66032100	2.48466100	-1.33731600
H	-2.38746900	2.96402500	-2.28569700
H	-3.47031300	3.08581700	-0.91641400
C	-0.17076900	2.65016300	-0.93992800
H	-0.05149500	2.85217100	-2.00290100
C	-1.45786400	2.49230300	-0.42682700
C	-1.58834800	2.27389000	0.94836600
C	-0.47325500	2.15325500	1.78844400
C	0.80300900	2.24813100	1.21407800
C	0.96997800	2.54931400	-0.14482000
C	2.33822100	2.79510700	-0.73046800
H	2.90976700	3.43035800	-0.04342500
H	2.22367300	3.37608700	-1.65312500
C	2.68890900	0.25967900	-0.89622900
H	1.66024000	0.10891600	-0.58010800
C	3.16877700	1.56135800	-1.03140300
C	4.48476900	1.73835100	-1.47172100
C	5.32688100	0.65663500	-1.75315900
C	4.81469600	-0.63089100	-1.55377400
C	3.50054400	-0.85213300	-1.12687000
C	3.03141300	-2.28760700	-0.93767400
H	3.10545600	-2.81270900	-1.89694600
H	3.73286300	-2.78988400	-0.26124700
C	0.53636000	-2.44247700	-1.28633600
H	0.72625000	-2.47359000	-2.35772000
C	1.62328600	-2.39789700	-0.41212900
C	1.35544300	-2.37240700	0.95863200
C	0.04637200	-2.34418800	1.46167400
C	-1.01235400	-2.34753500	0.54406400
C	-0.78224500	-2.43411200	-0.83793700
C	-1.93231300	-2.53415600	-1.81131900
H	-2.53816700	-3.41258100	-1.56951300
H	-1.52199700	-2.71628700	-2.81241500
C	-5.21042400	-3.33589700	-1.20398200
H	-6.03070700	-2.72376500	-0.79909800
H	-4.41552900	-3.37178400	-0.44438300
C	-5.70148400	-4.72749600	-1.54607700
H	-4.87270800	-5.29579500	-1.98405300
H	-6.48068400	-4.64807800	-2.31296800
C	-6.23972800	-5.44030600	-0.30896200
H	-5.45636600	-5.56025100	0.44732500
H	-6.61703900	-6.43545500	-0.56072500
H	-7.06075100	-4.87489800	0.14569100
C	-6.52623600	-0.54955600	-2.51534700
H	-7.11636500	-0.71621900	-1.60576700
H	-6.67289800	-1.41570500	-3.16530400
H	-6.92432800	0.34264000	-3.00529600
C	-5.98856800	2.19211100	-0.64900600
H	-5.20210500	2.20988500	0.11768900
H	-6.65924300	1.34926700	-0.42287000
C	-6.75904900	3.49631900	-0.68834500
H	-6.05748300	4.31499300	-0.89059800
H	-7.17900800	3.66952400	0.30971900
C	-7.86853800	3.48139800	-1.73594900
H	-7.45301500	3.34466500	-2.73836200
H	-8.43442800	4.41767900	-1.72729000
H	-8.56986300	2.66062400	-1.54619400
C	-3.44823900	3.35003600	1.93763900
H	-3.76511900	3.93349800	1.06190900
H	-2.71016900	3.94950200	2.48823200
C	-4.63351800	3.01664700	2.82586500
H	-5.34613900	2.40662300	2.25740700
H	-5.14325800	3.95686600	3.06711000
C	-4.23541500	2.28820600	4.10579800
H	-3.70390400	1.35871400	3.87727700
H	-5.11680400	2.03743200	4.70379000
H	-3.57780100	2.91116200	4.72251900
C	-0.65584200	1.94907300	3.26829400
H	-0.92162000	0.91124800	3.50354500
H	-1.46138000	2.57869900	3.65312900
H	0.26176800	2.19990600	3.80504900
C	2.18009900	0.75823300	2.42519500
H	2.17480200	0.09529900	1.55549500
H	1.39046600	0.42886900	3.11181800

C	3.53269100	0.71263400	3.10661000
H	3.65378500	-0.29973800	3.51082800
H	3.52921000	1.40391600	3.95842100
C	4.68043100	1.04336500	2.15770600
H	5.64760500	0.98422300	2.66755500
H	4.56565400	2.05507500	1.75698700
H	4.69807400	0.34815700	1.30837000
C	5.74236800	3.55985600	-0.64833700
H	6.58342400	2.88520200	-0.44090100
H	5.14087100	3.64378500	0.26800900
C	6.23025700	4.92617500	-1.08900700
H	6.83210400	4.80730500	-1.99791800
H	6.89561200	5.31414300	-0.30926700
C	5.08140800	5.89885400	-1.33830500
H	4.47945200	6.02930700	-0.43163600
H	4.42368300	5.52792300	-2.12943200
H	5.45407000	6.88259100	-1.63916200
C	6.71194600	0.87144500	-2.30121400
H	7.45807000	0.97628200	-1.50497900
H	6.74191100	1.78479800	-2.90153500
H	7.00909800	0.02254300	-2.92318400
C	6.54258600	-2.03388500	-0.80148200
H	6.02520600	-2.05818200	0.16599300
H	7.30887600	-1.24716800	-0.75684400
C	7.17320500	-3.37460700	-1.12143800
H	6.38584200	-4.13811500	-1.13481200
H	7.85676000	-3.62878300	-0.30285600
C	7.92023300	-3.36125700	-2.45191700
H	8.38447500	-4.33087400	-2.65522000
H	8.71174600	-2.60301100	-2.44473600
H	7.23971800	-3.13036000	-3.27640500
C	2.83463900	-3.65624600	2.25217800
H	3.21239400	-4.20209900	1.37524400
H	1.97864000	-4.21618300	2.65074300
C	3.91980900	-3.49306900	3.29751300
H	4.16248300	-4.48372000	3.69815300
H	3.51389700	-2.90035000	4.12657000
C	5.16964100	-2.83074100	2.72713800
H	5.91353900	-2.63684700	3.50601500
H	4.91680500	-1.87765900	2.25032200
H	5.63337700	-3.47547700	1.97092000
C	-0.20583600	-2.32189100	2.94581600
H	0.61115600	-2.79329100	3.49487100
H	-1.13818300	-2.84195700	3.18283500
H	-0.29218600	-1.29466500	3.31903100
C	-2.72907100	-1.06650800	1.56468900
H	-2.24656000	-0.24319600	1.02955600
H	-2.41552300	-1.03092200	2.61653700
C	-4.23805000	-0.95705500	1.47283900
H	-4.52686500	-0.96747700	0.41554600
H	-4.51457200	0.02747200	1.87013100
C	-4.95655600	-2.06357800	2.23947900
H	-4.71401300	-2.01727200	3.30781700
H	-4.66026900	-3.05202800	1.87381600
H	-6.04331800	-1.97704300	2.13829300

