

Supporting Information: Photocycloaddition Reaction of Atropisomeric Maleimides: Mechanism and Selectivity

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Table S1: Selected Dihedral Angles (in Degrees) and Drawings of Four Different Conformers (A-D) and Their Enantiomers (A'-D') Optimized at the B3LYP-D3/6-31G*/PCM (acetonitrile) Level

Dihedral Angles	A-S0-R	B-S0-R	C-S0-R	D-S0-R
C5-N-C6-C9	110.4	113.5	111.6	113.7
C1-C2-C7-C8	111.1	-117.7	111.4	-117.4
C2-C7-C8-C9	62.5	67.0	63.0	66.2
C7-C8-C9-C10	83.9	80.3	83.5	79.6
C8-C9-C10-C11	-178.5	-178.1	-178.2	-178.2

Dihedral Angles	A'-S0-R	B'-S0-R	C'-S0-R	D'-S0-R
C5-N-C6-C9	-110.4	-113.5	-111.6	-113.7
C1-C2-C7-C8	-111.1	117.7	-111.4	117.4
C2-C7-C8-C9	-62.5	-67.0	-63.0	-66.2
C7-C8-C9-C10	-83.9	-80.3	-83.5	-79.6
C8-C9-C10-C11	178.5	178.1	178.2	178.2

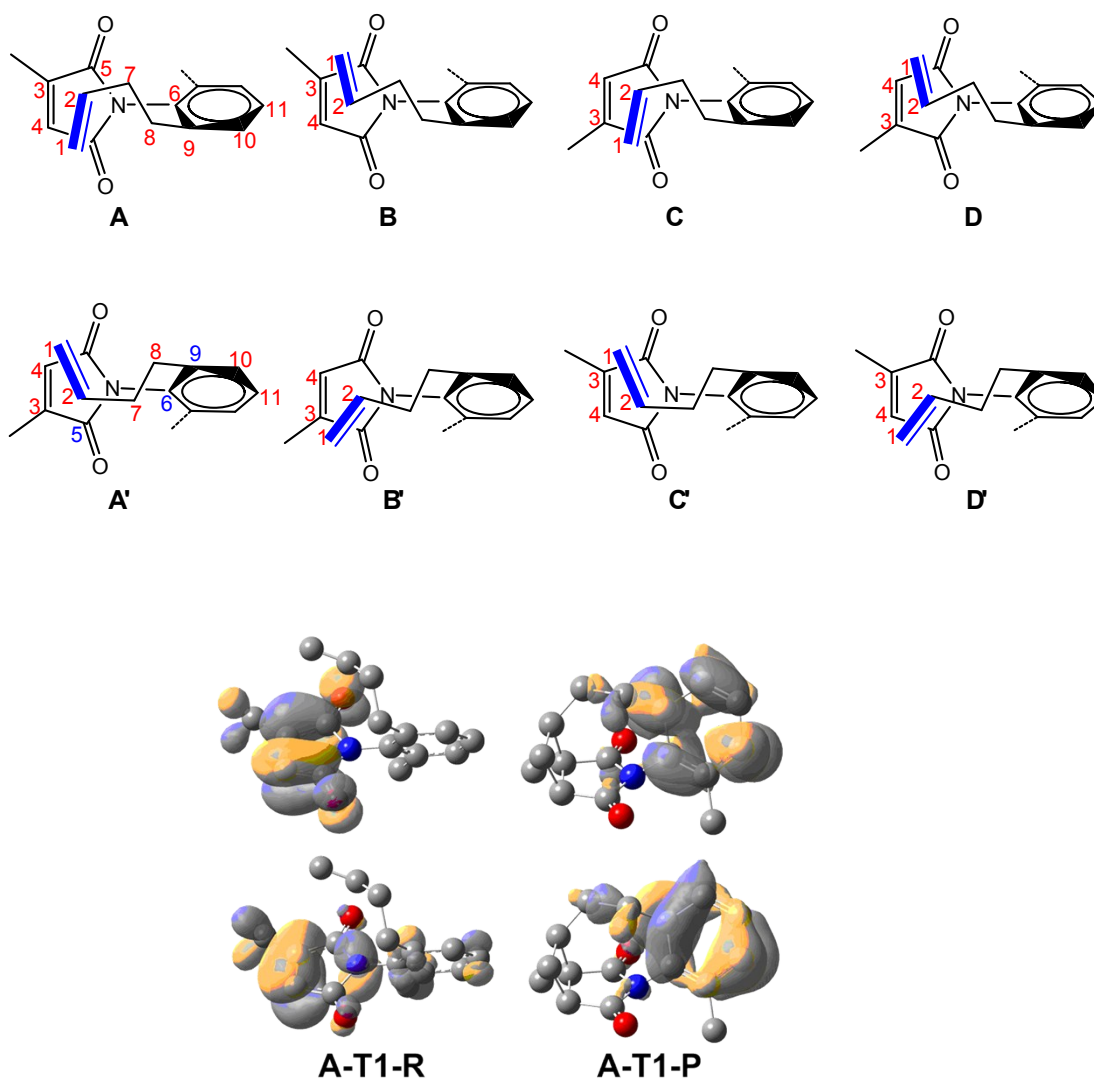


Fig. S1: Two singly-occupied molecular orbitals of the T_1 reactant and product of the A conformer.

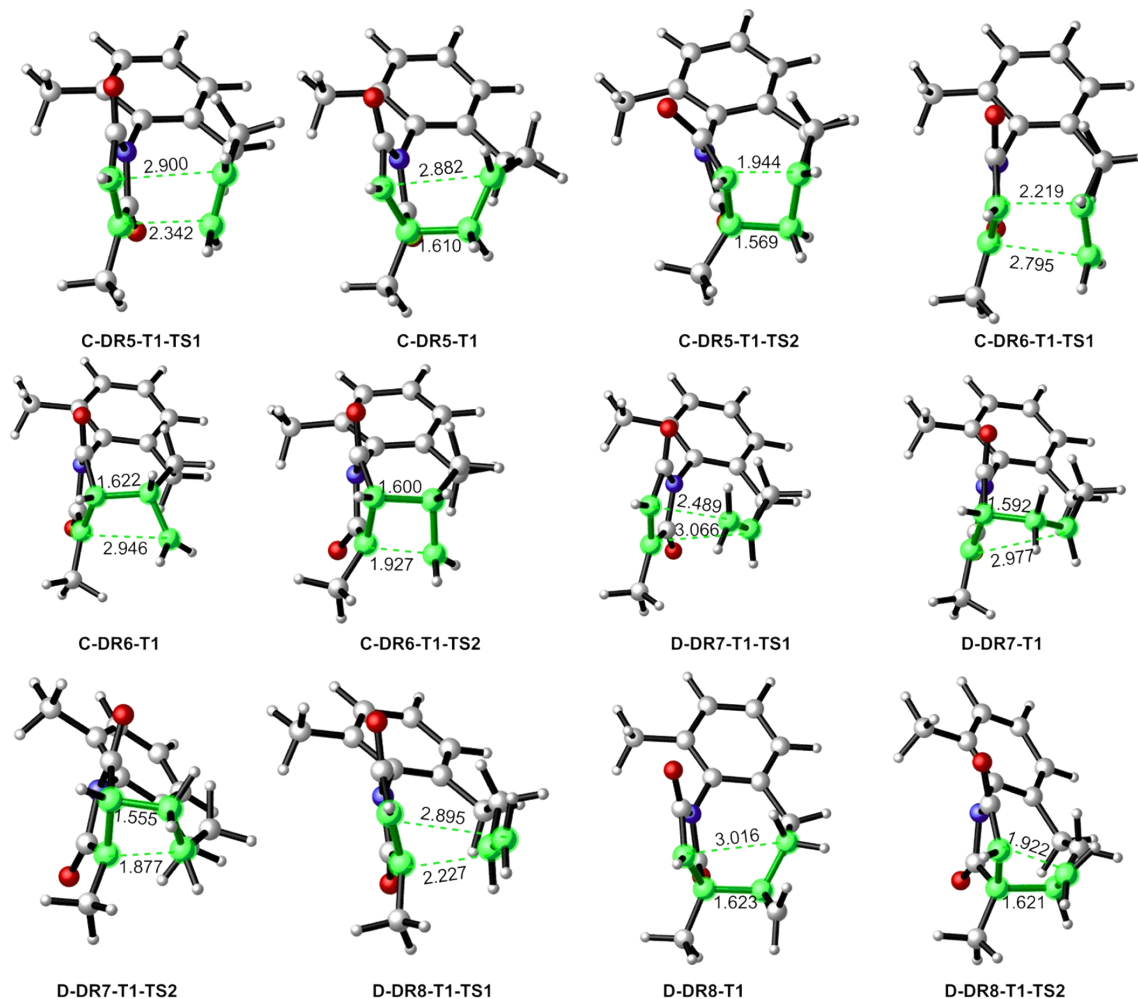


Fig. S2: B3LYP-D3/6-31G*/PCM (acetonitrile) optimized stationary points (diradical intermediates and transition states) involved in the triplet-state reaction starting from the conformers C and D. Selected distances are given in Å.

Comment on Fig. S3: According to our calculations, the second half reaction will not take place in any of the T_1 pathways DR1-DR8, because the Gibbs free energy of each transition state is more than 40 kcal/mol higher than that of the corresponding reactant (see main text and Fig. S10). Why is each second half reaction blocked in the T_1 state? This can be traced back to the evolution of two relevant SOMOs along the T_1 paths, e.g. of conformer A (Fig. S3). The two unpaired electrons are initially localized within the maleimide group of the triplet reactant (A-T1-R), become distributed over the maleimide and alkene groups in the intermediate (A-DR1-T1), and finally move to the phenyl moiety of the product (A-T1-P), forming a triplet exciton. Overall, the conversion from A-T1-R to A-T1-P may thus be viewed as a triplet exciton transfer from the maleimide to the phenyl group, which is energetically unfavorable.

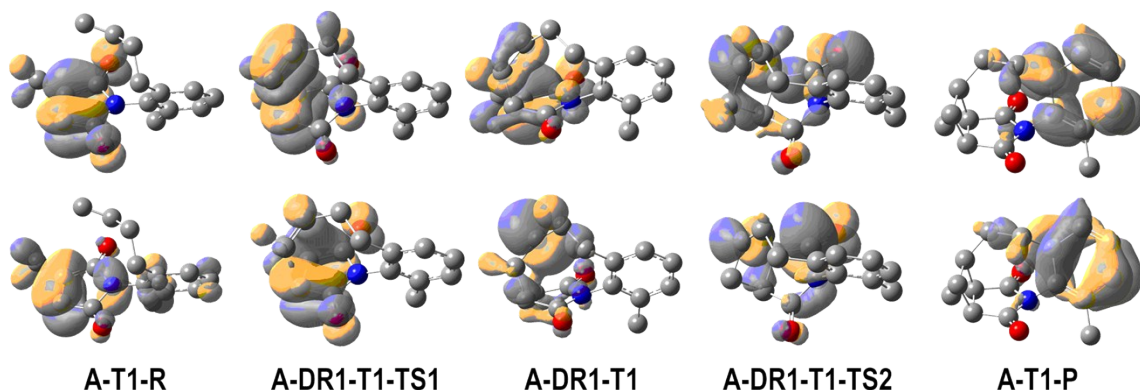


Fig. S3: Singly-occupied molecular orbitals along the T_1 photocyclization reaction path DR1 of the A conformer. See main text for discussion.

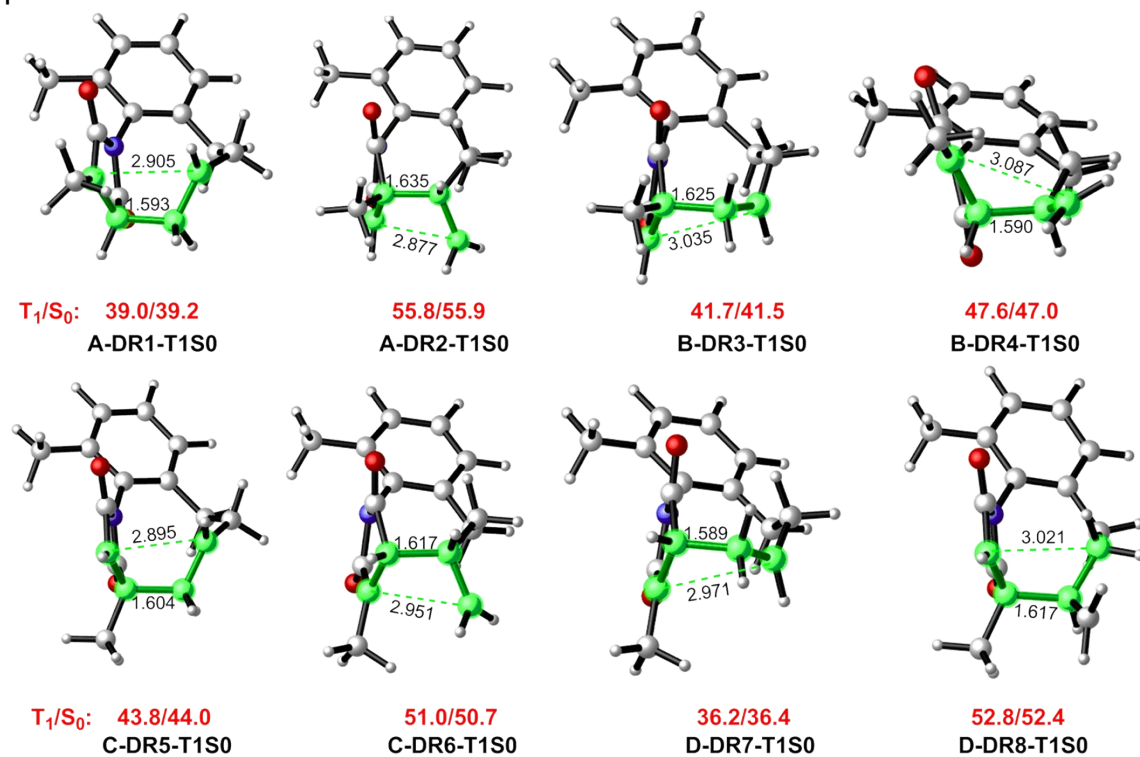


Fig. S4: T_1/S_0 crossing points optimized at the B3LYP-D3/6-31G*/PCM level. T_1/S_0 state energies in kcal/mol, selected distances in Å. See main text for discussion.

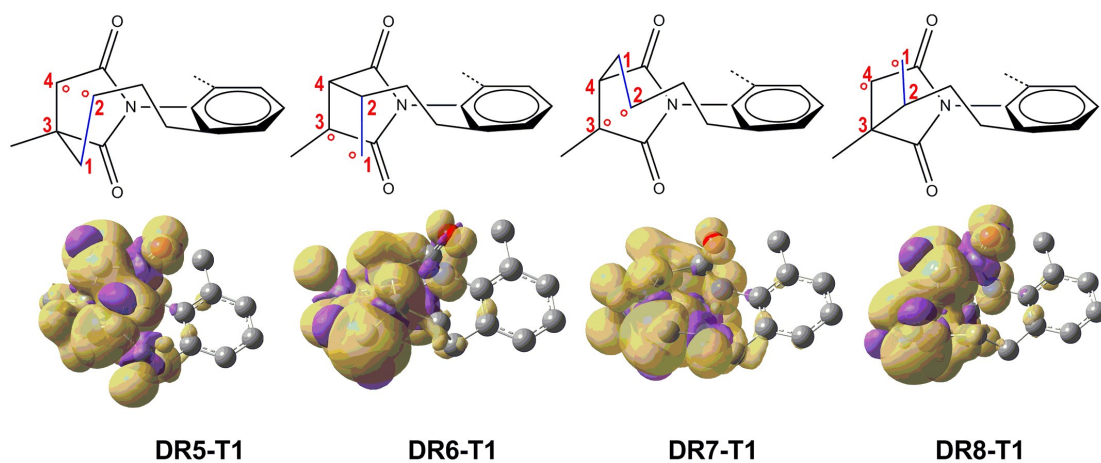


Fig. S5: Spin density plots for triplet diradical intermediates (paths DR5-DR8) obtained from B3LYP-D3/6-31G*/PCM (acetonitrile) calculations.