Monomer Open

O	-3.26082200	2.90300500	-0.74332300
O	1.34367800	4.06719700	-1.38675900
O	4.88786500	2.78038300	1.43389700
O	5.50165000	-1.22277900	-1.10543400
C	-0.30264600	2.22042100	1.29318800
H	-0.03307700	1.70585400	2.21395500
C	-1.63400400	2.21536100	0.88213200
C	-1.95951700	2.89876900	-0.29619700
C	-0.98762300	3.54273900	-1.07060400
C	0.34754700	3.47361300	-0.64541700
C	0.70136300	2.84801600	0.55539300
C	2.13234700	2.83652000	1.02767100
H	2.13896200	2.76724300	2.12293200
H	2.60892000	3.79005300	0.77911700
C	2.47175400	0.67462900	-0.30565000
H	1.39963500	0.62466300	-0.48761600
C	2.98634700	1.71815000	0.45691300
C	4.36830200	1.73925700	0.69651900
C	5.22637900	0.77019200	0.17249000
C	4.66186600	-0.25100500	-0.60547100
C	3.29022900	-0.32019400	-0.84877200
C	2.69046100	-1.45606000	-1.65309800
H	2.23066400	-1.05669400	-2.56483600
H	3.49276900	-2.12845300	-1.96733100
C	-4.08385100	3.93021000	-0.18229400
H	-3.59387700	4.90587900	-0.31708500
H	-4.21115000	3.75940500	0.89350600
C	-5.42197000	3.89336500	-0.89383900
H	-6.08836800	4.60912200	-0.39731300
H	-5.85216600	2.89620500	-0.74762500
C	-5.30516200	4.21890300	-2.37973900
H	-6.28057500	4.17106500	-2.87359600
H	-4.63681000	3.51111700	-2.87913600
H	-4.90306200	5.22781100	-2.52889000
C	-1.38219800	4.28799300	-2.31766200
H	-2.32527400	4.82082200	-2.17090500
H	-1.52715800	3.60661900	-3.16419200
H	-0.61158300	5.01334100	-2.58921900
C	1.68809700	3.36626800	-2.58885600
H	0.88050000	3.47071900	-3.32360400
H	1.81117500	2.29854100	-2.36299400
C	2.98176200	3.94926400	-3.12446100
H	2.85382200	5.03250100	-3.23798700
H	3.14293800	3.53964000	-4.12847200
C	4.18164100	3.63971600	-2.23482200
H	4.33812800	2.55637600	-2.16219000
H	4.03116400	4.02411200	-1.22074500
H	5.09653300	4.08772500	-2.63518000
C	5.05696600	2.47213200	2.82055900
H	5.77177600	1.64493100	2.92761800
H	4.09562000	2.14508000	3.24248500
C	5.55569100	3.72002100	3.52221000
H	6.51874300	4.00718000	3.08330000
H	5.74344900	3.46434600	4.57130000
C	4.56564100	4.87674700	3.42568000
H	3.59994800	4.60004900	3.86433300
H	4.39499900	5.15522400	2.38189300
H	4.93544300	5.75896800	3.95685100
C	6.70814900	0.80115700	0.43383600
H	7.00568500	1.77359600	0.83203600
H	7.27592100	0.61146700	-0.48172200
H	6.99737000	0.02804000	1.15540600
C	5.94001000	-0.96872900	-2.44284100

H	6.41172700	0.02383200	-2.49263200
H	5.07301400	-0.96217900	-3.11792900
C	6.92545900	-2.05525200	-2.82598200
H	7.19110900	-1.91604700	-3.88007100
H	6.42074800	-3.02616100	-2.74677600
C	8.17887600	-2.03841200	-1.95634300
H	8.87126500	-2.83478500	-2.24547800
H	7.92319100	-2.17656400	-0.90151800
H	8.70648000	-1.08267100	-2.05426800
O	3.26081900	-2.90298000	0.74332700
O	-1.34368200	-4.06718000	1.38676100
O	-4.88786600	-2.78040200	-1.43389800
O	-5.50164900	1.22275000	1.10544700
C	0.30264800	-2.22043700	-1.29320400
H	0.03308200	-1.70588000	-2.21397700
C	1.63400500	-2.21536900	-0.88214300
C	1.95951500	-2.89876100	0.29619600
C	0.98762000	-3.54272600	1.07060700
C	-0.34754800	-3.47360800	0.64541400
C	-0.70136100	-2.84802600	-0.55540500
C	-2.13234500	-2.83653300	-1.02768300
H	-2.13896000	-2.76725900	-2.12294500
H	-2.60891700	-3.79006500	-0.77912600
C	-2.47175100	-0.67463900	0.30563300
H	-1.39963100	-0.62467100	0.48759400
C	-2.98634500	-1.71816200	-0.45692800
C	-4.36830100	-1.73927400	-0.69652400
C	-5.22637900	-0.77021400	-0.17248700
C	-4.66186400	0.25098400	0.60547100
C	-3.29022500	0.32018000	0.84876100
C	-2.69045700	1.45604700	1.65308700
H	-2.23065500	1.05667700	2.56482100
H	-3.49276500	2.12843700	1.96732700
C	4.08386100	-3.93017800	0.18230400
H	3.59390500	-4.90585400	0.31710900
H	4.21115000	-3.75938200	-0.89349900
C	5.42198500	-3.89330000	0.89383800
H	6.08839300	-4.60905000	0.39731700
H	5.85216300	-2.89613300	0.74760800
C	5.30519400	-4.21882100	2.37974400
H	6.28061000	-4.17096000	2.87359200
H	4.63683400	-3.51104000	2.87913700
H	4.90311300	-5.22773400	2.52891000
C	1.38219300	-4.28796200	2.31767700
H	2.32527100	-4.82079000	2.17093000
H	1.52714900	-3.60657700	3.16419800
H	0.61157900	-5.01330800	2.58924100
C	-1.68811400	-3.36622700	2.58884100
H	-0.88052300	-3.47066100	3.32359800
H	-1.81119300	-2.29850500	2.36295600
C	-2.98178200	-3.94921600	3.12444600
H	-2.85384000	-5.03245100	3.23799600
H	-3.14296900	-3.53957100	4.12844700
C	-4.18165300	-3.63969100	2.23478900
H	-4.33814300	-2.55635300	2.16213200
H	-4.03116600	-4.02410800	1.22072200
H	-5.09654800	-4.08769400	2.63514800
C	-5.05698300	-2.47215100	-2.82055800
H	-5.77180000	-1.64495500	-2.92760800
H	-4.09564400	-2.14509200	-3.24249400
C	-5.55570700	-3.72004200	-3.52220500
H	-6.51875300	-4.00720700	-3.08328600
H	-5.74347700	-3.46436700	-4.57129400
C	-4.56564900	-4.87676200	-3.42568600
H	-3.59996100	-4.60005700	-3.86434800
H	-4.39499500	-5.15524000	-2.38190200
H	-4.93545000	-5.75898500	-3.95685600
C	-6.70815100	-0.80118600	-0.43382100
H	-7.00568500	-1.77362500	-0.83202200
H	-7.27591600	-0.61150300	0.48174200
H	-6.99738200	-0.02806800	-1.15538600
C	-5.93999500	0.96869200	2.44285700
H	-6.41170300	-0.02387300	2.49264900
H	-5.07299100	0.96214600	3.11793600
C	-6.92544800	2.05520500	2.82601200
H	-7.19108600	1.91599600	3.88010300
H	-6.42074500	3.02611900	2.74680400
C	-8.17887300	2.03836000	1.95638600
H	-8.87126600	2.83472600	2.24553000
H	-7.92320000	2.17651600	0.90155900
H	-8.70647000	1.08261300	2.05431300

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O	-6.59550800	2.52786600	-0.56119600
O	-6.86042700	0.15605700	3.59427300
O	-5.77437500	-3.74837100	1.04499500
O	-1.34258800	-5.45611000	0.51228600
O	2.08041700	-4.90310300	1.34579500
O	2.42448800	-2.57106300	-2.81424700
O	-1.14781700	-3.22680400	-3.35599100
O	-5.52776400	-1.38106000	-2.74389100
C	-4.76607700	-0.38579400	0.65611100
H	-3.95707100	-1.03706500	0.33443700
C	-5.17394700	0.65027900	-0.18320100
C	-6.21403700	1.47905400	0.24924200
C	-6.82842000	1.31813300	1.49716200
C	-6.36981400	0.27601400	2.31231500
C	-5.36088400	-0.60195300	1.89842800
C	-4.93509200	-1.72072200	2.83259800
H	-4.47170500	-1.27974100	3.72466100
H	-5.83419200	-2.24071400	3.18232300
C	-2.61343900	-2.65968500	2.50479300
H	-2.24794500	-1.87361300	3.16372600
C	-3.97952300	-2.71898800	2.22837600
C	-4.43398800	-3.71280100	1.35246300
C	-3.56053000	-4.68012000	0.83389500
C	-2.19475900	-4.56539200	1.12176900
C	-1.69530100	-3.54963300	1.94773500
C	-0.20795300	-3.36604500	2.16397700
H	0.23222200	-4.22325300	2.68026400
H	-0.06322900	-2.49896300	2.82096200
C	0.07995300	-2.17479400	-0.03912600
H	-0.81262100	-1.60086100	0.20907700
C	0.53227900	-3.13781300	0.86174500
C	1.65269600	-3.89615700	0.50739200
C	2.32855000	-3.69188000	-0.70449800
C	1.82162000	-2.72821600	-1.58748400
C	0.69770400	-1.95816400	-1.26842100
C	0.12324500	-0.96386600	-2.25526000

H	0.37684600	0.05722300	-1.94053000
H	0.59147200	-1.13465700	-3.22945500
C	-2.21569100	-0.04302000	-1.93693800
H	-1.77267000	0.84421500	-1.48593200
C	-1.37960500	-1.06748500	-2.37541600
C	-1.96847400	-2.22004200	-2.91238500
C	-3.35796900	-2.32405600	-3.07376300
C	-4.15664400	-1.26365300	-2.62581800
C	-3.60551400	-0.12100500	-2.03904000
C	-4.47267600	0.97983600	-1.48686400
H	-5.21616400	1.29938300	-2.22383600
H	-3.83692500	1.85597300	-1.30456100
C	-7.67932200	2.19897300	-1.43283100
H	-8.59237200	2.03577800	-0.84190600
H	-7.45055700	1.26015600	-1.96088300
C	-7.86494300	3.33573400	-2.41743200
H	-8.04921800	4.26003500	-1.85803200
H	-6.92853100	3.47459700	-2.97181400
C	-9.01475400	3.05540900	-3.38004000
H	-8.83247200	2.14006600	-3.95414800
H	-9.14136300	3.87673500	-4.09075900
H	-9.95928200	2.92954900	-2.84006700
C	-7.90528900	2.26289300	1.95773400
H	-8.90000600	1.92294800	1.64510600
H	-7.74814800	3.25656000	1.52974700
H	-7.90692800	2.33633300	3.04870000
C	-8.11769700	-0.51317200	3.71790500
H	-7.99853900	-1.57067300	3.44385600
H	-8.84762400	-0.06309200	3.03224900
C	-8.56756800	-0.39164100	5.16095300
H	-8.68956600	0.67083000	5.40353900
H	-9.55527400	-0.85876000	5.24666000
C	-7.58617800	-1.04630500	6.12893600
H	-6.60284400	-0.57129300	6.06651600
H	-7.46229600	-2.11008400	5.89558500
H	-7.93736100	-0.96673100	7.16207300
C	-6.07550500	-3.42592600	-0.32349100
H	-5.71452900	-4.22483600	-0.98213200
H	-5.56628100	-2.49624500	-0.59764700
C	-7.57668200	-3.26614600	-0.46292500
H	-7.79913500	-3.17030000	-1.53177400
H	-8.06462800	-4.18467800	-0.11405400
C	-8.11145900	-2.05467300	0.29118000
H	-7.64434000	-1.13352200	-0.08014600
H	-7.88276600	-2.13884500	1.35681900
H	-9.19647700	-1.95994400	0.17874300
C	-4.06009400	-5.84519400	0.02164600
H	-3.51576600	-6.75527000	0.28819700
H	-3.91912900	-5.68957600	-1.05506700
H	-5.12461400	-6.00957000	0.20630200
C	-0.84629400	-6.51636900	1.33509300
H	-1.68810600	-7.00590900	1.84674900
H	-0.16281300	-6.11784600	2.09192900
C	-0.12063500	-7.48980000	0.42648500
H	0.41556000	-8.21138100	1.05383300
H	0.63567700	-6.92470600	-0.13361300
C	-1.06628000	-8.21529000	-0.52543200
H	-1.77007600	-8.84515900	0.03121500
H	-0.51803000	-8.85796200	-1.22140900
H	-1.64892700	-7.49782200	-1.11124200
C	3.11177100	-4.50687800	2.25367000
H	2.73498500	-3.69893000	2.89914400
H	3.97287500	-4.11892900	1.68881600
C	3.50950300	-5.72196700	3.06892800
H	4.24089800	-5.40114900	3.81999500
H	2.62928200	-6.08503500	3.61373400
C	4.09338800	-6.83369500	2.20258200
H	4.41325400	-7.68460400	2.81160800
H	4.96363600	-6.47149200	1.64258100
H	3.35456600	-7.19213200	1.47987000
C	3.54598900	-4.50359400	-1.05673400
H	3.45822000	-5.51987400	-0.66155300
H	4.45570300	-4.06094700	-0.62801000
H	3.67533000	-4.54717100	-2.14053500
C	3.45077600	-1.57586700	-2.80530500
H	4.15947800	-1.80191500	-1.99832200
H	3.00245200	-0.59297200	-2.59605900
C	4.15362900	-1.59205400	-4.14749700
H	3.42072500	-1.39167300	-4.93876900
H	4.87976600	-0.77017700	-4.15708800
C	4.86890700	-2.91484200	-4.40325700
H	5.57733000	-3.12831800	-3.59290100
H	5.42833200	-2.89006200	-5.34349700
H	4.15445100	-3.74262200	-4.45356200
C	-1.15366000	-4.43096000	-2.57224400
H	-2.17989700	-4.66874900	-2.26558600
H	-0.55979500	-4.28081600	-1.66198000
C	-0.57184400	-5.53870500	-3.43016400
H	-0.67367600	-6.48276100	-2.88270000
H	-1.17600900	-5.62786500	-4.34193200
C	0.89278500	-5.29690800	-3.78348400
H	1.26961800	-6.06997200	-4.46101900
H	1.50915500	-5.30823100	-2.87762900
H	1.02660100	-4.32116600	-4.25842300
C	-3.98484500	-3.52471400	-3.72924400
H	-4.44275900	-4.19349500	-2.98996300
H	-3.23485700	-4.09173200	-4.28571900
H	-4.77501400	-3.22440600	-4.42244200
C	-6.07087000	-0.79919700	-3.93429800
H	-5.46986400	-1.10531700	-4.80230100
H	-6.02566200	0.29616800	-3.86595200
C	-7.50444900	-1.27492100	-4.07794400
H	-8.03908800	-1.04381600	-3.14741000
H	-7.98011700	-0.69137000	-4.87462300
C	-7.60033900	-2.76500000	-4.39163000
H	-7.06921200	-3.35673300	-3.63977300
H	-7.15381800	-2.98429800	-5.36826300
H	-8.64193500	-3.09980600	-4.41553800
O	6.14622100	-2.80426500	0.71190700
O	7.14514200	-0.10326500	-3.11422500
O	5.75642900	4.03672700	-0.75395500
O	1.21965800	5.52158900	-0.95131500
O	-2.02701100	4.63394300	-1.95676300
O	-2.47983700	3.07235900	2.53963500
O	1.52650100	3.59483800	3.38737600
O	5.50064300	0.94913100	3.01308900
C	4.76704000	0.39514900	-0.38934000
H	3.98945300	1.09752100	-0.09715100
C	4.97828500	-0.74862400	0.38459700
C	5.97000900	-1.64659400	-0.01900900
C	6.74518300	-1.43888100	-1.16585100
C	6.48237700	-0.29063000	-1.92088500
C	5.50461200	0.64129200	-1.54606100
C	5.26476900	1.83156000	-2.45779500