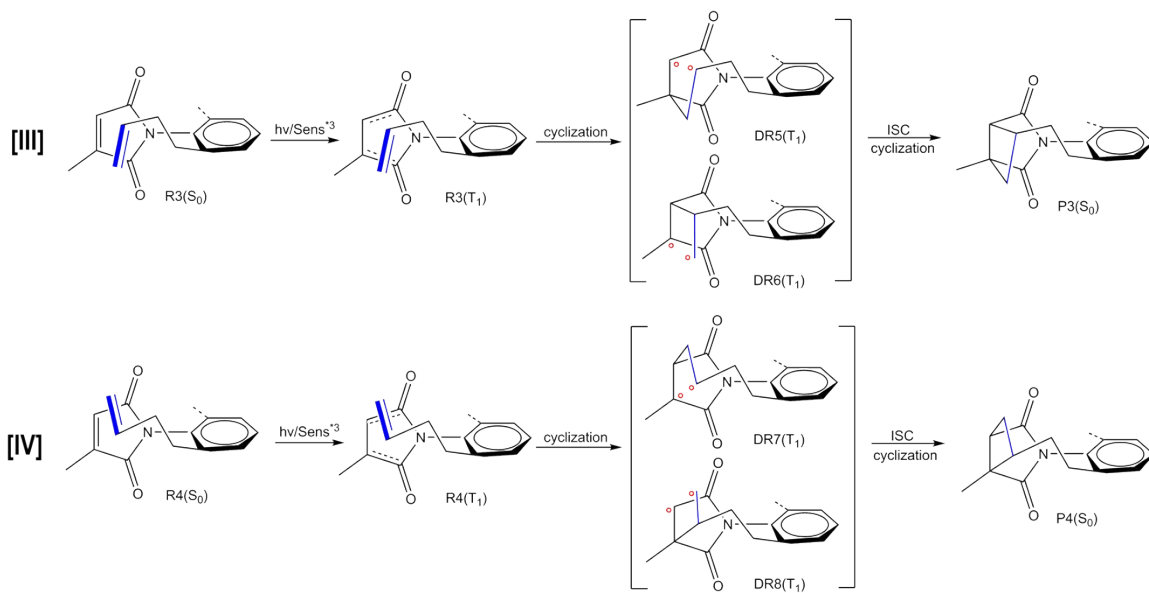


Fig. S6: Reaction paths for [2+2] photocyclization starting from the reactant conformers C and D.

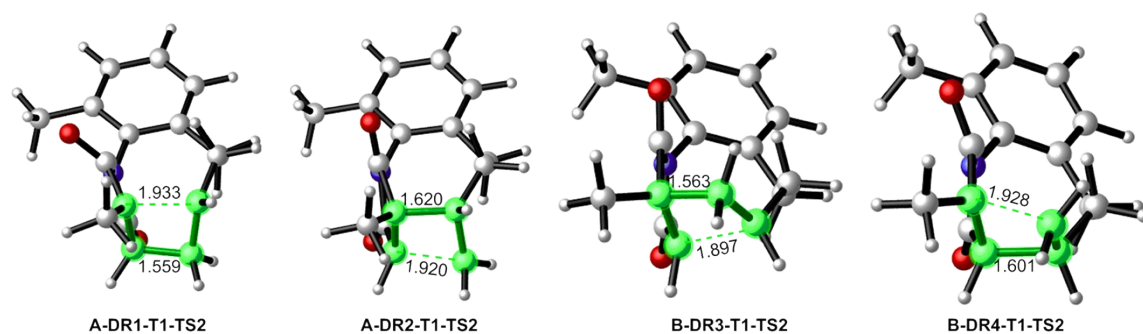


Fig. S7: B3LYP-D3/6-31G*/PCM (acetonitrile) optimized transition states involved in the triplet-state the second half reaction starting from the conformers A and B. Selected distances are given in Å.

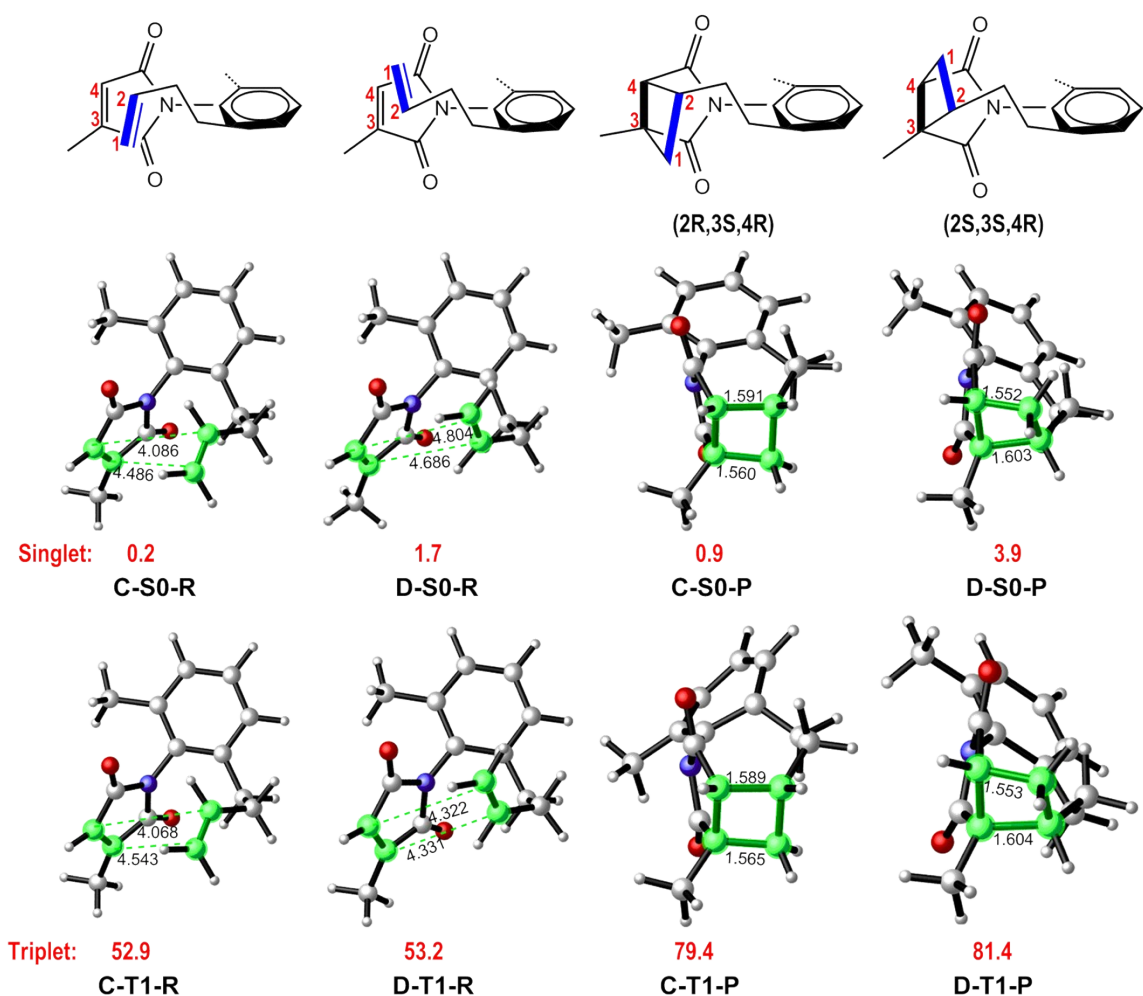


Fig. S8: B3LYP-D3/6-31G*/PCM (acetonitrile) optimized stationary points (reactants and products) starting from the conformers C and D. Selected distances are given in Å.

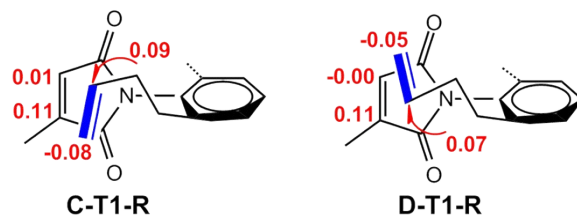


Fig. S9: Mulliken charges of the four carbon atoms involved in the [2+2] photoaddition reaction of the different triplet reactants starting from the conformers C and D.

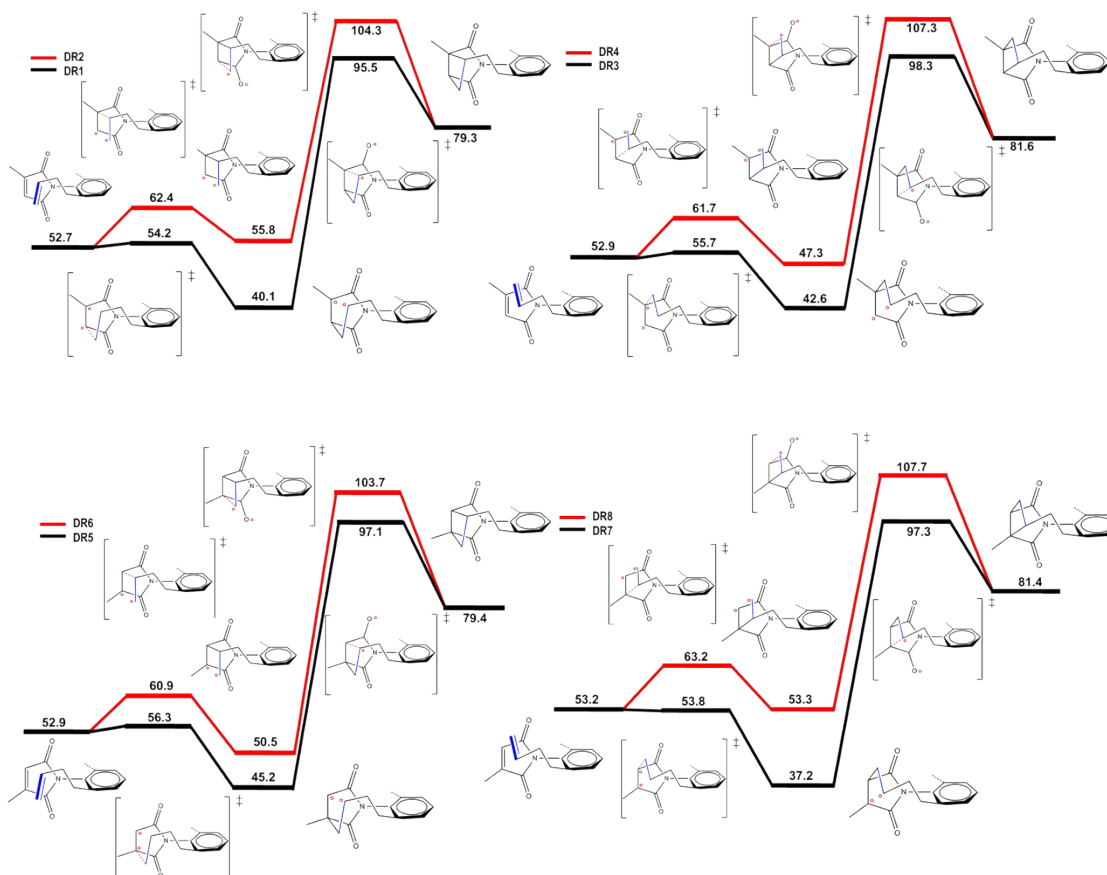


Fig. S10: Gibbs free energy profiles (in kcal/mol) for the [2+2] photocyclizations starting from the the reactant conformers A, B, C, and D computed at the B3LYP-D3/6-31G*/PCM level.

Comments on Fig. S11: As discussed in the main paper, phenyl substitution at the maleimide double bond makes the DR1 pathway much more favorable thermodynamically. This can be understood by considering the electronic structures of the triplet diradical intermediates (e.g. A-DR1-T1 and B-DR3-T1). Fig. S11 shows the computed spin density distributions in these intermediates for compounds 1, 2, 7, and 10. In the case of methyl substitution (compounds 1 and 2) the plots for DR1 and DR3 look fairly similar, whereas there are pronounced differences in the case of phenyl substitution (compounds 7 and 10). On pathway DR1, the phenyl substituent is located at the radical center of the original maleimide double bond so that the spin density can delocalize into the phenyl ring, which affords significant stabilization (Fig. S11). On pathway DR3, such delocalization and stabilization is not possible because the phenyl substituent is attached to a saturated carbon atom. In these compounds, the diastereoselectivity is thus ultimately governed by the ability of the substituents to stabilize the intermediate diradical triplet species.

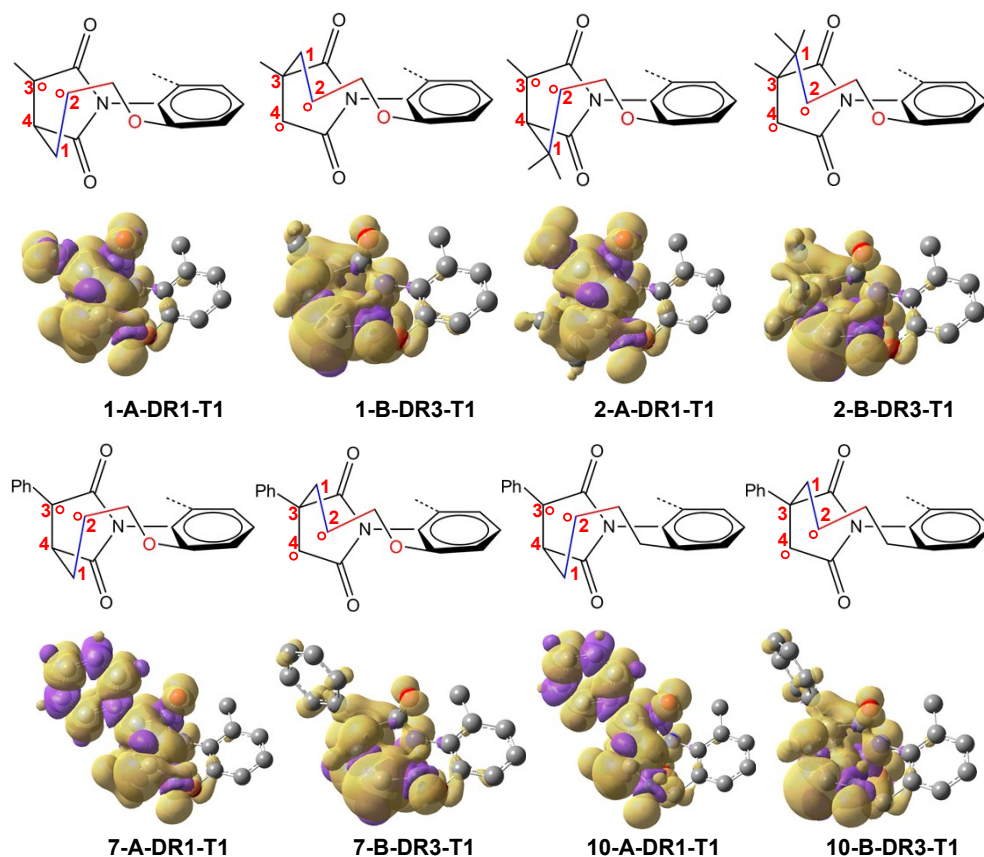


Fig. S11: Spin density plots of the diradical triplet intermediates on the DR1 and DR3 pathways of the substituted maleimides. Methyl-phenyl substitution on the

maleimide double bond stabilizes the DR1 diradical intermediates of compounds 7 and 10 (7-A-DR1-T1 and 10-A-DR1-T1) and makes no difference for the DR3 diradical intermediates (7-B-DR3-T1 and 10-B-DR3-T1).

Table S2: Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) Computed at the CAM-B3LYP-D3/6-31G*/PCM Level.

DR1	R-S0	P-S0	R-T1	TS1	DR	TS2	P-T1	T ₁ /S ₀
E	0.0	-11.2	59.3	57.5	35.5	95.7	72.5	35.5/35.7
H	0.0	-9.6	57.3	55.3	34.8	93.2	71.1	
G	0.0	-5.9	56.4	56.6	36.5	96.0	73.3	
DR2								
E	0.0	-11.2	59.3	64.8	52.1	106.2	72.5	52.1/52.3
H	0.0	-9.6	57.3	62.3	50.4	102.7	71.2	
G	0.0	-5.9	56.4	64.0	51.6	104.5	73.3	
DR3								
E	1.0	-8.5	61.2	58.5	37.6	98.8	75.6	38.2/38.1
H	1.0	-6.9	58.9	56.2	36.6	95.9	73.7	
G	0.9	-2.8	58.0	57.7	38.5	99.4	75.7	
DR4								
E	1.0	-8.5	61.2	64.7	43.6	108.4	75.6	43.6/43.2
H	1.0	-6.9	58.9	62.3	42.2	105.3	73.7	
G	0.9	-2.8	58.0	63.9	43.3	107.4	75.7	
DR5								
E	0.3	-11.0	58.5	59.0	40.2	97.7	72.7	40.2/40.4
H	0.2	-9.4	56.6	56.8	39.2	95.2	71.4	
G	0.2	-5.7	55.7	58.4	41.2	97.9	73.5	
DR6								
E	0.3	-11.0	58.5	64.0	47.5	105.4	72.7	47.5/47.3
H	0.2	-9.4	56.6	61.7	46.1	102.3	71.4	
G	0.2	-5.7	55.7	63.1	46.8	104.2	73.5	
DR7								
E	1.1	-8.8	61.3	57.0	32.6	97.4	75.4	32.6/32.8
H	1.1	-7.2	58.9	54.8	31.9	95.1	73.5	
G	1.0	-3.1	57.7	56.0	33.2	97.2	75.4	
DR8								
E	1.1	-8.8	61.3	65.8	48.9	110.5	75.4	48.9/48.6
H	1.1	-7.2	58.9	63.1	47.3	111.0	73.5	
G	1.0	-3.1	57.7	65.0	48.9	114.6	75.4	

Table S3: Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) Computed at the M06-2X/6-31G*/PCM Level.

DR1	R-S0	P-S0	R-T1	TS1	DR	TS2	P-T1	T ₁ /S ₀
E	0.0	-12.6	60.2	60.4	38.1	98.3	75.5	38.1/38.3
H	0.0	-11.1	58.1	58.2	37.5	95.7	74.4	
G	0.0	-7.1	59.5	59.6	39.2	98.9	76.9	
DR2								
E	0.0	-12.6	60.2	67.4	53.6	108.6	75.5	53.6/53.8
H	0.0	-11.1	58.1	64.9	52.0	104.2	74.4	
G	0.0	-7.1	59.5	66.7	53.8	107.3	76.9	
DR3								
E	0.9	-10.3	64.7	61.5	39.6	100.8	79.8	40.3/40.3
H	0.8	-8.7	62.6	59.1	38.6	97.7	77.9	
G	0.6	-4.4	61.5	60.5	40.6	101.4	80.1	
DR4								
E	0.9	-10.3	64.7	67.6	45.5	110.5	79.8	45.5/45.3
H	0.8	-8.7	62.6	65.1	44.0	106.7	77.9	
G	0.6	-4.4	61.5	66.8	45.2	110.3	80.1	
DR5								
E	0.3	-12.2	62.1	61.8	42.3	100.5	75.8	42.3/42.5
H	0.2	-10.7	60.4	59.5	41.2	97.8	74.7	
G	-0.1	-6.7	59.4	61.4	43.4	100.9	77.2	
DR6								
E	0.3	-12.2	62.1	66.9	49.3	108.0	75.8	49.3/49.3
H	0.2	-10.7	60.4	64.6	48.1	104.7	74.7	
G	-0.1	-6.7	59.4	66.3	49.3	106.5	77.2	
DR7								
E	1.0	-10.8	64.8	60.1	35.2	99.5	79.3	35.2/35.4
H	0.7	-9.3	61.9	58.0	34.5	97.1	77.5	
G	0.0	-4.8	62.4	59.5	35.6	99.4	79.7	
DR8								
E	1.0	-10.8	64.8	68.2	50.0	110.8	79.3	50.0/49.9
H	0.7	-9.3	61.9	65.6	48.4	106.6	77.5	
G	0.0	-4.8	62.4	67.5	50.3	110.4	79.7	

Table S4: Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) Computed at the PBE0-D3/6-31G*/PCM Level.

DR1	R-S0	P-S0	R-T1	TS1	DR	TS2	P-T1	T ₁ /S ₀
E	0.0	-16.6	55.7	53.1	30.6	85.7	65.8	30.6/30.8
H	0.0	-15.1	53.5	50.9	29.9	83.1	64.5	
G	0.0	-11.1	52.6	52.2	31.7	86.2	66.9	
DR2								
E	0.0	-16.6	55.7	58.7	47.5	96.4	65.8	47.5/47.7
H	0.0	-15.1	53.5	56.1	45.8	93.0	64.5	
G	0.0	-11.1	52.6	58.0	47.1	95.6	66.9	
DR3								
E	1.0	-14.1	56.8	53.8	33.1	88.9	68.8	33.7/33.6
H	0.9	-12.6	54.5	51.5	32.1	86.2	66.8	
G	0.8	-8.3	53.5	53.1	34.2	89.2	69.1	
DR4								
E	1.0	-14.1	56.8	59.2	39.1	98.4	68.8	39.1/38.6
H	0.9	-12.6	54.5	56.8	37.6	95.1	66.8	
G	0.8	-8.3	53.5	58.4	38.4	97.9	69.1	
DR5								
E	0.2	-16.5	55.4	53.8	35.5	87.7	66.0	35.5/35.8
H	0.2	-15.0	53.4	51.6	34.4	85.1	64.7	
G	0.1	-10.9	52.4	53.4	36.7	88.2	67.1	
DR6								
E	0.2	-16.5	55.4	58.0	42.7	95.4	66.0	42.7/42.5
H	0.2	-15.0	53.4	55.7	41.3	92.4	64.7	
G	0.1	-10.9	52.4	57.2	42.0	95.0	67.1	
DR7								
E	1.1	-14.3	57.0	52.8	28.0	87.3	68.6	28.0/28.3
H	1.1	-12.8	54.5	50.6	27.3	84.6	66.6	
G	0.9	-8.5	53.0	51.9	28.6	87.7	68.9	
DR8								
E	1.1	-14.3	57.0	59.9	44.4	99.2	68.6	44.4/44.0
H	1.1	-12.8	54.5	57.2	42.7	95.6	66.6	
G	0.9	-8.5	53.0	59.1	44.2	98.6	68.9	

Table S5: Relative Energies E, Enthalpies H, and Gibbs Free Energies G (in kcal/mol) Computed at the B3LYP-D3/6-31G*/PCM Level.

DR1	R-S0	P-S0	R-T1	TS1	DR	TS2	P- T1	T ₁ /S ₀
E	0.0	-5.2	55.6	54.2	38.8	94.2	77.9	39.0/39.2
H	0.0	-3.7	53.6	52.5	38.1	91.9	76.6	
G	0.0	0.7	52.7	54.2	40.1	95.5	79.3	
DR2								
E	0.0	-5.2	55.6	62.7	55.6	104.2	77.9	55.8/55.9
H	0.0	-3.7	53.6	60.2	54.0	101.3	76.6	
G	0.0	0.7	52.7	62.4	55.8	104.3	79.3	
DR3								
E	1.0	-2.4	56.4	55.9	41.2	97.5	80.8	41.7/41.5
H	0.8	-0.8	54.1	53.6	40.2	94.9	79.0	
G	0.5	4.0	52.9	55.7	42.6	98.3	81.6	
DR4								
E	1.0	-2.4	56.4	62.1	47.4	106.6	80.8	47.6/47.0
H	0.8	-0.8	54.1	59.7	46.0	103.7	79.0	
G	0.5	4.0	52.9	61.7	47.3	107.3	81.6	
DR5								
E	0.3	-5.1	55.9	56.3	43.7	95.9	78.0	43.8/44.0
H	0.3	-3.6	53.8	54.1	42.6	93.6	76.7	
G	0.2	0.9	52.9	56.3	45.2	97.1	79.4	
DR6								
E	0.3	-5.1	55.9	61.5	50.9	103.4	78.0	51.0/50.7
H	0.3	-3.6	53.8	59.2	49.5	100.7	76.7	
G	0.2	0.9	52.9	60.9	50.5	103.7	79.4	
DR7								
E	1.1	-2.5	56.4	54.3	36.1	96.1	80.7	36.2/36.4
H	0.4	-0.9	54.2	52.1	35.4	93.7	78.8	
G	1.7	3.9	53.2	53.8	37.2	97.3	81.4	
DR8								
E	1.1	-2.5	56.4	63.3	52.7	107.4	80.7	52.8/52.4
H	0.4	-0.9	54.2	60.7	51.2	104.2	78.8	
G	1.7	3.9	53.2	63.2	53.3	107.7	81.4	

Effects of Different Functionals on Energy Profiles of DR3-DR8

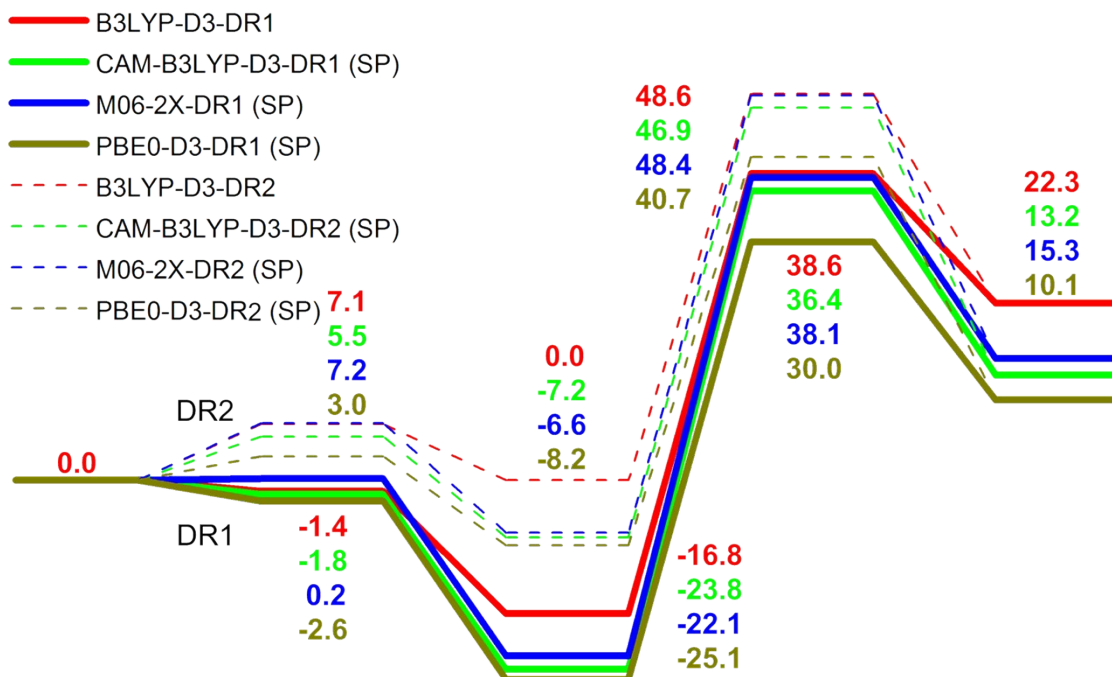


Fig. S12: Single-point energies from CAM-B3LYP-D3, M06-2X, and PBE0-D3 calculations on the B3LYP-D3 optimized geometries for pathways DR1 and DR2 (see text in the main article). The T₁ reactant serves as reference point in each potential energy profile.

Table S6: Computed Differences (in kcal/mol) in the Potential Energy Barriers $\Delta\Delta E^\ddagger_{\text{DR3:DR4}}$ and the Reaction Energies $\Delta\Delta E^{\text{rx}}_{\text{DR3:DR4}}$ between Paths DR1 and DR2 by Different Exchange-Correlation Functionals (B3LYP-D3, CAM-B3LYP-D3, M06-2X, and PBE0-D3). See Fig. S12 for the Associated Potential Energy Profiles.

	first half reaction		second half reaction	
	$\Delta\Delta E^\ddagger_{\text{DR1:DR2}}$	$\Delta\Delta E^{\text{rx}}_{\text{DR1:DR2}}$	$\Delta\Delta E^\ddagger_{\text{DR1:DR2}}$	$\Delta\Delta E^{\text{rx}}_{\text{DR1:DR2}}$
B3LYP-D3	-8.5	-16.8	6.8	16.8
CAM-B3LYP-D3	-7.3	-16.6	6.1	16.6
M06-2X	-7.0	-15.5	5.2	15.5
PBE0-D3	-5.6	-16.9	6.2	16.9

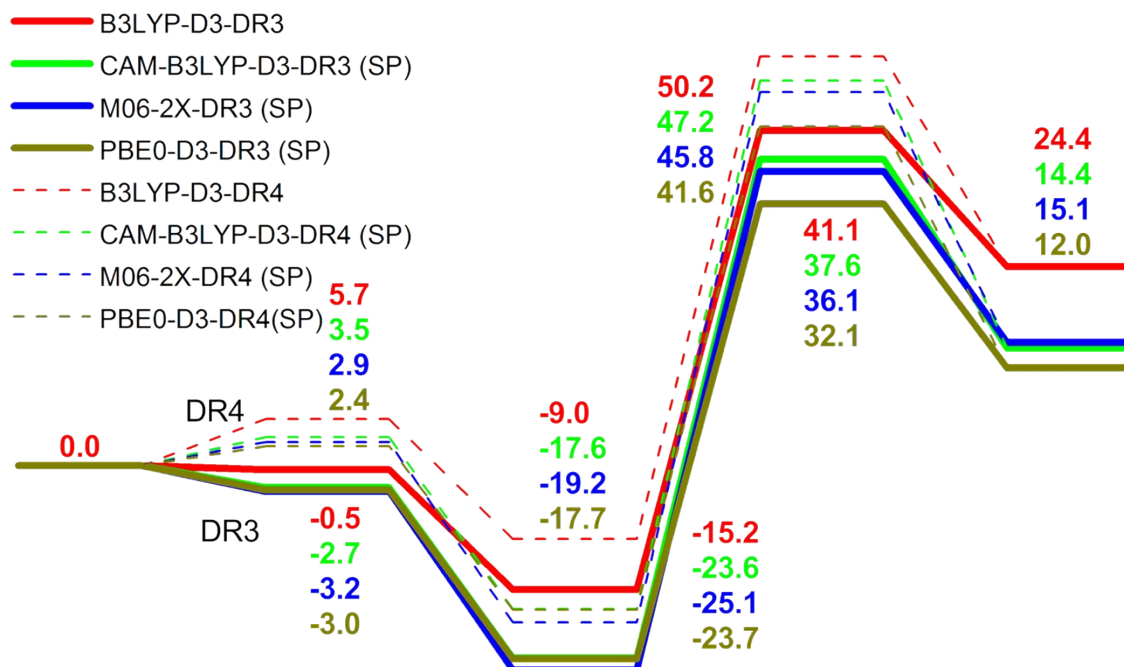


Fig. S13: Single-point energies from CAM-B3LYP-D3, M06-2X, and PBE0-D3 calculations on the B3LYP-D3 optimized geometries for pathways DR3 and DR4 (see text in the main article). The T₁ reactant serves as reference point in each potential energy profile.