H	5.01401100	1.44736000	-3.45478500
H	6.20556300	2.38119100	-2.57459700
C	2.85732800	2.60339400	-2.43516400
H	2.60982500	1.72408800	-3.02919000
C	4.18125800	2.79063300	-2.03133600
C	4.47358300	3.89990200	-1.23138800
C	3.50247400	4.87009200	-0.93900400
C	2.18830800	4.63000500	-1.35115900
C	1.83793700	3.48343100	-2.07785300
C	0.38727500	3.16455700	-2.36067100
H	-0.06952600	3.89863700	-3.02951400
H	0.33833200	2.19742600	-2.87685500
C	0.05150900	2.35612600	0.00626500
H	0.99545300	1.82129000	-0.09140300
C	-0.41562700	3.10107800	-1.07750900
C	-1.60591700	3.81882500	-0.92766200
C	-2.33775400	3.78630600	0.26797300
C	-1.82407500	3.03291000	1.33012500
C	-0.62882500	2.31146100	1.22086000
C	-0.12121500	1.51075300	2.40365700
H	-0.54112100	0.49722200	2.35124300
H	-0.51495500	1.96953200	3.31540700
C	2.03773200	0.23602000	2.07106000
H	1.46048500	-0.55559400	1.59502800
C	1.37929500	1.38538900	2.50605600
C	2.15053100	2.41592600	3.05437500
C	3.52527900	2.26111700	3.29031300
C	4.13778000	1.08514000	2.84449300
C	3.41637500	0.07833000	2.19613300
C	4.11655400	-1.10255000	1.58245900
H	4.72974900	-1.62781700	2.32163000
H	3.35828500	-1.82611700	1.25393200
C	7.13616000	-2.68163300	1.73589700
H	8.13500000	-2.62336700	1.27983800
H	6.96656100	-1.74828100	2.29274800
C	7.02640100	-3.88066700	2.65529900
H	7.14516100	-4.79402700	2.06071000
H	6.01478100	-3.90031400	3.08095500
C	8.06914000	-3.82797000	3.76753900
H	7.94968600	-2.92447900	4.37600700
H	7.98001100	-4.69264900	4.43102600
H	9.08420000	-3.82282700	3.35625600
C	7.77495600	-2.44691000	-1.59864600
H	8.74038800	-2.27253700	-1.10875300
H	7.45216700	-3.45807800	-1.33578700
H	7.93486200	-2.38895400	-2.67825000
C	8.43382100	0.50404200	-2.99084500
H	8.32563300	1.50567900	-2.55103700
H	9.06184300	-0.09660900	-2.31935500
C	9.04212400	0.59509000	-4.37667500
H	9.14924700	-0.41880300	-4.78052200
H	10.05130100	1.01009300	-4.27439400
C	8.20787900	1.45518600	-5.32137300
H	7.20774300	1.03190200	-5.45207000
H	8.09584100	2.47109400	-4.92541000
H	8.67709900	1.52826100	-6.30707000
C	5.85636200	3.85831700	0.66652000
H	5.44358300	4.73831100	1.17587300
H	5.26579900	2.97938500	0.96533000
C	7.31593600	3.66430700	1.02771300
H	7.40948700	3.78096700	2.11368200
H	7.89756400	4.47462300	0.57150900
C	7.84880500	2.30225600	0.59649000
H	7.28199500	1.49967100	1.08422400
H	7.74841900	2.17601700	-0.48618300
H	8.90608900	2.18664200	0.85703500
C	3.84443000	6.15458700	-0.23204500
H	3.30171800	6.99111500	-0.68152600
H	3.57092500	6.12983500	0.82905800
H	4.91617700	6.35605600	-0.30333800
C	0.77294900	6.43799800	-1.95580600
H	1.63678500	6.99445200	-2.34917600
H	0.31026600	5.89171600	-2.78524500
C	-0.22936600	7.37415300	-1.30986200
H	-0.66565800	8.00044600	-2.09722700
H	-1.04159900	6.76378400	-0.89593500
C	0.39977900	8.24398900	-0.22679400
H	1.15733800	8.91210400	-0.65311200
H	-0.35089300	8.86237400	0.27509800
H	0.88701100	7.62054500	0.52843900
C	-3.01200100	4.04938400	-2.80985400
H	-2.64102200	3.08461000	-3.18690200
H	-3.93108600	3.86213200	-2.23508400
C	-3.28750300	5.01706600	-3.94402100
H	-3.98902700	4.53489400	-4.63469300
H	-2.35553600	5.18695500	-4.49689500
C	-3.85945700	6.34178700	-3.44805200
H	-4.06572300	7.02062500	-4.28103700
H	-4.79779500	6.17949500	-2.90476500
H	-3.15876400	6.83865100	-2.77030400
C	-3.60559100	4.57880700	0.43763600
H	-3.64750700	5.39539600	-0.28793300
H	-4.49565500	3.95121700	0.28936500
H	-3.66215700	4.99370500	1.44773400
C	-3.41375900	2.00384800	2.72382100
H	-4.13566100	2.01372200	1.89686800
H	-2.88056600	1.04256300	2.69931700
C	-4.11919300	2.21084100	4.04865800
H	-3.37218400	2.22534400	4.85185800
H	-4.77040900	1.34640600	4.22385500
C	-4.94213300	3.49543600	4.06272500
H	-5.64248800	3.51034900	3.21852400
H	-5.52266500	3.58700000	4.98602700
H	-4.29622700	4.37458100	3.97812200
C	1.85716200	4.65790600	2.48100500
H	2.94226000	4.82295100	2.50298600
H	1.57643000	4.36491200	1.45793600
C	1.11047100	5.90614500	2.90626700
H	1.56758000	6.76053300	2.39308000
H	1.27232300	6.05861500	3.98051200
C	-0.37807700	5.83616900	2.58168300
H	-0.89686000	6.74996400	2.89017800
H	-0.52079600	5.70898200	1.50108700
H	-0.85235300	4.98627000	3.08365100
C	4.33157600	3.31069700	4.00736100
H	4.97832200	3.86785700	3.31900900
H	3.67280900	4.02153900	4.51169000
H	4.98391800	2.85255800	4.75627700
C	5.87094400	0.23688300	4.19920000
H	5.33260700	0.65513900	5.06159600
H	5.58066500	-0.81874000	4.10413000
C	7.36965400	0.37242400	4.39005500
H	7.87573700	-0.01535100	3.49728100
H	7.66152000	-0.26896900	5.23000800

C	7.79727900	1.81258800	4.65043900
H	7.47399000	2.46099000	3.83111300
H	7.35167900	2.19033600	5.57779200
H	8.88461100	1.89358600	4.74174800