Table S7: Computed Differences (in kcal/mol) in the Potential Energy Barriers $\Delta\Delta E^{\ddagger}_{\text{DR3:DR4}}$ and the Reaction Energies $\Delta\Delta E^{\text{rx}}_{\text{DR3:DR4}}$ between Paths DR3 and DR4 by Different Exchange-Correlation Functionals (B3LYP-D3, CAM-B3LYP-D3, M06-2X, and PBE0-D3). See Fig. S13 for the Associated Potential Energy Profiles.

	first half reaction		second half reaction	
	$\Delta\Delta E^{\ddagger}_{\text{DR3:DR4}}$	$\Delta\Delta E^{\text{rx}}_{\text{DR3:DR4}}$	$\Delta\Delta E^{\ddagger}_{\text{DR3:DR4}}$	$\Delta\Delta E^{\text{rx}}_{\text{DR3:DR4}}$
B3LYP-D3	-6.2	-6.2	-2.9	6.2
CAM-B3LYP-D3	-6.2	-6.0	-3.6	6.0
M06-2X	-6.1	-5.9	-3.8	5.9
PBE0-D3	-5.4	-6.0	-3.5	6.0

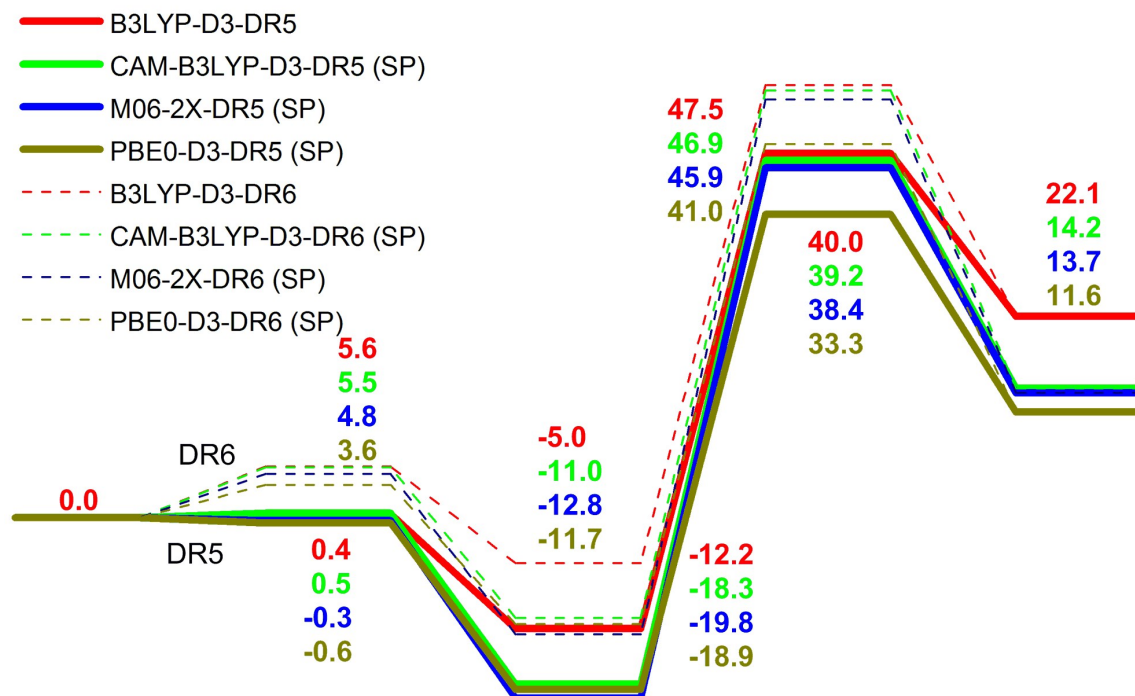


Fig. S14: Single-point energies from CAM-B3LYP-D3, M06-2X, and PBE0-D3 calculations on the B3LYP-D3 optimized geometries for pathways DR5 and DR6 (see text in the main article). The T_1 reactant serves as reference point in each potential energy profile.

Table S8: Computed Differences (in kcal/mol) in the Potential Energy Barriers $\Delta\Delta E^\ddagger_{\text{DR5:DR6}}$ and the Reaction Energies $\Delta\Delta E^{\text{rx}}_{\text{DR5:DR6}}$ between Paths DR5 and DR6 by Different Exchange-Correlation Functionals (B3LYP-D3, CAM-B3LYP-D3, M06-2X, and PBE0-D3). See Fig. S14 for the Associated Potential Energy Profiles.

	first half reaction		second half reaction	
	$\Delta\Delta E^\ddagger_{\text{DR5:DR6}}$	$\Delta\Delta E^{\text{rx}}_{\text{DR5:DR6}}$	$\Delta\Delta E^\ddagger_{\text{DR5:DR6}}$	$\Delta\Delta E^{\text{rx}}_{\text{DR5:DR6}}$
B3LYP-D3	-5.2	-7.2	-0.3	7.2
CAM-B3LYP-D3	-5.0	-7.3	-0.4	7.3
M06-2X	-5.1	-7.0	-0.5	7.0
PBE0-D3	-4.2	-7.2	-0.5	7.2

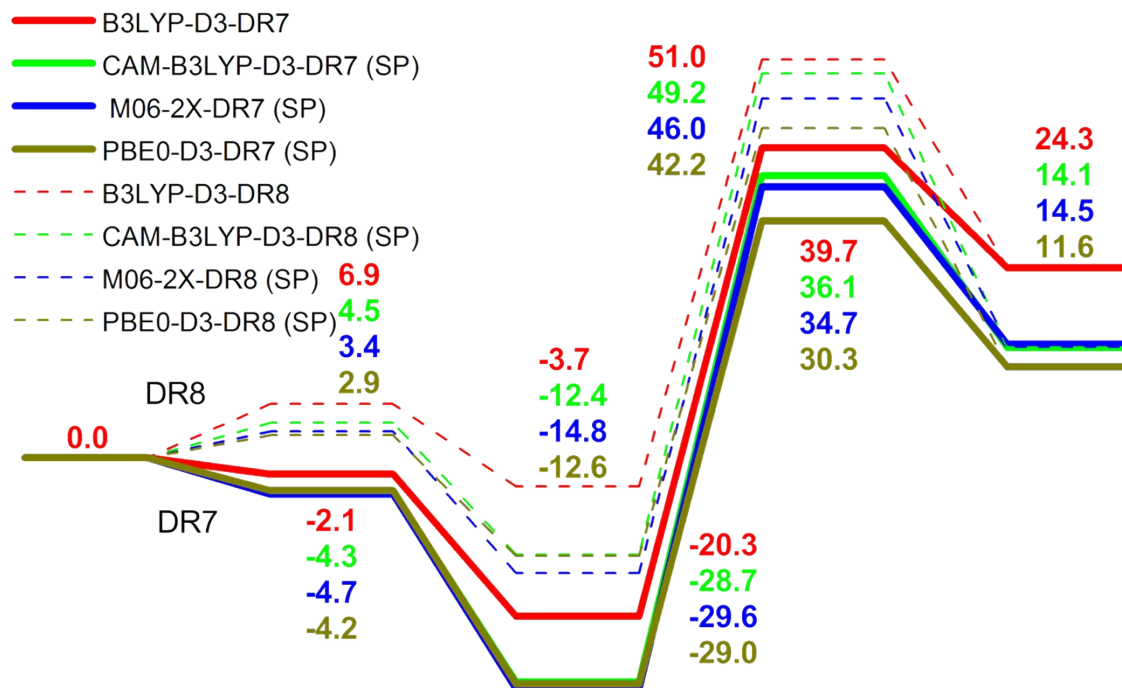


Fig. S15: Single-point energies from CAM-B3LYP-D3, M06-2X, and PBE0-D3 calculations on the B3LYP-D3 optimized geometries for pathways DR7 and DR8 (see text in the main article). The T₁ reactant serves as reference point in each potential energy profile.

Table S9: Computed Differences (in kcal/mol) in the Potential Energy Barriers $\Delta\Delta E^{\ddagger}_{\text{DR7:DR8}}$ and the Reaction Energies $\Delta\Delta E^{\text{rx}}_{\text{DR7:DR8}}$ between Paths DR7 and DR8 by Different Exchange-Correlation Functionals (B3LYP-D3, CAM-B3LYP-D3, M06-2X, and PBE0-D3). See Fig. S15 for the Associated Potential Energy Profiles.

	first half reaction		second half reaction	
	$\Delta\Delta E^{\ddagger}_{\text{DR7:DR8}}$	$\Delta\Delta E^{\text{rx}}_{\text{DR7:DR8}}$	$\Delta\Delta E^{\ddagger}_{\text{DR7:DR8}}$	$\Delta\Delta E^{\text{rx}}_{\text{DR7:DR8}}$
B3LYP-D3	-9.0	-16.6	5.3	16.6
CAM-B3LYP-D3	-8.8	-16.3	3.2	16.3
M06-2X	-8.1	-14.8	3.5	14.8
PBE0-D3	-7.1	-16.4	4.5	16.4

Table S10: Computed Gibbs Free Energy Barriers (in kcal/mol) for A-C Interconversion Paths and A-B Interconversion Paths: Results from (I) B3LYP-D3/6-31G*/PCM//B3LYP-D3/6-31G*/PCM and (II) B3LYP-D3/6-31+G*/PCM//B3LYP-D3/6-31+G*/PCM.

B3LYP-D3	Barrier-S0-AC	Barrier-T1-AC	Barrier-S0-AB	Barrier-T1-AB
I	33.8	19.7	4.0	4.3
II	34.3	18.8	4.1	4.2

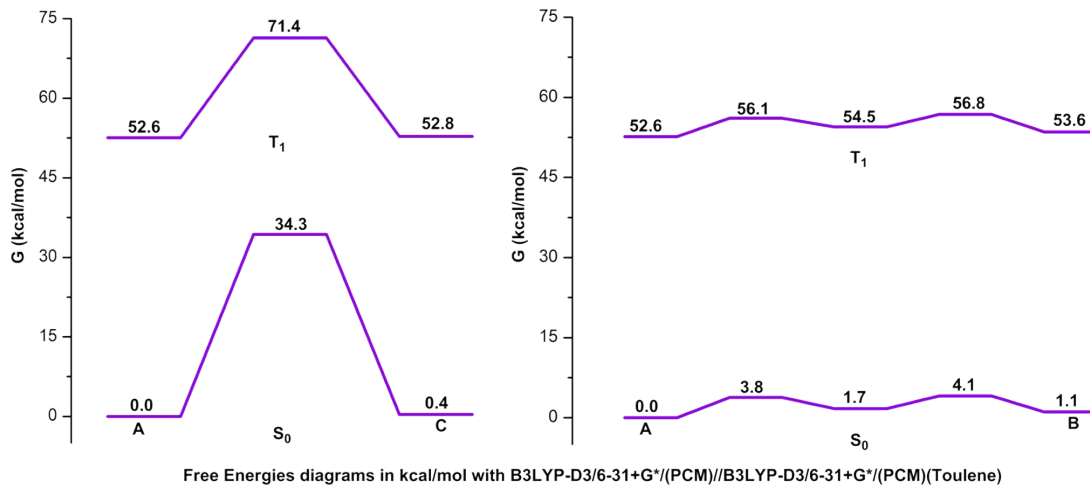


Fig. S16: Gibbs free energy profiles (kcal/mol) in the S₀ and T₁ states from B3LYP-D3/6-31+G*/PCM//B3LYP-D3/6-31+G*/PCM calculations.

Cartesian Coordinates of All Optimized Structures

In xyz format (unit: Ångstrom)

UB3LYP-D3/6-31G*/PCM level in acetonitrile solution

A-S0-R

C	-0.985878000	-0.704512000	1.629982000
C	-2.454476000	-0.803762000	1.397764000
C	-2.700300000	-0.750735000	0.081176000
C	-1.374998000	-0.630501000	-0.629361000
N	-0.388064000	-0.577390000	0.359777000
H	-3.158859000	-0.895806000	2.214520000
O	-0.382543000	-0.714564000	2.685701000
O	-1.188309000	-0.601134000	-1.831269000
C	1.019101000	-0.460430000	0.117994000
C	1.691924000	-1.560520000	-0.446923000
C	1.683974000	0.733734000	0.449714000
C	3.060535000	-1.433329000	-0.705458000
C	3.057736000	0.811496000	0.183167000
C	3.740609000	-0.255556000	-0.395362000
H	3.596319000	-2.270766000	-1.144339000
H	3.590757000	1.724943000	0.435332000
H	4.805489000	-0.174899000	-0.595447000
C	0.982787000	1.935967000	1.049676000
H	1.670305000	2.421196000	1.752327000
H	0.108642000	1.632676000	1.629450000
C	0.545183000	2.992099000	-0.000303000
H	0.128507000	3.855557000	0.532546000
H	1.441077000	3.339791000	-0.533889000
C	-0.456921000	2.458899000	-0.985005000
H	-0.096039000	1.683269000	-1.658821000
C	-1.737382000	2.829767000	-1.054975000
H	-2.151106000	3.590470000	-0.394946000
H	-2.419478000	2.384199000	-1.774942000
C	-3.973989000	-0.789810000	-0.686342000
H	-3.948236000	-1.596557000	-1.428016000
H	-4.107956000	0.146117000	-1.242443000
H	-4.832653000	-0.935417000	-0.027024000
C	0.961266000	-2.841963000	-0.766597000
H	1.666012000	-3.640404000	-1.014495000
H	0.285364000	-2.706693000	-1.618404000

H	0.350085000	-3.175423000	0.079804000
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B-S0-R

C	-1.260458000	-0.621078000	1.590808000
C	-2.713597000	-0.419064000	1.330506000
C	-2.903467000	-0.197886000	0.022226000
C	-1.555801000	-0.257697000	-0.655889000
N	-0.607237000	-0.479811000	0.349269000
H	-3.448966000	-0.458354000	2.123936000
O	-0.705527000	-0.853813000	2.647533000
O	-1.332342000	-0.153427000	-1.846013000
C	0.802133000	-0.628341000	0.142881000
C	1.259753000	-1.768146000	-0.546641000
C	1.683482000	0.347629000	0.640338000
C	2.635159000	-1.898483000	-0.763754000
C	3.054220000	0.167491000	0.411070000
C	3.528708000	-0.937458000	-0.290898000
H	3.006149000	-2.769237000	-1.297851000
H	3.751657000	0.910889000	0.789403000
H	4.595243000	-1.057428000	-0.460345000
C	1.226290000	1.592174000	1.372496000
H	1.936484000	1.798770000	2.181771000
H	0.255081000	1.440402000	1.848633000
C	1.155407000	2.842920000	0.458831000
H	0.959475000	3.712372000	1.102450000
H	2.132464000	3.004051000	-0.013489000
C	-4.140231000	0.063791000	-0.762221000
H	-4.255119000	-0.686714000	-1.553157000
H	-4.075359000	1.038583000	-1.260479000
H	-5.026941000	0.049345000	-0.124418000
C	0.085122000	2.738977000	-0.590677000
H	-0.934265000	2.631292000	-0.215085000
C	0.297353000	2.738317000	-1.907183000
H	1.299725000	2.831598000	-2.321633000
H	-0.517723000	2.632503000	-2.617616000
C	0.301080000	-2.824639000	-1.040105000
H	0.838274000	-3.732500000	-1.328130000
H	-0.260931000	-2.469576000	-1.911098000
H	-0.432547000	-3.090447000	-0.270673000

C-S0-R

C	1.387041000	-0.765854000	-1.008078000
C	2.765814000	-0.749337000	-0.395628000
C	2.623341000	-0.547174000	0.921686000
C	1.175276000	-0.427818000	1.251005000
N	0.477573000	-0.545056000	0.032265000

O	1.103456000	-0.928413000	-2.179529000
O	0.660214000	-0.272682000	2.342015000
C	-0.947402000	-0.507002000	-0.111249000
C	-1.697834000	-1.582979000	0.400532000
C	-1.552009000	0.585772000	-0.758502000
C	-3.090072000	-1.532055000	0.277611000
C	-2.949164000	0.587509000	-0.869132000
C	-3.714038000	-0.454551000	-0.350994000
H	-3.686105000	-2.351919000	0.669481000
H	-3.435505000	1.421925000	-1.368369000
H	-4.796229000	-0.433757000	-0.445542000
C	-0.771602000	1.764596000	-1.304371000
H	-1.264574000	2.110849000	-2.220323000
H	0.241040000	1.470584000	-1.587859000
C	-0.687883000	2.961592000	-0.319942000
H	-0.191844000	3.795766000	-0.831169000
H	-1.711239000	3.286236000	-0.083968000
C	0.043948000	2.622196000	0.947871000
H	-0.436489000	1.887726000	1.592469000
C	1.234663000	3.111074000	1.301117000
H	1.762306000	3.836433000	0.683756000
H	1.727107000	2.800176000	2.219089000
C	-1.025626000	-2.760170000	1.064264000
H	-1.731659000	-3.583374000	1.203749000
H	-0.627127000	-2.481861000	2.046271000
H	-0.183515000	-3.128583000	0.467603000
C	3.978502000	-0.935168000	-1.237312000
H	4.889707000	-0.893970000	-0.636244000
H	3.937430000	-1.899167000	-1.758207000
H	4.026178000	-0.160449000	-2.011887000
H	3.390415000	-0.476258000	1.682120000

D-S0-R

C	1.695030000	-0.437631000	-0.920716000
C	2.999070000	-0.104435000	-0.238763000
C	2.736840000	0.106485000	1.058588000
C	1.278787000	-0.080020000	1.307782000
N	0.696290000	-0.377654000	0.058063000
O	1.525973000	-0.701157000	-2.095979000
O	0.683083000	-0.015393000	2.364923000
C	-0.689375000	-0.664340000	-0.164231000
C	-1.219662000	-1.853857000	0.372991000
C	-1.471548000	0.227602000	-0.918562000
C	-2.577130000	-2.121032000	0.169011000
C	-2.823565000	-0.088639000	-1.108423000
C	-3.376944000	-1.244768000	-0.564580000

H	-3.004366000	-3.031968000	0.579879000
H	-3.443965000	0.588550000	-1.690393000
H	-4.428119000	-1.470664000	-0.721358000
C	-0.939079000	1.520431000	-1.501175000
H	-1.379290000	1.661188000	-2.495380000
H	0.142146000	1.474953000	-1.648663000
C	-1.283071000	2.761797000	-0.638163000
H	-0.975508000	3.653410000	-1.202980000
H	-2.370419000	2.822662000	-0.505280000
C	-0.599211000	2.746939000	0.699541000
H	0.492064000	2.743527000	0.670985000
C	-1.220565000	2.704069000	1.878628000
H	-2.306929000	2.693074000	1.948879000
H	-0.669434000	2.664652000	2.814060000
C	-0.355073000	-2.818789000	1.147278000
H	-0.863480000	-3.778176000	1.276818000
H	-0.115560000	-2.421825000	2.139884000
H	0.596978000	-3.002073000	0.636454000
C	4.273188000	-0.059141000	-1.005904000
H	5.118486000	0.185726000	-0.358745000
H	4.461405000	-1.025028000	-1.489518000
H	4.209128000	0.686922000	-1.806978000
H	3.424215000	0.363020000	1.854519000

A'-S0-R

C	0.985878000	-0.704512000	1.629982000
C	2.454476000	-0.803762000	1.397764000
C	2.700300000	-0.750735000	0.081176000
C	1.374998000	-0.630501000	-0.629361000
N	0.388064000	-0.577390000	0.359777000
O	0.382543000	-0.714564000	2.685701000
O	1.188309000	-0.601134000	-1.831269000
C	-1.019101000	-0.460430000	0.117994000
C	-1.691924000	-1.560520000	-0.446923000
C	-1.683974000	0.733734000	0.449714000
C	-3.060535000	-1.433329000	-0.705458000
C	-3.057736000	0.811496000	0.183167000
C	-3.740609000	-0.255556000	-0.395362000
C	-0.982787000	1.935967000	1.049676000
C	-0.545183000	2.992099000	-0.000303000
C	0.456921000	2.458899000	-0.985005000
C	1.737382000	2.829767000	-1.054975000
C	3.973989000	-0.789810000	-0.686342000
C	-0.961266000	-2.841963000	-0.766597000
H	3.158859000	-0.895806000	2.214520000
H	-3.596319000	-2.270766000	-1.144339000

H	-3.590757000	1.724943000	0.435332000
H	-4.805489000	-0.174899000	-0.595447000
H	-1.670305000	2.421196000	1.752327000
H	-0.108642000	1.632676000	1.629450000
H	-0.128507000	3.855557000	0.532546000
H	-1.441077000	3.339791000	-0.533889000
H	0.096039000	1.683269000	-1.658821000
H	2.151106000	3.590470000	-0.394946000
H	2.419478000	2.384199000	-1.774942000
H	3.948236000	-1.596557000	-1.428016000
H	4.107956000	0.146117000	-1.242443000
H	4.832653000	-0.935417000	-0.027024000
H	-1.666012000	-3.640404000	-1.014495000
H	-0.285364000	-2.706693000	-1.618404000
H	-0.350085000	-3.175423000	0.079804000

B'-S0-R

C	1.260458000	-0.621078000	1.590808000
C	2.713597000	-0.419064000	1.330506000
C	2.903467000	-0.197886000	0.022226000
C	1.555801000	-0.257697000	-0.655889000
N	0.607237000	-0.479811000	0.349269000
O	0.705527000	-0.853813000	2.647533000
O	1.332342000	-0.153427000	-1.846013000
C	-0.802133000	-0.628341000	0.142881000
C	-1.259753000	-1.768146000	-0.546641000
C	-1.683482000	0.347629000	0.640338000
C	-2.635159000	-1.898483000	-0.763754000
C	-3.054220000	0.167491000	0.411070000
C	-3.528708000	-0.937458000	-0.290898000
C	-1.226290000	1.592174000	1.372496000
C	-1.155407000	2.842920000	0.458831000
C	4.140231000	0.063791000	-0.762221000
C	-0.085122000	2.738977000	-0.590677000
C	-0.297353000	2.738317000	-1.907183000
C	-0.301080000	-2.824639000	-1.040105000
H	3.448966000	-0.458354000	2.123936000
H	-3.006149000	-2.769237000	-1.297851000
H	-3.751657000	0.910889000	0.789403000
H	-4.595243000	-1.057428000	-0.460345000
H	-1.936484000	1.798770000	2.181771000
H	-0.255081000	1.440402000	1.848633000
H	-0.959475000	3.712372000	1.102450000
H	-2.132464000	3.004051000	-0.013489000
H	4.255119000	-0.686714000	-1.553157000
H	4.075359000	1.038583000	-1.260479000

H	5.026941000	0.049345000	-0.124418000
H	0.934265000	2.631292000	-0.215085000
H	-1.299725000	2.831598000	-2.321633000
H	0.517723000	2.632503000	-2.617616000
H	-0.838274000	-3.732500000	-1.328130000
H	0.260931000	-2.469576000	-1.911098000
H	0.432547000	-3.090447000	-0.270673000

C'-S0-R

C	1.387041000	-0.765854000	1.008078000
C	2.765814000	-0.749337000	0.395628000
C	2.623341000	-0.547174000	-0.921686000
C	1.175276000	-0.427818000	-1.251005000
N	0.477573000	-0.545056000	-0.032265000
O	1.103456000	-0.928413000	2.179529000
O	0.660214000	-0.272682000	-2.342015000
C	-0.947402000	-0.507002000	0.111249000
C	-1.697834000	-1.582979000	-0.400532000
C	-1.552009000	0.585772000	0.758502000
C	-3.090072000	-1.532055000	-0.277611000
C	-2.949164000	0.587509000	0.869132000
C	-3.714038000	-0.454551000	0.350994000
C	-0.771602000	1.764596000	1.304371000
C	-0.687883000	2.961592000	0.319942000
C	0.043948000	2.622196000	-0.947871000
C	1.234663000	3.111074000	-1.301117000
C	-1.025626000	-2.760170000	-1.064264000
C	3.978502000	-0.935168000	1.237312000
H	3.390415000	-0.476258000	-1.682120000
H	-3.686105000	-2.351919000	-0.669481000
H	-3.435505000	1.421925000	1.368369000
H	-4.796229000	-0.433757000	0.445542000
H	-1.264574000	2.110849000	2.220323000
H	0.241040000	1.470584000	1.587859000
H	-0.191844000	3.795766000	0.831169000
H	-1.711239000	3.286236000	0.083968000
H	-0.436489000	1.887726000	-1.592469000
H	1.762306000	3.836433000	-0.683756000
H	1.727107000	2.800176000	-2.219089000
H	-1.731659000	-3.583374000	-1.203749000
H	-0.627127000	-2.481861000	-2.046271000
H	-0.183515000	-3.128583000	-0.467603000
H	4.889707000	-0.893970000	0.636244000
H	3.937430000	-1.899167000	1.758207000
H	4.026178000	-0.160449000	2.011887000

D'-S0-R

C	-1.695030000	-0.437631000	-0.920716000
C	-2.999070000	-0.104435000	-0.238763000
C	-2.736840000	0.106485000	1.058588000
C	-1.278787000	-0.080020000	1.307782000
N	-0.696290000	-0.377654000	0.058063000
O	-1.525973000	-0.701157000	-2.095979000
O	-0.683083000	-0.015393000	2.364923000
C	0.689375000	-0.664340000	-0.164231000
C	1.219662000	-1.853857000	0.372991000
C	1.471548000	0.227602000	-0.918562000
C	2.577130000	-2.121032000	0.169011000
C	2.823565000	-0.088639000	-1.108423000
C	3.376944000	-1.244768000	-0.564580000
C	0.939079000	1.520431000	-1.501175000
C	1.283071000	2.761797000	-0.638163000
C	0.599211000	2.746939000	0.699541000
C	1.220565000	2.704069000	1.878628000
C	0.355073000	-2.818789000	1.147278000
C	-4.273188000	-0.059141000	-1.005904000
H	-3.424215000	0.363020000	1.854519000
H	3.004366000	-3.031968000	0.579879000
H	3.443965000	0.588550000	-1.690393000
H	4.428119000	-1.470664000	-0.721358000
H	1.379290000	1.661188000	-2.495380000
H	-0.142146000	1.474953000	-1.648663000
H	0.975508000	3.653410000	-1.202980000
H	2.370419000	2.822662000	-0.505280000
H	-0.492064000	2.743527000	0.670985000
H	2.306929000	2.693074000	1.948879000
H	0.669434000	2.664652000	2.814060000
H	0.863480000	-3.778176000	1.276818000
H	0.115560000	-2.421825000	2.139884000
H	-0.596978000	-3.002073000	0.636454000
H	-5.118486000	0.185726000	-0.358745000
H	-4.461405000	-1.025028000	-1.489518000
H	-4.209128000	0.686922000	-1.806978000

A-S0-P

C	-0.769336000	-0.479006000	1.480574000
C	-2.237403000	-0.435423000	1.098288000
C	-2.219846000	-0.529925000	-0.449478000
C	-0.824368000	-0.924548000	-0.822307000
N	-0.021652000	-0.700169000	0.313706000
H	-2.839321000	-1.139571000	1.677390000
O	-0.280067000	-0.274484000	2.575332000

O	-0.390389000	-1.249346000	-1.910763000
C	1.295578000	-0.166977000	0.129265000
C	2.409806000	-1.008384000	0.072383000
C	1.358336000	1.222984000	-0.073332000
C	3.651348000	-0.415429000	-0.186931000
C	2.618970000	1.773565000	-0.333628000
C	3.753471000	0.961525000	-0.389961000
H	4.539325000	-1.040002000	-0.236070000
H	2.711514000	2.844775000	-0.492538000
H	4.723648000	1.405638000	-0.595278000
C	0.128565000	2.115286000	0.049855000
H	0.474458000	3.142846000	-0.097765000
H	-0.221229000	2.081679000	1.088797000
C	-1.086990000	1.911583000	-0.916446000
H	-1.484693000	2.914992000	-1.105283000
H	-0.726200000	1.547475000	-1.886450000
C	-2.321656000	1.065839000	-0.498267000
H	-3.140362000	1.361409000	-1.161306000
C	-2.725966000	1.038692000	1.005032000
H	-2.253894000	1.756770000	1.680744000
H	-3.809134000	1.100992000	1.135529000
C	-3.324570000	-1.276385000	-1.170680000
H	-3.301922000	-2.343448000	-0.923580000
H	-3.203350000	-1.170688000	-2.253643000
H	-4.306389000	-0.880315000	-0.891652000
C	2.251655000	-2.495012000	0.270213000
H	3.219177000	-3.003615000	0.235598000
H	1.608759000	-2.921099000	-0.508706000
H	1.779271000	-2.716326000	1.234232000

B-S0-P

C	0.765527000	-0.140506000	1.457258000
C	2.126967000	-0.447837000	0.942264000
C	2.419490000	0.576817000	-0.181912000
C	0.996036000	0.981408000	-0.586818000
N	0.102671000	0.513500000	0.391994000
H	2.888385000	-0.590626000	1.708057000
O	0.234874000	-0.441892000	2.507654000
O	0.664718000	1.577958000	-1.593660000
C	-1.268735000	0.195443000	0.123406000
C	-2.235942000	1.204879000	0.054613000
C	-1.559215000	-1.170074000	-0.077149000
C	-3.553242000	0.820361000	-0.224151000
C	-2.890929000	-1.506385000	-0.344600000
C	-3.878390000	-0.521998000	-0.417856000
H	-4.326402000	1.581721000	-0.284615000

H	-3.153425000	-2.548435000	-0.507748000
H	-4.905737000	-0.803689000	-0.631848000
C	-0.489017000	-2.260215000	-0.012212000
H	-0.953896000	-3.184999000	-0.366524000
H	-0.219936000	-2.452865000	1.033473000
C	0.793088000	-2.003246000	-0.862522000
H	1.033346000	-2.921770000	-1.409403000
H	0.535910000	-1.277203000	-1.641525000
C	3.315712000	1.782988000	0.053705000
H	2.916418000	2.426487000	0.846117000
H	3.394128000	2.376787000	-0.863473000
H	4.319278000	1.457644000	0.345142000
C	2.129934000	-1.582075000	-0.178341000
H	2.672557000	-2.470979000	0.150636000
C	2.926636000	-0.589574000	-1.077603000
H	2.676895000	-0.557881000	-2.142813000
H	4.009606000	-0.699208000	-0.964277000
C	-1.856611000	2.647603000	0.276974000
H	-2.741387000	3.290209000	0.288362000
H	-1.182733000	2.993820000	-0.514091000
H	-1.326292000	2.772414000	1.228289000

C-S0-P

C	1.009453000	-0.761366000	-0.933640000
C	2.400173000	-0.520879000	-0.354137000
C	2.085250000	-0.130491000	1.113015000
C	0.668569000	-0.514676000	1.374588000
N	0.072532000	-0.688726000	0.105736000
O	0.723698000	-0.926957000	-2.104664000
O	0.053479000	-0.545655000	2.422319000
C	-1.266855000	-0.221392000	-0.095169000
C	-2.356158000	-1.087442000	0.032353000
C	-1.393313000	1.157648000	-0.339048000
C	-3.636089000	-0.537791000	-0.108720000
C	-2.691565000	1.665600000	-0.469491000
C	-3.801104000	0.825728000	-0.355517000
H	-4.505417000	-1.183525000	-0.017863000
H	-2.833033000	2.725715000	-0.662843000
H	-4.801140000	1.237938000	-0.458542000
C	-0.182413000	2.064388000	-0.527352000
H	-0.574370000	3.061617000	-0.749203000
H	0.341575000	1.758166000	-1.441204000
C	0.854101000	2.243454000	0.633209000
H	1.192797000	3.283319000	0.566432000
H	0.340214000	2.159344000	1.598908000
C	2.159130000	1.401916000	0.690109000

H	2.848520000	1.939774000	1.345503000
C	2.814259000	0.953991000	-0.648645000
H	2.447533000	1.394628000	-1.579966000
H	3.902920000	1.058628000	-0.621735000
C	-2.135255000	-2.550232000	0.326398000
H	-3.083781000	-3.093099000	0.364425000
H	-1.624816000	-2.676435000	1.288129000
H	-1.501751000	-3.015151000	-0.437862000
C	3.380169000	-1.635521000	-0.681837000
H	3.469077000	-1.749220000	-1.767527000
H	4.369024000	-1.404237000	-0.273504000
H	3.047100000	-2.591444000	-0.261933000
H	2.790295000	-0.421648000	1.890705000

D-S0-P

C	0.902018000	0.133552000	1.236570000
C	2.246861000	0.077874000	0.587940000
C	2.205764000	1.126141000	-0.551774000
C	0.707648000	1.307385000	-0.780419000
N	0.022928000	0.676200000	0.275113000
O	0.556631000	-0.276845000	2.327356000
O	0.163007000	1.842139000	-1.727054000
C	-1.295175000	0.127973000	0.144878000
C	-2.422096000	0.956356000	0.205225000
C	-1.369612000	-1.265798000	-0.059099000
C	-3.677119000	0.353288000	0.056997000
C	-2.645874000	-1.823695000	-0.192887000
C	-3.788417000	-1.023370000	-0.136293000
H	-4.570301000	0.970936000	0.098330000
H	-2.743476000	-2.894114000	-0.354453000
H	-4.769853000	-1.475889000	-0.248520000
C	-0.130329000	-2.157899000	-0.136616000
H	-0.468744000	-3.144812000	-0.465940000
H	0.278612000	-2.312168000	0.869215000
C	0.990328000	-1.679144000	-1.108783000
H	1.322762000	-2.539003000	-1.701054000
H	0.532313000	-1.002774000	-1.838932000
C	2.301968000	-1.040144000	-0.559273000
H	3.019803000	-1.825734000	-0.307554000
C	2.813270000	0.076914000	-1.520582000
H	2.441436000	0.064295000	-2.549241000
H	3.903220000	0.156931000	-1.533566000
C	-2.274219000	2.441056000	0.426200000
H	-3.249941000	2.919993000	0.546830000
H	-1.758459000	2.906358000	-0.420595000
H	-1.674846000	2.647632000	1.320586000