Dimer closed-II

O	1.37893100	-1.68687700	2.74180100
O	1.70178000	-2.51806000	-1.96929100
O	-2.15628700	-4.43673500	-1.92923400
O	-6.61449100	-2.66335400	-2.01397000
O	-7.38387800	2.11749500	-3.09621800
O	-7.78968200	2.78445000	1.63723000
O	-6.93092400	-2.07133400	2.42231000
O	-2.37887400	-3.61190500	2.48205500
C	-1.12007600	-1.44131300	0.08491000
H	-2.17095300	-1.18441800	-0.03153600
C	-0.55414200	-1.39594600	1.35732100
C	0.79983800	-1.72133900	1.48769400
C	1.58583400	-2.09140700	0.38977800
C	0.96414400	-2.14012300	-0.86329300
C	-0.38781500	-1.82501900	-1.03761100
C	-1.00584500	-1.85360800	-2.42481700
H	-0.82938800	-0.88319100	-2.90873300
H	-0.48618200	-2.60053700	-3.03161300
C	-3.39089900	-1.05972000	-2.61714300
H	-2.99527600	-0.07451200	-2.86170400
C	-2.49227700	-2.10558500	-2.41008300
C	-3.01403500	-3.37182100	-2.12914600
C	-4.39167800	-3.59221200	-1.99918500
C	-5.25512400	-2.49711500	-2.15391600
C	-4.77076500	-1.23193300	-2.51247600
C	-5.70662000	-0.08566900	-2.80346500
H	-6.56302300	-0.45910000	-3.37820400
H	-5.19194600	0.62851000	-3.45698800
C	-5.88640000	0.34188100	-0.28286500
H	-5.17487400	-0.46061900	-0.10859500
C	-6.23567800	0.66203100	-1.59377900
C	-7.10790900	1.73567400	-1.80203500
C	-7.64849100	2.47201900	-0.74149000
C	-7.30557300	2.08086100	0.55795800
C	-6.43025400	1.01822200	0.80936400
C	-6.11338100	0.66529500	2.25409700
H	-5.70771500	1.55441500	2.75038000
H	-7.05647500	0.43604700	2.76506400
C	-3.76646000	-0.24066900	2.42956500
H	-3.40017200	0.78524000	2.39576400
C	-5.14165500	-0.47717100	2.40230500
C	-5.57634800	-1.80470200	2.44026400
C	-4.67906800	-2.88272300	2.46567600
C	-3.30740600	-2.59709200	2.46146900
C	-2.83669900	-1.27637500	2.48149700
C	-1.36090700	-0.97723400	2.56905900
H	-0.94128400	-1.45591300	3.45953800
H	-1.24679000	0.10468900	2.71812500
C	1.32173700	-2.95415800	3.40390900
H	1.85174500	-3.70789500	2.80266300
H	0.27126600	-3.27035500	3.48663100
C	1.95881300	-2.81459500	4.77108400
H	1.44227500	-2.01845000	5.31991100
H	3.00115900	-2.49838400	4.64449500
C	1.89133400	-4.12673600	5.54693900
H	0.85245600	-4.43145800	5.71376100
H	2.37377900	-4.03139500	6.52375800
H	2.39402800	-4.93290900	5.00130200
C	3.04383400	-2.42541200	0.55248000
H	3.19342200	-3.48557800	0.79242700
H	3.48228100	-1.83906400	1.36507100
H	3.59132600	-2.21448000	-0.37059300
C	1.70645400	-3.93904700	-2.14172300
H	0.66983200	-4.29945700	-2.09050500
H	2.26742100	-4.40310100	-1.31680200
C	2.34208100	-4.27082100	-3.47641700
H	1.72169700	-3.85578600	-4.28031100
H	2.32719600	-5.36168100	-3.58785900
C	3.76990500	-3.74360600	-3.59282700
H	3.77809100	-2.64975200	-3.59240500
H	4.24180200	-4.08268400	-4.52002400
H	4.38664700	-4.08729500	-2.75346000
C	-1.82215300	-5.15539400	-3.12251600
H	-1.14290100	-4.54954600	-3.73830100
H	-2.73274800	-5.33785000	-3.71014400
C	-1.17180100	-6.46914800	-2.72770600
H	-0.27824700	-6.25896100	-2.12748300
H	-0.82887800	-6.96108800	-3.64556300
C	-2.11055500	-7.38959600	-1.95388200
H	-2.48380500	-6.89575300	-1.05082700
H	-1.59867500	-8.30854200	-1.65231900
H	-2.97428800	-7.67195900	-2.56646700
C	-4.91779700	-4.97432300	-1.72024300
H	-4.79508400	-5.24661300	-0.66479600
H	-4.38093200	-5.72366900	-2.30676300
H	-5.97908700	-5.03730200	-1.97075400
C	-7.05636700	-2.83881000	-0.65845600
H	-6.62498600	-2.05413400	-0.03099100
H	-6.71507500	-3.80913900	-0.27596400
C	-8.56942000	-2.75466700	-0.62979900
H	-8.88439000	-2.97117500	0.39839100
H	-8.98552000	-3.54282100	-1.26937200
C	-9.08958800	-1.38837900	-1.06631800
H	-10.18286900	-1.34744900	-1.02346700
H	-8.77891000	-1.17259600	-2.09318600
H	-8.69205300	-0.59345300	-0.42271400
C	-8.62912200	1.63190700	-3.60286500
H	-9.44974800	1.96556300	-2.95394900
H	-8.62044700	0.53278300	-3.60103000
C	-8.79709400	2.15998400	-5.01425600
H	-8.81638900	3.25584700	-4.97884700
H	-9.77566000	1.83156700	-5.38278000
C	-7.68983300	1.68055700	-5.94826800
H	-7.66477100	0.58558300	-5.99126500
H	-6.71205400	2.02695000	-5.60136500
H	-7.84155100	2.05375500	-6.96557200
C	-8.52030200	3.67265700	-0.99264500
H	-9.58078700	3.40349700	-1.06063900
H	-8.24136500	4.15034400	-1.93574500
H	-8.41439400	4.39501100	-0.17838500
C	-9.13667600	2.45516600	1.98786800
H	-9.24383500	1.36338200	2.02103900
H	-9.82429500	2.84093900	1.22199700
C	-9.43757100	3.07859400	3.33653100
H	-8.75691900	2.64838800	4.08133600