C	3.424613000	0.060640000	1.541699000
H	3.452740000	0.976551000	2.141835000
H	3.342521000	-0.792942000	2.222280000
H	4.370199000	-0.022621000	0.996821000
H	2.716646000	2.084839000	-0.426942000

A-T1-R

C	-0.982425000	-0.448263000	1.717383000
C	-2.383621000	-0.651937000	1.510103000
C	-2.644241000	-0.811777000	0.067465000
C	-1.385737000	-0.779012000	-0.614604000
N	-0.401946000	-0.538871000	0.405091000
H	-3.104052000	-0.762933000	2.308929000
O	-0.331788000	-0.279364000	2.748840000
O	-1.130646000	-0.859055000	-1.818945000
C	0.986078000	-0.452052000	0.149095000
C	1.643731000	-1.587949000	-0.385482000
C	1.680960000	0.747506000	0.435450000
C	3.013683000	-1.493922000	-0.636506000
C	3.051172000	0.787266000	0.160556000
C	3.715035000	-0.317010000	-0.371518000
H	3.538041000	-2.359851000	-1.030928000
H	3.599487000	1.704241000	0.359837000
H	4.780991000	-0.264005000	-0.573669000
C	1.000553000	2.008925000	0.922329000
H	1.709614000	2.558163000	1.552386000
H	0.138928000	1.779102000	1.550068000
C	0.554326000	2.951989000	-0.229345000
H	0.171091000	3.877357000	0.217793000
H	1.443301000	3.219401000	-0.818109000
C	-0.486396000	2.343246000	-1.127273000
H	-0.173010000	1.477254000	-1.708650000
C	-1.750994000	2.758910000	-1.224808000
H	-2.120937000	3.610903000	-0.656463000
H	-2.464559000	2.258254000	-1.874698000
C	-3.960210000	-0.846239000	-0.599502000
H	-3.841335000	-1.010640000	-1.673181000
H	-4.501398000	0.100661000	-0.445874000
H	-4.597392000	-1.634674000	-0.174738000
C	0.911698000	-2.881446000	-0.638158000
H	1.617901000	-3.704968000	-0.773351000
H	0.291490000	-2.803695000	-1.537432000
H	0.243256000	-3.134521000	0.192168000

B-T1-R

C	-1.163335000	0.241283000	-1.724363000
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C	-2.570230000	0.212061000	-1.478708000
C	-2.819296000	0.336345000	-0.035493000
C	-1.561003000	0.513361000	0.621793000
N	-0.567833000	0.417554000	-0.422737000
H	-3.318038000	0.199649000	-2.259891000
O	-0.520772000	0.189666000	-2.774018000
O	-1.301167000	0.663912000	1.816457000
C	0.817435000	0.560241000	-0.204064000
C	1.292347000	1.773679000	0.361349000
C	1.701317000	-0.488009000	-0.565978000
C	2.664168000	1.902168000	0.580312000
C	3.064591000	-0.304150000	-0.319068000
C	3.546874000	0.871990000	0.252484000
H	3.046333000	2.830398000	0.995781000
H	3.754869000	-1.104610000	-0.571884000
H	4.611418000	0.991953000	0.432043000
C	1.246170000	-1.827305000	-1.101850000
H	2.019951000	-2.201208000	-1.782127000
H	0.335340000	-1.734340000	-1.694008000
C	1.032586000	-2.888132000	0.012285000
H	0.892001000	-3.857798000	-0.485611000
H	1.942725000	-2.964805000	0.619810000
C	-4.119043000	0.216105000	0.656287000
H	-3.997403000	0.374405000	1.730565000
H	-4.565544000	-0.776121000	0.491302000
H	-4.841741000	0.945160000	0.261793000
C	-0.153100000	-2.592379000	0.885975000
H	-1.120412000	-2.581671000	0.380748000
C	-0.095015000	-2.316398000	2.189580000
H	0.852665000	-2.300858000	2.725295000
H	-0.984718000	-2.078894000	2.765115000
C	0.371350000	2.928004000	0.665135000
H	0.941103000	3.854519000	0.776445000
H	-0.184990000	2.746242000	1.590213000
H	-0.368119000	3.073281000	-0.130007000

C-T1-R

C	1.412545000	-0.603057000	-1.102234000
C	2.716824000	-0.699647000	-0.516173000
C	2.562392000	-0.644780000	0.949948000
C	1.172259000	-0.575729000	1.275737000
N	0.498770000	-0.538224000	0.007199000
O	1.065029000	-0.616642000	-2.284631000
O	0.599797000	-0.499071000	2.364492000
C	-0.907794000	-0.500875000	-0.133840000
C	-1.664476000	-1.587305000	0.372647000

C	-1.520408000	0.597956000	-0.782306000
C	-3.051684000	-1.545776000	0.221751000
C	-2.913093000	0.588930000	-0.902739000
C	-3.675590000	-0.467695000	-0.407030000
H	-3.646842000	-2.377239000	0.588865000
H	-3.403437000	1.431265000	-1.383629000
H	-4.756318000	-0.454847000	-0.515488000
C	-0.758762000	1.821449000	-1.244873000
H	-1.260136000	2.222858000	-2.133123000
H	0.257676000	1.567772000	-1.547521000
C	-0.705945000	2.945549000	-0.173697000
H	-0.240710000	3.829324000	-0.627187000
H	-1.738188000	3.219460000	0.087180000
C	0.044252000	2.547536000	1.066663000
H	-0.383497000	1.731040000	1.647074000
C	1.194137000	3.091209000	1.470928000
H	1.670606000	3.900777000	0.920137000
H	1.703560000	2.743316000	2.366185000
C	-1.005236000	-2.780970000	1.014777000
H	-1.704249000	-3.618792000	1.082256000
H	-0.659962000	-2.533122000	2.024259000
H	-0.127883000	-3.110054000	0.447038000
C	3.967725000	-0.914976000	-1.268972000
H	4.708818000	-0.140723000	-1.021298000
H	4.431429000	-1.876135000	-1.000020000
H	3.776912000	-0.901026000	-2.344653000
H	3.359338000	-0.571520000	1.677126000

D-T1-R

C	1.587816000	-0.300263000	-1.069845000
C	2.861565000	-0.278019000	-0.418313000
C	2.637358000	-0.377878000	1.029893000
C	1.241959000	-0.526238000	1.289582000
N	0.617376000	-0.437045000	-0.011852000
O	1.302986000	-0.270017000	-2.269616000
O	0.624881000	-0.650642000	2.346975000
C	-0.771006000	-0.548839000	-0.224604000
C	-1.426262000	-1.736937000	0.197232000
C	-1.476570000	0.501777000	-0.866722000
C	-2.802591000	-1.835787000	-0.008203000
C	-2.854431000	0.347296000	-1.041583000
C	-3.517555000	-0.801908000	-0.614058000
H	-3.315832000	-2.744693000	0.293010000
H	-3.414914000	1.149831000	-1.513662000
H	-4.588978000	-0.898454000	-0.764367000
C	-0.847763000	1.815245000	-1.276609000

H	-1.389021000	2.189897000	-2.152855000
H	0.188546000	1.683333000	-1.589119000
C	-0.921312000	2.902023000	-0.168585000
H	-0.615222000	3.852688000	-0.627277000
H	-1.962584000	3.019479000	0.156103000
C	-0.039989000	2.603302000	1.010068000
H	1.030151000	2.557824000	0.800889000
C	-0.473656000	2.363910000	2.248554000
H	-1.534566000	2.382536000	2.492089000
H	0.208769000	2.122389000	3.057752000
C	-0.670415000	-2.899093000	0.789111000
H	-1.267327000	-3.813464000	0.733333000
H	-0.422910000	-2.706007000	1.837889000
H	0.274976000	-3.073453000	0.263864000
C	4.162649000	-0.265711000	-1.118052000
H	4.791736000	0.560813000	-0.757043000
H	4.728839000	-1.188599000	-0.920497000
H	4.017664000	-0.164479000	-2.196307000
H	3.387319000	-0.282347000	1.803105000

A-T1-P

C	-0.671441000	1.454613000	-0.684663000
C	-2.151237000	1.139378000	-0.619359000
C	-2.290040000	0.148027000	0.564177000
C	-0.947197000	0.121911000	1.226080000
N	-0.032338000	0.774864000	0.375510000
H	-2.771646000	2.037674000	-0.644637000
O	-0.084757000	2.086496000	-1.540319000
O	-0.620313000	-0.470160000	2.238133000
C	1.267997000	0.215015000	0.244757000
C	2.418896000	0.931666000	0.190607000
C	1.232324000	-1.251740000	-0.055437000
C	3.655734000	0.194169000	0.005895000
C	2.527424000	-1.962823000	0.093675000
C	3.680504000	-1.251303000	0.042594000
H	4.588725000	0.746782000	-0.039278000
H	2.530059000	-3.044919000	0.202420000
H	4.644577000	-1.752343000	0.093625000
C	0.216593000	-1.739575000	-1.068651000
H	0.616388000	-2.655224000	-1.518775000
H	0.136628000	-1.013988000	-1.894730000
C	-1.226453000	-2.104951000	-0.564780000
H	-1.595806000	-2.868582000	-1.260260000
H	-1.142700000	-2.594859000	0.412667000
C	-2.356210000	-1.050973000	-0.487597000
H	-3.282708000	-1.612171000	-0.328582000

C	-2.491831000	-0.000236000	-1.628202000
H	-1.819901000	-0.096395000	-2.485382000
H	-3.515949000	0.082286000	-1.999522000
C	-3.469707000	0.254695000	1.511566000
H	-3.444587000	1.199661000	2.065319000
H	-3.444315000	-0.568513000	2.233076000
H	-4.414216000	0.203902000	0.960443000
C	2.480935000	2.425667000	0.361639000
H	3.239924000	2.693765000	1.107084000
H	1.519062000	2.838496000	0.672427000
H	2.765658000	2.908454000	-0.580799000

B-T1-P

C	0.786217000	-0.186942000	1.457460000
C	2.123851000	-0.511319000	0.896029000
C	2.418096000	0.564691000	-0.181006000
C	1.005264000	1.036138000	-0.539162000
N	0.102425000	0.523623000	0.427773000
H	2.896173000	-0.699037000	1.641064000
O	0.267262000	-0.490905000	2.514987000
O	0.680220000	1.696134000	-1.504901000
C	-1.249450000	0.236213000	0.193565000
C	-2.248822000	1.262676000	0.041348000
C	-1.579672000	-1.254834000	-0.009872000
C	-3.521152000	0.876952000	-0.248325000
C	-2.880591000	-1.554829000	-0.333141000
C	-3.872819000	-0.559852000	-0.444580000
H	-4.310851000	1.617654000	-0.332042000
H	-3.152059000	-2.591618000	-0.521408000
H	-4.896537000	-0.823133000	-0.685023000
C	-0.484410000	-2.297356000	0.008926000
H	-0.935940000	-3.244685000	-0.301709000
H	-0.122975000	-2.466487000	1.031234000
C	0.736782000	-1.988802000	-0.922266000
H	0.946791000	-2.876143000	-1.529762000
H	0.432523000	-1.223268000	-1.645069000
C	3.358308000	1.727973000	0.098898000
H	2.998719000	2.337339000	0.935967000
H	3.434742000	2.369940000	-0.785284000
H	4.357179000	1.355131000	0.346502000
C	2.094524000	-1.591898000	-0.276869000
H	2.646447000	-2.493208000	-0.000334000
C	2.869991000	-0.563614000	-1.152970000
H	2.578283000	-0.472140000	-2.203855000
H	3.954640000	-0.694204000	-1.091159000
C	-1.864931000	2.702065000	0.262018000

H	-2.739483000	3.355488000	0.197068000
H	-1.127089000	3.022839000	-0.480865000
H	-1.404510000	2.834773000	1.249250000

C-T1-P

C	-0.974468000	1.183475000	-0.403915000
C	-2.375409000	0.632093000	-0.175538000
C	-2.168205000	-0.408840000	0.954157000
C	-0.785165000	-0.210801000	1.473424000
N	-0.104950000	0.608154000	0.544982000
O	-0.619445000	1.928040000	-1.296159000
O	-0.237501000	-0.751990000	2.415399000
C	1.244987000	0.283071000	0.239655000
C	2.241253000	1.188856000	0.069663000
C	1.420425000	-1.162401000	-0.110488000
C	3.551259000	0.678794000	-0.290776000
C	2.825868000	-1.641543000	-0.141559000
C	3.825660000	-0.740412000	-0.307969000
H	4.363681000	1.384805000	-0.430185000
H	3.026187000	-2.708077000	-0.069878000
H	4.859605000	-1.067747000	-0.391442000
C	0.389368000	-1.794908000	-1.023968000
H	0.882263000	-2.617465000	-1.554446000
H	0.092114000	-1.075160000	-1.804092000
C	-0.902616000	-2.414938000	-0.378951000
H	-1.218626000	-3.212278000	-1.062673000
H	-0.623524000	-2.907920000	0.559981000
C	-2.175247000	-1.570842000	-0.129594000
H	-2.972095000	-2.282381000	0.103514000
C	-2.615702000	-0.528115000	-1.197798000
H	-2.038927000	-0.479325000	-2.125852000
H	-3.675232000	-0.615872000	-1.454432000
C	2.068098000	2.668708000	0.282823000
H	2.868634000	3.059436000	0.923036000
H	1.104267000	2.902007000	0.740192000
H	2.124206000	3.203228000	-0.672871000
C	-3.432494000	1.717497000	-0.054934000
H	-3.434185000	2.341308000	-0.955075000
H	-4.424988000	1.270658000	0.061268000
H	-3.239515000	2.361611000	0.810367000
H	-2.929315000	-0.500457000	1.728395000

D-T1-P

C	0.914966000	0.065624000	1.247850000
C	2.243925000	0.026936000	0.569404000
C	2.200941000	1.166542000	-0.481437000

C	0.708047000	1.403540000	-0.673598000
N	0.014868000	0.681200000	0.334978000
O	0.572149000	-0.385557000	2.325366000
O	0.167895000	2.027928000	-1.563381000
C	-1.276827000	0.152947000	0.203525000
C	-2.459929000	0.975580000	0.209312000
C	-1.346590000	-1.366508000	-0.042033000
C	-3.663284000	0.364270000	0.036730000
C	-2.598027000	-1.897992000	-0.238263000
C	-3.763226000	-1.106475000	-0.192281000
H	-4.580574000	0.944231000	0.074736000
H	-2.692767000	-2.961091000	-0.450230000
H	-4.741192000	-1.551738000	-0.335358000
C	-0.083369000	-2.183820000	-0.195990000
H	-0.384448000	-3.183017000	-0.525758000
H	0.407063000	-2.331499000	0.774550000
C	0.958315000	-1.606338000	-1.212053000
H	1.263247000	-2.406550000	-1.895731000
H	0.448884000	-0.875531000	-1.850171000
C	2.278900000	-0.996845000	-0.664683000
H	3.005799000	-1.795029000	-0.487941000
C	2.767470000	0.190903000	-1.548008000
H	2.362450000	0.263860000	-2.561387000
H	3.857126000	0.264500000	-1.591000000
C	-2.328846000	2.454159000	0.462824000
H	-3.311723000	2.929278000	0.527976000
H	-1.755307000	2.933343000	-0.337353000
H	-1.789522000	2.641678000	1.399969000
C	3.436684000	-0.072220000	1.500150000
H	3.472736000	0.785886000	2.179930000
H	3.367876000	-0.984159000	2.101900000
H	4.372939000	-0.102425000	0.934082000
H	2.738083000	2.099070000	-0.287638000