H	-10.45564100	2.78908700	3.62224700
C	-9.30373300	4.59849200	3.31413400
H	-9.54663900	5.03203100	4.28882800
H	-9.98030300	5.03685600	2.57139500
H	-8.28265700	4.89324300	3.05552100
C	-7.51215400	-2.14061200	3.72936100
H	-7.36199700	-1.18341400	4.24961300
H	-7.00901700	-2.92154300	4.31448600
C	-8.98875300	-2.44012300	3.56439100
H	-9.41813500	-2.61237200	4.55775700
H	-9.09056400	-3.37650500	3.00212200
C	-9.72449600	-1.30685400	2.85647200
H	-10.77018700	-1.56448000	2.66192500
H	-9.24502500	-1.07567000	1.89907200
H	-9.70981400	-0.39855100	3.47095700
C	-5.17849200	-4.30238300	2.50541200
H	-6.17201900	-4.36218600	2.95329200
H	-4.49222900	-4.93259900	3.07830300
H	-5.25402200	-4.72527000	1.49680300
C	-2.29080600	-4.37791200	1.26723500
H	-2.49243400	-3.72281000	0.41414800
H	-3.04515600	-5.17636100	1.28155200
C	-0.90297100	-4.97951900	1.16485300
H	-0.17024000	-4.16497100	1.12290000
H	-0.84971700	-5.50702100	0.20449600
C	-0.58718000	-5.93135600	2.31487100
H	-1.28122200	-6.78026500	2.31910300
H	-0.67648800	-5.42414200	3.28088200
H	0.42947800	-6.32967700	2.23440300
O	-1.37893500	1.68706200	-2.74161300
O	-1.70157200	2.51845900	1.96945100
O	2.15669900	4.43691800	1.92927100
O	6.61476800	2.66318700	2.01400100
O	7.38341700	-2.11804300	3.09598600
O	7.78911300	-2.78470900	-1.63751200
O	6.93090500	2.07177300	-2.42229700
O	2.37878100	3.61207000	-2.48179400
C	1.12018700	1.44150800	-0.08479900
H	2.17106700	1.18460300	0.03161100
C	0.55420700	1.39611400	-1.35719100
C	-0.79978100	1.72150500	-1.48752500
C	-1.58572500	2.09161900	-0.38958400
C	-0.96398800	2.14038600	0.86346000
C	0.38797900	1.82526000	1.03773700
C	1.00607000	1.85386700	2.42492000
H	0.82958400	0.88347500	2.90888300
H	0.48647700	2.60084500	3.03171500
C	3.39107200	1.05980900	2.61717300
H	2.99538600	0.07462600	2.86172400
C	2.49251900	2.10574300	2.41013600
C	3.01437200	3.37194500	2.12919500
C	4.39203300	3.59222800	1.99920600
C	5.25539100	2.49706700	2.15394100
C	4.77094400	1.23192200	2.51248500
C	5.70672300	0.08557900	2.80339400
H	6.56321800	0.45894300	3.37804100
H	5.19205600	-0.62855500	3.45696900
C	5.88643800	-0.34179800	0.28275900
H	5.17511300	0.46089400	0.10854500
C	6.23560000	-0.66215900	1.59365400
C	7.10754500	-1.73604500	1.80183400
C	7.64792900	-2.47246000	0.74123400
C	7.30515100	-2.08109700	-0.55818900
C	6.43014300	-1.01818100	-0.80951800
C	6.11350500	-0.66496300	-2.25423000
H	5.70800000	-1.55401000	-2.75077200
H	7.05667500	-0.43552500	-2.76497000
C	3.76654800	0.24090300	-2.42958400
H	3.40030800	-0.78502900	-2.39587600
C	5.14173000	0.47746900	-2.40235800
C	5.57634800	1.80503300	-2.44024500
C	4.67901100	2.88300400	-2.46557700
C	3.30736600	2.59730300	-2.46132500
C	2.83672900	1.27656800	-2.48141700
C	1.36094400	0.97737200	-2.56893100
H	0.94127600	1.45599000	-3.45942200
H	1.24686000	-0.10456000	-2.71793400
C	-1.32163400	2.95433100	-3.40373600
H	-1.85169000	3.70809000	-2.80255700
H	-0.27114600	3.27049700	-3.48634800
C	-1.95856600	2.81476400	-4.77097700
H	-1.44197000	2.01861900	-5.31975100
H	-3.00092500	2.49855400	-4.64450000
C	-1.89100200	4.12690500	-5.54682600
H	-0.85210400	4.43161600	-5.71354800
H	-2.37335200	4.03157000	-6.52369100
H	-2.39373900	4.93308200	-5.00123500
C	-3.04370800	2.42570600	-0.55226000
H	-3.19322900	3.48584400	-0.79238000
H	-3.48224300	1.83925400	-1.36472600
H	-3.59116000	2.21497100	0.37087900
C	-1.70624700	3.93947700	2.14166200
H	-0.66965300	4.29991700	2.09012100
H	-2.26743900	4.40337500	1.31680500
C	-2.34153800	4.27149200	3.47645100
H	-1.72099400	3.85654800	4.28026700
H	-2.32654200	5.36237200	3.58770600
C	-3.76939500	3.74446500	3.59332800
H	-3.77776000	2.65061500	3.59335300
H	-4.24107100	4.08397200	4.52048300
H	-4.38625200	4.08792500	2.75395200
C	1.82249800	5.15553800	3.12255900
H	1.14309200	4.54972000	3.73820600
H	2.73302900	5.33784800	3.71032900
C	1.17235300	6.46939700	2.72774600
H	0.27888300	6.25935400	2.12734700
H	0.82931900	6.96130000	3.64558100
C	2.11134200	7.38980900	1.95416500
H	2.48470300	6.89599800	1.05113900
H	1.59961400	8.30883200	1.65258000
H	2.97499500	7.67203700	2.56692500
C	4.91829300	4.97426500	1.72016300
H	4.79569500	5.24645900	0.66468000
H	4.38146000	5.72372300	2.30656100
H	5.97957500	5.03716100	1.97074000
C	7.05668600	2.83856500	0.65849900
H	6.62515300	2.05397400	0.03102600
H	6.71558900	3.80896600	0.27601000
C	8.56972400	2.75411900	0.62987400
H	8.88475200	2.97048200	-0.39832900
H	8.98596000	3.54224800	1.26938900
C	9.08961800	1.38777400	1.06653600
H	10.18289300	1.34664700	1.02374900
H	8.77884500	1.17214100	2.09340900

H	8.69197300	0.59285700	0.42299200
C	8.62873000	-1.63270700	3.60269800
H	9.44931400	-1.96644900	2.95377100
H	8.62024000	-0.53358100	3.60094900
C	8.79658500	-2.16092400	5.01405100
H	8.81572100	-3.25678800	4.97855200
H	9.77519000	-1.83268100	5.38262900
C	7.68936800	-1.68141300	5.94807100
H	7.66444500	-0.58643900	5.99113600
H	6.71155100	-2.02765900	5.60112700
H	7.84101900	-2.05469600	6.96535400
C	8.51942200	-3.67334500	0.99231100
H	9.57996700	-3.40444400	1.06039800
H	8.24031900	-4.15106300	1.93534600
H	8.41338500	-4.39558600	0.17797100
C	9.13618300	-2.45571100	-1.98812700
H	9.24367900	-1.36394900	-2.02093500
H	9.82373600	-2.84195700	-1.22243400
C	9.43681000	-3.07877300	-3.33701900
H	8.75625800	-2.64810000	-4.08164600
H	10.45495900	-2.78949200	-3.62268100
C	9.30249300	-4.59863800	-3.31513500
H	9.54523600	-5.03191900	-4.28998400
H	9.97894300	-5.03746600	-2.57256300
H	8.28133100	-4.89315400	-3.05659400
C	7.51211100	2.14120400	-3.72935100
H	7.36174100	1.18415200	-4.24980700
H	7.00911300	2.92236500	-4.31428700
C	8.98877900	2.44037400	-3.56436600
H	9.41816500	2.61273300	-4.55771100
H	9.09081200	3.37661900	-3.00191100
C	9.72429900	1.30679900	-2.85670500
H	10.77007300	1.56411900	-2.66220100
H	9.24484300	1.07556800	-1.89930800
H	9.70932900	0.39860500	-3.47134700
C	5.17837200	4.30268600	-2.50528800
H	6.17182800	4.36255200	-2.95331500
H	4.49200200	4.93291100	-3.07804000
H	5.25404200	4.72551200	-1.49666700
C	2.29070400	4.37793800	-1.26688800
H	2.49235600	3.72274300	-0.41387800
H	3.04503400	5.17640800	-1.28112100
C	0.90284900	4.97948700	-1.16443000
H	0.17014500	4.16491200	-1.12254900
H	0.84959400	5.50688100	-0.20401500
C	0.58701500	5.93143700	-2.31434100
H	1.28102200	6.78037400	-2.31848600
H	0.67633700	5.42433200	-3.28040900
H	-0.42966000	6.32970600	-2.23382500

Dimer open

O	6.13497400	-2.90118400	-1.06544300
O	1.73452600	-4.78565800	-1.07031300
O	-1.00499200	-5.05578900	2.88415200
O	-2.77604200	-0.61861200	2.98650100
C	3.64929100	-3.16508100	1.59285900
H	3.55233300	-2.92522400	2.65079200
C	4.83086100	-2.84031900	0.93136800
C	4.95765200	-3.19843100	-0.41857200
C	3.91913000	-3.82738500	-1.11286700
C	2.74430500	-4.12606400	-0.40672600
C	2.59546700	-3.82284100	0.95025400
C	1.37953400	-4.28952400	1.71192000
H	1.71856100	-4.72614600	2.66077000
H	0.91108300	-5.10828600	1.15772800
C	0.42745600	-1.89739900	1.74813300
H	1.34364600	-1.52361000	1.29250300
C	0.30993800	-3.25741900	2.02251000
C	-0.87163900	-3.70817800	2.63264400
C	-1.91581300	-2.84076200	2.96092900
C	-1.75595200	-1.48185300	2.65479300
C	-0.59724600	-0.99241700	2.05053300
C	-0.46452800	0.48373000	1.74090700
H	-0.42354600	0.63771200	0.65688200
H	-1.36434200	0.99735800	2.08728600
C	7.07683300	-3.97634900	-1.08677900
H	6.59776300	-4.87422100	-1.50521300
H	7.39272000	-4.20979300	-0.06049000
C	8.25365500	-3.54468600	-1.93929400
H	9.02151700	-4.32543800	-1.88040400
H	8.67162600	-2.63453800	-1.49514900
C	7.85596000	-3.29791400	-3.39133500
H	8.71407300	-2.97507600	-3.98890600
H	7.08827600	-2.51970800	-3.45194500
H	7.45121200	-4.20893700	-3.84762900
C	4.05773600	-4.22169500	-2.55890600
H	4.96550400	-3.79258200	-2.98812300
H	3.20093300	-3.87927800	-3.14857800
H	4.10298600	-5.31143400	-2.66528200
C	0.75130200	-3.89241200	-1.60801700
H	1.20565400	-3.30636200	-2.41853200
H	0.43245000	-3.19141300	-0.82297600
C	-0.43077000	-4.69564100	-2.11213000
H	-0.05837600	-5.50300800	-2.75438900
H	-1.03584800	-4.03491400	-2.74402500
C	-1.28338000	-5.25284800	-0.97607000
H	-1.61827400	-4.43904100	-0.31950300
H	-0.71731500	-5.96541800	-0.36665300
H	-2.17153100	-5.76670700	-1.35859300
C	-0.67232000	-5.43045400	4.22450500
H	-1.35291100	-4.93078000	4.92638300
H	0.35127300	-5.10060800	4.45337600
C	-0.78852800	-6.93813400	4.33288300
H	-1.82214700	-7.22607800	4.10624200
H	-0.59808400	-7.21580400	5.37590100
C	0.17810100	-7.66625600	3.40400000
H	1.21479900	-7.38602300	3.62359700
H	-0.02517700	-7.41648600	2.35872800
H	0.09230300	-8.75121400	3.51669100
C	-3.15908500	-3.32996200	3.65340600
H	-3.28306800	-4.40642700	3.51019200
H	-4.04859600	-2.81457600	3.28238000
H	-3.10796900	-3.13272300	4.73138300
C	-3.69332300	-0.39777100	1.90888300
H	-4.01436400	-1.36886400	1.50629800
H	-3.18845000	0.15030300	1.09757000
C	-4.87991100	0.37940500	2.43610300
H	-5.53922300	0.60383500	1.59013400
H	-4.52764700	1.34678800	2.81949400
C	-5.64215900	-0.37752600	3.51920400
H	-6.50518000	0.19679600	3.87056400
H	-5.00049000	-0.58972700	4.38021800

H	-6.01496100	-1.33339100	3.13170000
O	-0.08898500	0.73781800	4.56216200
O	4.25373800	2.68568400	4.01376400
O	6.54114100	3.30671200	0.07185000
O	8.37737200	-1.09765700	0.42289800
C	1.80958300	1.57113000	1.54638000
H	1.70867100	1.51339000	0.46133900
C	0.76637000	1.10957800	2.34854200
C	0.89873100	1.22488100	3.73707700
C	2.04679600	1.76950800	4.32618500
C	3.09417200	2.16998300	3.48253700
C	2.97921500	2.10277100	2.08820700
C	4.10005200	2.57462900	1.20052100
H	3.67949400	2.86197900	0.22565300
H	4.54869100	3.48070500	1.61932400
C	5.08665400	0.21737000	1.35240800
H	4.15763500	-0.13343900	1.79884400
C	5.20332900	1.55466300	0.98537200
C	6.40600300	1.97390300	0.39610300
C	7.47487100	1.09744700	0.19446000
C	7.32115500	-0.23475600	0.61260900
C	6.13536000	-0.69333200	1.18901500
C	5.97181100	-2.13473000	1.62928000
H	5.79089100	-2.16399000	2.71026300
H	6.90655200	-2.66727200	1.43750500
C	-1.18661200	1.62231200	4.80638400
H	-0.80325200	2.60654200	5.11628700
H	-1.77314500	1.75222100	3.88964900
C	-2.05052700	1.00429900	5.88827000
H	-2.94312400	1.63140100	6.00270600
H	-2.38935000	0.02620900	5.52739200
C	-1.32276800	0.86455000	7.22134800
H	-1.96841000	0.40897100	7.97842900
H	-0.43273800	0.23776900	7.11232200
H	-1.00425400	1.84371600	7.59761900
C	2.13004000	1.92278300	5.82129800
H	1.16664500	2.23567300	6.23218600
H	2.39604300	0.97820100	6.31000000
H	2.88093800	2.67046000	6.08752400
C	5.10712200	1.71921400	4.64026600
H	4.64265700	1.35564000	5.56465200
H	5.24297900	0.86400200	3.96461700
C	6.43738000	2.38561300	4.93367800
H	6.24854600	3.29074800	5.52333600
H	7.02036800	1.70707200	5.56725800
C	7.21953100	2.72127500	3.66801600
H	7.45644700	1.80753900	3.10959500
H	6.64111600	3.37527400	3.00727200
H	8.16103800	3.22593300	3.90654300
C	6.19949600	3.60477200	-1.28420000
H	6.96872800	3.19237700	-1.95242300
H	5.24163400	3.12503900	-1.52725400
C	6.08333800	5.10792600	-1.44364900
H	7.03119600	5.56947200	-1.14193300
H	5.94927200	5.31883100	-2.51131600
C	4.92449200	5.69188000	-0.64096800
H	3.97279400	5.23986000	-0.94800700
H	5.05897200	5.50507800	0.42860300
H	4.84482700	6.77312600	-0.78944900
C	8.75653500	1.55322300	-0.44900500
H	8.80797200	2.64386300	-0.46649400
H	9.62938600	1.17105400	0.08800300
H	8.82816400	1.18544800	-1.47953800
C	9.23342500	-1.21925000	1.56189700
H	9.59717900	-0.22420200	1.85857900
H	8.66498500	-1.63408500	2.40570700
C	10.38827700	-2.12460100	1.18034100
H	10.99017600	-2.30602800	2.07802600
H	9.97954900	-3.09332300	0.86590000
C	11.25356800	-1.52906600	0.07393100
H	12.06420400	-2.20937700	-0.20407100
H	10.65819600	-1.32505600	-0.82118600
H	11.70453500	-0.58511600	0.40112600
O	0.08869900	-0.73761900	-4.56234700
O	-4.25389800	-2.68561400	-4.01352600
O	-6.54106400	-3.30673500	-0.07167800
O	-8.37733200	1.09761800	-0.42265300
C	-1.80950300	-1.57109000	-1.54636900
H	-1.70848000	-1.51337900	-0.46133700
C	-0.76637800	-1.10949600	-2.34862700
C	-0.89889700	-1.22474000	-3.73715300
C	-2.04701900	-1.76936400	-4.32615500
C	-3.09429300	-2.16989300	-3.48240900
C	-2.97918900	-2.10272100	-2.08808800
C	-4.09994300	-2.57458600	-1.20030000
H	-3.67930800	-2.86184700	-0.22543900
H	-4.54856500	-3.48071000	-1.61901500
C	-5.08660500	-0.21735900	-1.35219600
H	-4.15759800	0.13346300	-1.79864600
C	-5.20325300	-1.55465400	-0.98515300
C	-6.40592100	-1.97391800	-0.39589100
C	-7.47479900	-1.09747500	-0.19423400
C	-7.32110700	0.23472900	-0.61237900
C	-6.13532900	0.69332100	-1.18881000
C	-5.97183800	2.13470900	-1.62913200
H	-5.79104500	2.16394100	-2.71013800
H	-6.90656600	2.66724200	-1.43726600
C	1.18632700	-1.62206000	-4.80675600
H	0.80296500	-2.60628600	-5.11666700
H	1.77298700	-1.75200000	-3.89010900
C	2.05006800	-1.00395200	-5.88872700
H	2.94267200	-1.63101200	-6.00332800
H	2.38890400	-0.02586900	-5.52784400
C	1.32211000	-0.86415900	-7.22169200
H	1.96762200	-0.40850700	-7.97884000
H	0.43206600	-0.23742800	-7.11250200
H	1.00358700	-1.84331900	-7.59797400
C	-2.13043400	-1.92256800	-5.82126600
H	-1.16706700	-2.23535800	-6.23229100
H	-2.39657800	-0.97798400	-6.30988900
H	-2.88130700	-2.67029100	-6.08743600
C	-5.10734700	-1.71918200	-4.63999600
H	-4.64293900	-1.35559600	-5.56440500
H	-5.24320800	-0.86397100	-3.96434600
C	-6.43759000	-2.38564000	-4.93334400
H	-6.24874100	-3.29077100	-5.52300700
H	-7.02063800	-1.70713000	-5.56690100
C	-7.21966700	-2.72133300	-3.66764400
H	-7.45662100	-1.80760200	-3.10923000
H	-6.64118000	-3.37528000	-3.00691200
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C	-6.19944400	-3.60485600	1.28435900
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H	-5.24151300	-3.12526000	1.52741100