A-DR1-T1

C	-0.947424000	0.039866000	1.423357000
C	-2.378343000	0.019079000	0.921049000
C	-2.355188000	-1.054446000	-0.112351000
C	-0.979246000	-1.232469000	-0.529214000
N	-0.171461000	-0.520687000	0.410543000
H	-3.111016000	-0.101904000	1.722306000
O	-0.520904000	0.552782000	2.443113000
O	-0.537501000	-1.850506000	-1.492640000
C	1.203041000	-0.205733000	0.179789000
C	2.146054000	-1.248405000	0.167244000
C	1.554764000	1.138623000	-0.071083000

C	3.47240000	-0.93242800	-0.14880000
C	2.89684900	1.40107300	-0.37799400
C	3.84496300	0.38010000	-0.43043700
H	4.21558000	-1.72528200	-0.16491400
H	3.19955400	2.42599600	-0.57612500
H	4.87784700	0.61187800	-0.67541600
C	0.59151500	2.31319300	0.03313300
H	1.20072000	3.22241600	-0.00177900
H	0.11745100	2.31723000	1.01881800
C	-0.50324800	2.48191200	-1.06524100
H	-0.81185400	3.54079800	-0.99894500
H	-0.03621000	2.36873400	-2.05024800
C	-1.73456700	1.63060800	-1.00071200
H	-2.06464000	1.14701900	-1.91633400
C	-2.58883900	1.43854000	0.21501700
H	-2.40417900	2.20771600	0.97419800
H	-3.65074700	1.48479600	-0.05633500
C	-3.51983200	-1.65946000	-0.79570300
H	-4.17850200	-2.16776900	-0.07866300
H	-3.19314100	-2.37700900	-1.55292800
H	-4.13203700	-0.88797000	-1.28665200
C	1.74951400	-2.66674300	0.49629900
H	2.63106800	-3.27499900	0.71823000
H	1.21350100	-3.12451700	-0.34154900
H	1.07959900	-2.70038700	1.36263200

A-DR2-T1

C	-0.58276100	-0.85531500	1.49998900
C	-1.99606000	-0.81844600	1.20774700
C	-2.20664900	-0.57502800	-0.24461200
C	-0.83332900	-0.89657800	-0.82033800
N	0.08230200	-0.83296700	0.24099800
H	-2.76738000	-0.86756800	1.96431100
O	-0.00234300	-0.85600900	2.57976900
O	-0.53946400	-1.05747500	-1.98888600
C	1.33785800	-0.16055300	0.07548900
C	2.51371000	-0.88231400	-0.14649800
C	1.28984000	1.24549700	0.12555600
C	3.69595000	-0.15168600	-0.31980600
C	2.49334900	1.93660000	-0.05107900
C	3.68538100	1.24287800	-0.27133100
H	4.62799600	-0.68244900	-0.49484900
H	2.49504100	3.02296800	-0.01905600
H	4.61174800	1.79395000	-0.40833000
C	-0.02120700	1.98438100	0.36003200
H	0.21853300	3.04400300	0.48625400

H	-0.459059000	1.671712000	1.316051000
C	-1.079681000	1.850152000	-0.784221000
H	-1.432610000	2.856643000	-1.034809000
H	-0.587969000	1.478274000	-1.687756000
C	-2.379735000	1.029300000	-0.543737000
H	-2.899223000	1.022638000	-1.512795000
C	-3.265071000	1.648007000	0.478738000
H	-2.871830000	2.343862000	1.212776000
H	-4.285430000	1.300300000	0.605186000
C	-3.359060000	-1.352225000	-0.881010000
H	-3.298693000	-2.415262000	-0.627836000
H	-3.316568000	-1.252147000	-1.969698000
H	-4.322584000	-0.969433000	-0.530516000
C	2.482324000	-2.389285000	-0.198420000
H	3.477155000	-2.799002000	-0.394411000
H	1.802600000	-2.735804000	-0.985152000
H	2.117460000	-2.806355000	0.747585000

B-DR3-T1

C	-0.800670000	-0.355604000	1.593718000
C	-2.215812000	-0.489933000	1.321359000
C	-2.448159000	-0.509535000	-0.148652000
C	-1.039559000	-0.746769000	-0.694888000
N	-0.144325000	-0.498400000	0.340061000
H	-2.977009000	-0.460290000	2.089989000
O	-0.217492000	-0.146070000	2.651480000
O	-0.734045000	-1.002171000	-1.846133000
C	1.238668000	-0.205317000	0.115357000
C	2.137760000	-1.262878000	-0.079104000
C	1.621634000	1.146182000	0.051731000
C	3.474925000	-0.941802000	-0.339840000
C	2.969354000	1.421767000	-0.209860000
C	3.887422000	0.389047000	-0.404240000
H	4.193280000	-1.742598000	-0.493710000
H	3.298364000	2.456184000	-0.263564000
H	4.928563000	0.623348000	-0.608588000
C	0.630983000	2.274749000	0.271662000
H	1.185914000	3.217070000	0.243737000
H	0.221312000	2.194033000	1.285561000
C	-0.561476000	2.351266000	-0.754455000
H	-0.575928000	3.376484000	-1.156039000
H	-0.358891000	1.700329000	-1.612358000
C	-3.474442000	-1.522820000	-0.658100000
H	-3.226460000	-2.534398000	-0.321584000
H	-3.490025000	-1.516367000	-1.752039000
H	-4.474065000	-1.270040000	-0.291055000

C	-1.905859000	2.043317000	-0.165912000
H	-2.187989000	2.581967000	0.736466000
C	-2.818928000	0.965546000	-0.651573000
H	-2.821262000	0.905755000	-1.748720000
H	-3.846011000	1.152143000	-0.319761000
C	1.662916000	-2.693577000	-0.015607000
H	2.499580000	-3.390061000	-0.118848000
H	0.943360000	-2.898469000	-0.816603000
H	1.157296000	-2.902202000	0.934350000

B-DR4-T1

C	0.750502000	0.029912000	1.417462000
C	2.157420000	0.097838000	0.858752000
C	2.074913000	1.214153000	-0.128960000
C	0.679977000	1.426957000	-0.448589000
N	-0.077500000	0.641204000	0.472089000
H	2.928155000	0.216919000	1.624703000
O	0.368683000	-0.574299000	2.401852000
O	0.186091000	2.107727000	-1.342878000
C	-1.353678000	0.088312000	0.141589000
C	-2.495751000	0.902280000	0.159255000
C	-1.381069000	-1.268892000	-0.239462000
C	-3.710794000	0.327220000	-0.229217000
C	-2.622453000	-1.798844000	-0.615865000
C	-3.773802000	-1.011521000	-0.614966000
H	-4.611295000	0.935608000	-0.225073000
H	-2.683437000	-2.841091000	-0.918400000
H	-4.723882000	-1.444266000	-0.916122000
C	-0.164697000	-2.191248000	-0.203471000
H	-0.458226000	-3.104802000	-0.728891000
H	0.003606000	-2.497537000	0.837378000
C	1.195457000	-1.722369000	-0.815870000
H	1.586761000	-2.568891000	-1.389761000
H	1.032994000	-0.925939000	-1.551122000
C	3.193816000	1.935724000	-0.776378000
H	3.860685000	2.381133000	-0.025457000
H	2.813990000	2.724034000	-1.431833000
H	3.809928000	1.247537000	-1.371604000
C	2.341617000	-1.324382000	0.162859000
H	2.312600000	-2.039523000	1.005638000
C	3.679202000	-1.390706000	-0.494239000
H	3.835660000	-1.994174000	-1.382514000
H	4.547071000	-0.947850000	-0.015663000
C	-2.407370000	2.344364000	0.593150000
H	-3.402499000	2.790452000	0.676392000
H	-1.820873000	2.927094000	-0.124702000

H	-1.906681000	2.432659000	1.564305000
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C-DR5-T1

C	1.135056000	-0.347275000	-1.020610000
C	2.471259000	-0.420344000	-0.287868000
C	2.130393000	-1.275756000	0.880709000
C	0.697751000	-1.250791000	1.082903000
N	0.144963000	-0.647619000	-0.087442000
O	0.943594000	0.012217000	-2.168639000
O	0.035095000	-1.636687000	2.038570000
C	-1.204282000	-0.183729000	-0.167396000
C	-2.246525000	-1.126890000	-0.173066000
C	-1.438570000	1.207907000	-0.200794000
C	-3.562915000	-0.651621000	-0.171164000
C	-2.774618000	1.630641000	-0.202781000
C	-3.827025000	0.716323000	-0.175828000
H	-4.382924000	-1.364896000	-0.174359000
H	-2.988639000	2.695886000	-0.228785000
H	-4.853685000	1.071991000	-0.174079000
C	-0.341771000	2.259360000	-0.294680000
H	-0.836053000	3.212552000	-0.509070000
H	0.292360000	2.057074000	-1.162886000
C	0.558955000	2.504917000	0.954637000
H	0.995308000	3.508363000	0.800791000
H	-0.080402000	2.590823000	1.840664000
C	1.675168000	1.547197000	1.240812000
H	1.798261000	1.204429000	2.264621000
C	2.689709000	1.083820000	0.243751000
H	2.718466000	1.727594000	-0.644305000
H	3.691468000	1.087865000	0.691777000
C	-1.961909000	-2.608707000	-0.193910000
H	-2.854201000	-3.171480000	-0.482619000
H	-1.636863000	-2.956332000	0.792362000
H	-1.159129000	-2.848852000	-0.899839000
C	3.638450000	-0.863210000	-1.164104000
H	4.574531000	-0.833214000	-0.597814000
H	3.487164000	-1.883022000	-1.531343000
H	3.729547000	-0.196525000	-2.026760000
H	2.825784000	-1.704214000	1.590623000

C-DR6-T1

C	0.780229000	-1.241727000	-0.849543000
C	2.138622000	-1.063472000	-0.383631000
C	2.095058000	-0.339801000	0.922221000
C	0.657764000	-0.534295000	1.370404000
N	-0.076815000	-0.838900000	0.213482000

O	0.379160000	-1.629305000	-1.942942000
O	0.177153000	-0.327012000	2.467611000
C	-1.323697000	-0.180828000	-0.046756000
C	-2.539380000	-0.824151000	0.200871000
C	-1.230948000	1.136586000	-0.535405000
C	-3.714295000	-0.109620000	-0.064908000
C	-2.428438000	1.813943000	-0.789508000
C	-3.658700000	1.194827000	-0.557194000
H	-4.676282000	-0.581421000	0.116927000
H	-2.395896000	2.832681000	-1.166941000
H	-4.579858000	1.734772000	-0.758675000
C	0.119480000	1.803376000	-0.765282000
H	-0.067776000	2.757251000	-1.266792000
H	0.713125000	1.215091000	-1.475826000
C	0.952260000	2.078721000	0.530691000
H	1.273586000	3.125964000	0.511374000
H	0.296396000	1.988994000	1.401330000
C	2.255199000	1.269386000	0.796698000
H	2.567791000	1.555311000	1.811550000
C	3.343884000	1.615572000	-0.158186000
H	3.131775000	2.117925000	-1.096338000
H	4.361532000	1.286688000	0.027225000
C	-2.557033000	-2.231911000	0.741936000
H	-3.581062000	-2.590468000	0.879036000
H	-2.039388000	-2.281511000	1.706724000
H	-2.037759000	-2.918949000	0.063659000
C	3.332177000	-1.552009000	-1.111965000
H	3.943448000	-2.200493000	-0.468866000
H	3.031817000	-2.111710000	-2.001882000
H	3.979009000	-0.720936000	-1.422359000
H	2.833648000	-0.693932000	1.645479000

D-DR7-T1

C	1.000127000	-0.828439000	-1.067795000
C	2.339785000	-0.914033000	-0.522729000
C	2.287846000	-0.539808000	0.919538000
C	0.803388000	-0.599947000	1.246120000
N	0.124677000	-0.612508000	0.032275000
O	0.628863000	-0.904045000	-2.235464000
O	0.281383000	-0.526415000	2.344866000
C	-1.242907000	-0.210618000	-0.094986000
C	-2.258940000	-1.136016000	0.179415000
C	-1.500099000	1.125896000	-0.449182000
C	-3.584321000	-0.695826000	0.083841000
C	-2.840015000	1.523040000	-0.535007000
C	-3.872388000	0.621969000	-0.271074000

H	-4.391970000	-1.392899000	0.290780000
H	-3.072894000	2.548831000	-0.808292000
H	-4.906060000	0.949631000	-0.340584000
C	-0.381339000	2.108748000	-0.744587000
H	-0.837868000	3.044400000	-1.080700000
H	0.204741000	1.736624000	-1.593093000
C	0.595352000	2.416824000	0.453669000
H	0.607098000	3.509716000	0.586448000
H	0.183932000	2.010884000	1.384384000
C	2.003136000	1.941439000	0.247272000
H	2.498719000	2.244360000	-0.672973000
C	2.714872000	0.977439000	1.142927000
H	2.517770000	1.191432000	2.201866000
H	3.796687000	1.030876000	0.983737000
C	-1.917632000	-2.551867000	0.572768000
H	-2.821901000	-3.153122000	0.701906000
H	-1.355985000	-2.566510000	1.513808000
H	-1.289788000	-3.033961000	-0.185657000
C	3.551935000	-1.163183000	-1.333802000
H	4.148786000	-1.983289000	-0.912584000
H	3.281889000	-1.407769000	-2.364453000
H	4.204949000	-0.277591000	-1.346408000
H	2.884395000	-1.174104000	1.582348000

D-DR8-T1

C	-0.888701000	-0.395358000	1.090839000
C	-2.223822000	-0.467460000	0.368867000
C	-1.904849000	-1.351987000	-0.785270000
C	-0.472822000	-1.409082000	-0.969154000
N	0.096705000	-0.766317000	0.170245000
O	-0.681164000	0.030789000	2.211423000
O	0.180173000	-1.856327000	-1.905580000
C	1.356339000	-0.092455000	0.126499000
C	2.549368000	-0.828963000	0.149402000
C	1.320207000	1.312382000	0.019713000
C	3.752204000	-0.119904000	0.055491000
C	2.550260000	1.976835000	-0.066704000
C	3.753248000	1.270583000	-0.052378000
H	4.691955000	-0.665583000	0.071052000
H	2.562541000	3.060296000	-0.152517000
H	4.695127000	1.807247000	-0.126001000
C	0.031728000	2.130084000	0.048373000
H	0.305121000	3.146691000	-0.249240000
H	-0.302988000	2.213138000	1.090250000
C	-1.177293000	1.695527000	-0.841248000
H	-1.560197000	2.604785000	-1.315907000

H	-0.836442000	1.063382000	-1.669520000
C	-2.421007000	1.056618000	-0.152324000
H	-2.628194000	1.618903000	0.769474000
C	-3.603605000	1.124641000	-1.059540000
H	-3.470338000	1.074964000	-2.135931000
H	-4.613822000	1.089645000	-0.667045000
C	2.527089000	-2.331505000	0.279972000
H	3.534944000	-2.726103000	0.437049000
H	2.108423000	-2.790877000	-0.621757000
H	1.898134000	-2.644113000	1.121495000
C	-3.384994000	-0.908686000	1.258521000
H	-3.474798000	-0.234865000	2.115822000
H	-4.326642000	-0.900119000	0.703550000
H	-3.215782000	-1.922543000	1.634273000
H	-2.616163000	-1.793938000	-1.469851000

A-DR1-T1-TS1

C	-0.868306000	-0.132168000	1.510554000
C	-2.284626000	-0.338198000	1.164506000
C	-2.324379000	-1.067917000	-0.097702000
C	-0.969829000	-1.117299000	-0.619659000
N	-0.138285000	-0.536089000	0.372836000
H	-3.039632000	-0.401297000	1.939859000
O	-0.386759000	0.381327000	2.510363000
O	-0.576633000	-1.537286000	-1.706147000
C	1.226792000	-0.185467000	0.144139000
C	2.200873000	-1.193701000	0.116962000
C	1.539562000	1.167693000	-0.074538000
C	3.527192000	-0.816732000	-0.119861000
C	2.877574000	1.503482000	-0.299920000
C	3.865827000	0.519867000	-0.320610000
H	4.298473000	-1.582314000	-0.143876000
H	3.143317000	2.544143000	-0.468741000
H	4.901533000	0.796043000	-0.499697000
C	0.459121000	2.233197000	-0.091153000
H	0.942012000	3.206914000	-0.218541000
H	-0.017597000	2.266658000	0.893187000
C	-0.596390000	2.043500000	-1.221625000
H	-0.620994000	2.950306000	-1.848402000
H	-0.257975000	1.254419000	-1.909985000
C	-2.018664000	1.736938000	-0.852054000
H	-2.661981000	1.489448000	-1.695068000
C	-2.596520000	1.703279000	0.425449000
H	-2.101569000	2.166929000	1.273805000
H	-3.680418000	1.665994000	0.490394000
C	-3.504044000	-1.603398000	-0.816935000