C	-6.08347200	-5.10803000	1.44377800
H	-7.03139100	-5.56945500	1.14206900
H	-5.94941100	-5.31897500	2.51143800
C	-4.92470900	-5.69210800	0.64106600
H	-3.97295300	-5.24020600	0.94809600
H	-5.05918500	-5.50527400	-0.42850000
H	-4.84516800	-6.77336600	0.78952800
C	-8.75645600	-1.55327900	0.44922700
H	-8.80789500	-2.64392000	0.46666800
H	-9.62931200	-1.17108300	-0.08775400
H	-8.82807400	-1.18555000	1.47977700
C	-9.23340600	1.21919800	-1.56163800
H	-9.59715700	0.22414500	-1.85830500
H	-8.66498500	1.63403200	-2.40546200
C	-10.38825900	2.12454200	-1.18006900
H	-10.99018400	2.30594300	-2.07774200
H	-9.97953600	3.09327700	-0.86565800
C	-11.25351200	1.52901900	-0.07362400
H	-12.06416000	2.20931800	0.20437400
H	-10.65811800	1.32505200	0.82148900
H	-11.70446200	0.58504800	-0.40078100
O	-6.13472500	2.90120400	1.06557300
O	-1.73427000	4.78570400	1.06994500
O	1.00504400	5.05585500	-2.88435200
O	2.77618000	0.61871200	-2.98650700
C	-3.64933200	3.16510300	-1.59299400
H	-3.55248700	2.92523900	-2.65093600
C	-4.83082200	2.84033100	-0.93136800
C	-4.95746600	3.19845100	0.41858400
C	-3.91887300	3.82740800	1.11276600
C	-2.74412600	4.12609200	0.40649100
C	-2.59544400	3.82287500	-0.95050600
C	-1.37959200	4.28954300	-1.71231000
H	-1.71870900	4.72595900	-2.66122300
H	-0.91118900	5.10844200	-1.15828300
C	-0.42742900	1.89745500	-1.74837800
H	-1.34364500	1.52365300	-1.29281100
C	-0.30992000	3.25747500	-2.02276900
C	0.87169200	3.70824900	-2.63281900
C	1.91591400	2.84084900	-2.96100300
C	1.75605300	1.48194000	-2.65487300
C	0.59730500	0.99248600	-2.05070200
C	0.46457800	-0.48366400	-1.74108700
H	0.42366800	-0.63765100	-0.65706000
H	1.36436100	-0.99730700	-2.08752400
C	-7.07656600	3.97638300	1.08705900
H	-6.59745600	4.87421300	1.50553400
H	-7.39252000	4.20991700	0.06081200
C	-8.25333200	3.54465800	1.93962100
H	-9.02117900	4.32543600	1.88088000
H	-8.67136200	2.63456800	1.49541400
C	-7.85551800	3.29771900	3.39160200
H	-8.71358100	2.97481200	3.98920600
H	-7.08783000	2.51950400	3.45205500
H	-7.45073100	4.20868800	3.84796700
C	-4.05734600	4.22175100	2.55881100
H	-4.96511100	3.79270600	2.98810200
H	-3.20053000	3.87928800	3.14843800
H	-4.10251600	5.31149500	2.66516800
C	-0.75105400	3.89246800	1.60768300
H	-1.20539300	3.30648200	2.41824900
H	-0.43224600	3.19140900	0.82268000
C	0.43105600	4.69570400	2.11170300
H	0.05869300	5.50321700	2.75379500
H	1.03606100	4.03505500	2.74374900
C	1.28376400	5.25262000	0.97557200
H	1.61869600	4.43864300	0.31923700
H	0.71775500	5.96504100	0.36592800
H	2.17189400	5.76656400	1.35803200
C	0.67245200	5.43047600	-4.22473600
H	1.35313200	4.93083400	-4.92655100
H	-0.35110100	5.10055800	-4.45368200
C	0.78857000	6.93816100	-4.33314100
H	1.82215200	7.22617900	-4.10642700
H	0.59818900	7.21579100	-5.37618100
C	-0.17817900	7.66624600	-3.40435300
H	-1.21484000	7.38591300	-3.62400100
H	0.02505400	7.41654600	-2.35905600
H	-0.09246700	8.75120500	-3.51709300
C	3.15922500	3.33008100	-3.65339000
H	3.28324600	4.40652500	-3.51004500
H	4.04870800	2.81460400	-3.28242800
H	3.10811400	3.13298700	-4.73139500
C	3.69333600	0.39782300	-1.90879100
H	4.01429900	1.36890100	-1.50610500
H	3.18836900	-0.15030100	-1.09756900
C	4.87999000	-0.37933300	-2.43589300
H	5.53922100	-0.60374300	-1.58985600
H	4.52778000	-1.34672200	-2.81931500
C	5.64234200	0.37758400	-3.51893100
H	6.50542500	-0.19672600	-3.87015900
H	5.00077200	0.58972700	-4.38003400
H	6.01506800	1.33347700	-3.13142600