H	-4.002662000	-2.394036000	-0.237278000
H	-3.196037000	-2.017355000	-1.781026000
H	-4.258491000	-0.822010000	-0.989314000
C	1.815729000	-2.636387000	0.323785000
H	2.701316000	-3.274830000	0.394572000
H	1.199096000	-2.987334000	-0.511533000
H	1.227262000	-2.761515000	1.240028000

A-DR1-T1-TS2

C	0.750702000	0.232765000	1.473856000
C	2.232256000	0.244776000	1.088876000
C	2.220745000	0.631773000	-0.383431000
C	0.855013000	1.042329000	-0.745841000
N	0.020810000	0.652788000	0.380159000
H	2.853435000	0.824447000	1.779188000
O	0.282193000	-0.196203000	2.519667000
O	0.656218000	2.133363000	-1.410191000
C	-1.294710000	0.145545000	0.122971000
C	-2.388335000	1.020899000	0.120582000
C	-1.411701000	-1.224224000	-0.182071000
C	-3.647218000	0.492700000	-0.192051000
C	-2.688191000	-1.711528000	-0.485147000
C	-3.796131000	-0.861204000	-0.491362000
H	-4.512418000	1.150457000	-0.201400000
H	-2.814392000	-2.765039000	-0.721201000
H	-4.778557000	-1.256923000	-0.734269000
C	-0.216977000	-2.167275000	-0.143881000
H	-0.592922000	-3.170150000	-0.366431000
H	0.153090000	-2.221936000	0.885785000
C	0.961845000	-1.883088000	-1.126640000
H	1.237215000	-2.834061000	-1.603910000
H	0.606976000	-1.242943000	-1.948247000
C	2.260048000	-1.285502000	-0.626154000
H	3.068979000	-1.414750000	-1.345593000
C	2.675116000	-1.228993000	0.838899000
H	2.186460000	-1.948002000	1.503846000
H	3.758778000	-1.320084000	0.945615000
C	3.416747000	1.272968000	-1.018584000
H	3.560087000	2.280518000	-0.608208000
H	3.287946000	1.360044000	-2.100935000
H	4.325146000	0.699991000	-0.806110000
C	-2.194046000	2.481257000	0.446528000
H	-3.125247000	3.041053000	0.319472000
H	-1.423278000	2.921621000	-0.195740000
H	-1.855225000	2.609786000	1.481928000

A-DR2-T1-TS1

C	-0.686213000	-0.736223000	1.508654000
C	-2.089640000	-0.877737000	1.175542000
C	-2.236368000	-0.805867000	-0.266950000
C	-0.877177000	-0.919337000	-0.816390000
N	0.006040000	-0.748358000	0.270640000
H	-2.879512000	-0.978051000	1.906640000
O	-0.142635000	-0.591367000	2.602363000
O	-0.527648000	-1.043376000	-1.986136000
C	1.299441000	-0.165996000	0.093420000
C	2.422734000	-0.985242000	-0.066980000
C	1.367102000	1.238118000	0.050690000
C	3.660011000	-0.361298000	-0.269176000
C	2.620805000	1.824047000	-0.152812000
C	3.758321000	1.029855000	-0.311130000
H	4.549232000	-0.973004000	-0.396937000
H	2.704708000	2.907128000	-0.189106000
H	4.725730000	1.498413000	-0.470112000
C	0.119275000	2.083955000	0.239766000
H	0.426431000	3.132220000	0.289955000
H	-0.311372000	1.856919000	1.221443000
C	-0.963847000	1.932511000	-0.875458000
H	-1.215623000	2.935656000	-1.249001000
H	-0.548254000	1.405051000	-1.738427000
C	-2.311952000	1.324928000	-0.515813000
H	-2.948420000	1.178050000	-1.387357000
C	-2.971210000	1.685366000	0.681274000
H	-2.445511000	2.148737000	1.508751000
H	-4.017115000	1.438918000	0.829956000
C	-3.427111000	-1.319260000	-1.018860000
H	-3.545927000	-2.398662000	-0.860019000
H	-3.302880000	-1.146102000	-2.091608000
H	-4.348107000	-0.831170000	-0.682659000
C	2.278802000	-2.486342000	-0.030850000
H	3.247403000	-2.979519000	-0.152211000
H	1.612363000	-2.830054000	-0.830398000
H	1.839003000	-2.816947000	0.917233000

A-DR2-T1-TS2

C	-0.763729000	-0.901294000	1.326174000
C	-2.150578000	-0.704917000	1.010357000
C	-2.222172000	-0.415604000	-0.476898000
C	-0.813954000	-0.657047000	-0.999327000
N	0.011898000	-0.777412000	0.105848000
H	-2.910396000	-1.295116000	1.522007000
O	-0.313233000	-1.582170000	2.333224000

O	-0.447613000	-0.605960000	-2.161104000
C	1.304189000	-0.157361000	0.060256000
C	2.446903000	-0.945010000	-0.122125000
C	1.345124000	1.245768000	0.155732000
C	3.680750000	-0.290301000	-0.220555000
C	2.597710000	1.860970000	0.046997000
C	3.753866000	1.100642000	-0.143642000
H	4.585352000	-0.876276000	-0.360584000
H	2.668255000	2.943442000	0.117973000
H	4.717174000	1.596554000	-0.226557000
C	0.104968000	2.074091000	0.462368000
H	0.436964000	3.112060000	0.560145000
H	-0.248633000	1.788049000	1.460009000
C	-1.097714000	2.075603000	-0.536144000
H	-1.495410000	3.097177000	-0.537813000
H	-0.738901000	1.891239000	-1.554223000
C	-2.338697000	1.185852000	-0.265147000
H	-3.138413000	1.528011000	-0.934333000
C	-2.789650000	1.098082000	1.175527000
H	-2.267658000	1.648284000	1.953821000
H	-3.860155000	0.992347000	1.346338000
C	-3.337426000	-1.028393000	-1.300807000
H	-3.288101000	-2.121927000	-1.263062000
H	-3.245565000	-0.713972000	-2.345020000
H	-4.316533000	-0.715655000	-0.924220000
C	2.323717000	-2.445560000	-0.210495000
H	3.307125000	-2.924373000	-0.206998000
H	1.801046000	-2.741097000	-1.128276000
H	1.737482000	-2.834952000	0.629257000

B-DR3-T1-TS1

C	-0.823320000	-0.096738000	1.580609000
C	-2.221643000	-0.370357000	1.354314000
C	-2.389191000	-0.879483000	-0.009091000
C	-1.057542000	-0.969416000	-0.589715000
N	-0.164964000	-0.456913000	0.377435000
H	-3.001037000	-0.197323000	2.083567000
O	-0.258316000	0.370373000	2.575082000
O	-0.728087000	-1.353206000	-1.716152000
C	1.216749000	-0.206952000	0.121994000
C	2.092044000	-1.299229000	-0.000648000
C	1.653640000	1.123860000	-0.014981000
C	3.439670000	-1.035206000	-0.273033000
C	3.010368000	1.342725000	-0.279861000
C	3.897684000	0.274160000	-0.410236000
H	4.132162000	-1.866929000	-0.373069000

H	3.370136000	2.362220000	-0.392166000
H	4.946780000	0.463473000	-0.620499000
C	0.705767000	2.300534000	0.121164000
H	1.288401000	3.218418000	0.003691000
H	0.308396000	2.319532000	1.142170000
C	-0.477066000	2.314807000	-0.900595000
H	-0.485040000	3.297686000	-1.396737000
H	-0.310996000	1.579508000	-1.696149000
C	-3.561353000	-1.618688000	-0.550660000
H	-3.619543000	-2.624270000	-0.107249000
H	-3.464563000	-1.738308000	-1.633686000
H	-4.504206000	-1.110053000	-0.324382000
C	-1.835881000	2.118219000	-0.301794000
H	-2.045426000	2.637103000	0.632234000
C	-2.812424000	1.335237000	-0.857545000
H	-2.685073000	0.908488000	-1.848505000
H	-3.815958000	1.325267000	-0.444949000
C	1.590896000	-2.713511000	0.156304000
H	2.422267000	-3.423565000	0.183053000
H	0.930656000	-2.981329000	-0.675928000
H	1.008632000	-2.828633000	1.077773000

B-DR3-T1-TS2

C	0.824949000	-0.064563000	1.485450000
C	2.132255000	-0.392435000	0.991131000
C	2.409878000	0.566639000	-0.160886000
C	0.980723000	0.998699000	-0.560867000
N	0.099054000	0.573491000	0.432507000
H	2.926077000	-0.660750000	1.683188000
O	0.299628000	-0.373314000	2.628172000
O	0.654101000	1.554745000	-1.596953000
C	-1.256759000	0.206846000	0.143914000
C	-2.233602000	1.207059000	0.022651000
C	-1.545182000	-1.166506000	-0.010310000
C	-3.543216000	0.807219000	-0.265503000
C	-2.871436000	-1.517275000	-0.288198000
C	-3.862661000	-0.543031000	-0.413760000
H	-4.317382000	1.563267000	-0.367850000
H	-3.125237000	-2.566466000	-0.416797000
H	-4.886077000	-0.837266000	-0.629721000
C	-0.474522000	-2.243111000	0.089352000
H	-0.960197000	-3.203805000	-0.104144000
H	-0.091242000	-2.302060000	1.113319000
C	0.721955000	-2.079964000	-0.919992000
H	0.839382000	-3.042574000	-1.435521000
H	0.419105000	-1.367567000	-1.695628000

C	3.354270000	1.747595000	0.014328000
H	3.006263000	2.409444000	0.815163000
H	3.407135000	2.327368000	-0.913082000
H	4.360248000	1.397126000	0.266225000
C	2.094128000	-1.698592000	-0.383765000
H	2.680427000	-2.539005000	-0.011940000
C	2.844817000	-0.589964000	-1.117606000
H	2.550724000	-0.426744000	-2.161502000
H	3.930190000	-0.714656000	-1.056320000
C	-1.869440000	2.660446000	0.194417000
H	-2.761007000	3.293798000	0.178724000
H	-1.195239000	2.985065000	-0.605673000
H	-1.343324000	2.824561000	1.142114000

B-DR4-T1-TS1

C	0.789848000	0.001548000	1.469443000
C	2.168531000	0.228044000	1.086267000
C	2.180517000	1.170922000	-0.026576000
C	0.812593000	1.314210000	-0.480186000
N	0.012237000	0.575362000	0.431671000
H	2.993827000	0.066199000	1.767222000
O	0.326653000	-0.626702000	2.423366000
O	0.380345000	1.912598000	-1.471315000
C	-1.307208000	0.127664000	0.130936000
C	-2.365256000	1.050777000	0.109487000
C	-1.489675000	-1.238593000	-0.165687000
C	-3.639879000	0.580517000	-0.227716000
C	-2.782944000	-1.664375000	-0.490282000
C	-3.849208000	-0.765356000	-0.524891000
H	-4.472722000	1.278546000	-0.250689000
H	-2.951874000	-2.711745000	-0.727072000
H	-4.844326000	-1.115646000	-0.785121000
C	-0.355996000	-2.251573000	-0.110293000
H	-0.742306000	-3.195710000	-0.504794000
H	-0.113966000	-2.443381000	0.941033000
C	0.947890000	-1.895404000	-0.882369000
H	1.162627000	-2.712984000	-1.584040000
H	0.802164000	-1.017711000	-1.521653000
C	3.326899000	1.927348000	-0.585680000
H	3.555064000	2.802807000	0.042919000
H	3.086659000	2.294264000	-1.588102000
H	4.235272000	1.318142000	-0.627810000
C	2.224073000	-1.734125000	-0.077257000
H	2.264093000	-2.239618000	0.885779000
C	3.418895000	-1.459762000	-0.731754000
H	3.426639000	-1.142814000	-1.770537000

H	4.366710000	-1.480522000	-0.204181000
C	-2.132127000	2.501385000	0.451643000
H	-3.079508000	3.041475000	0.535703000
H	-1.519879000	2.984083000	-0.317539000
H	-1.591835000	2.600565000	1.400262000

B-DR4-T1-TS2

C	0.711189000	-0.151819000	1.422684000
C	2.113004000	-0.388283000	0.917783000
C	2.359864000	0.646317000	-0.156455000
C	1.026590000	1.070292000	-0.580008000
N	0.055230000	0.543261000	0.418256000
H	2.870493000	-0.497155000	1.693783000
O	0.204210000	-0.586525000	2.442648000
O	0.797025000	2.169199000	-1.212673000
C	-1.289682000	0.182345000	0.102975000
C	-2.283201000	1.176431000	0.041714000
C	-1.573384000	-1.185061000	-0.126794000
C	-3.587345000	0.783853000	-0.277912000
C	-2.894825000	-1.529838000	-0.429481000
C	-3.892514000	-0.556981000	-0.510876000
H	-4.369557000	1.536413000	-0.331873000
H	-3.142162000	-2.572011000	-0.614418000
H	-4.910797000	-0.846478000	-0.755754000
C	-0.510595000	-2.276185000	-0.047313000
H	-0.960064000	-3.192207000	-0.442219000
H	-0.279948000	-2.491938000	1.002670000
C	0.792173000	-1.992884000	-0.844307000
H	1.055423000	-2.888539000	-1.419720000
H	0.573085000	-1.224029000	-1.592382000
C	3.470565000	1.660748000	-0.094736000
H	3.239447000	2.403851000	0.681414000
H	3.557914000	2.192422000	-1.047189000
H	4.428547000	1.197726000	0.155701000
C	2.108083000	-1.610107000	-0.116990000
H	2.546517000	-2.489361000	0.371066000
C	3.017908000	-0.901029000	-1.099686000
H	2.767045000	-0.893690000	-2.158852000
H	4.085156000	-0.902658000	-0.885331000
C	-1.950375000	2.614679000	0.346254000
H	-2.839685000	3.247307000	0.272610000
H	-1.182819000	2.991065000	-0.337300000
H	-1.539808000	2.710183000	1.359090000

C-DR5-T1-TS1

C	1.084316000	-0.628389000	-1.009705000
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C	2.393170000	-0.805084000	-0.384212000
C	2.151111000	-1.023701000	1.037576000
C	0.739029000	-0.877101000	1.297845000
N	0.140856000	-0.626515000	0.036802000
O	0.815624000	-0.441539000	-2.198422000
O	0.117555000	-0.913700000	2.364658000
C	-1.213580000	-0.201082000	-0.116338000
C	-2.243870000	-1.148774000	-0.021641000
C	-1.464568000	1.165312000	-0.336007000
C	-3.562432000	-0.700765000	-0.166412000
C	-2.795348000	1.571473000	-0.482141000
C	-3.837038000	0.646500000	-0.399554000
H	-4.376641000	-1.417470000	-0.097373000
H	-3.014285000	2.622322000	-0.652980000
H	-4.865636000	0.978259000	-0.511972000
C	-0.332598000	2.174327000	-0.396600000
H	-0.758007000	3.151310000	-0.642261000
H	0.322499000	1.916958000	-1.234552000
C	0.478327000	2.296000000	0.926548000
H	0.465032000	3.343426000	1.266983000
H	-0.037336000	1.750037000	1.729881000
C	1.915418000	1.865313000	0.943054000
H	2.371275000	1.851837000	1.931522000
C	2.707392000	1.501700000	-0.124859000
H	2.396037000	1.658923000	-1.152269000
H	3.769914000	1.349198000	0.032004000
C	-1.927355000	-2.600557000	0.238536000
H	-2.831212000	-3.214730000	0.194860000
H	-1.473089000	-2.721731000	1.228697000
H	-1.210210000	-2.988473000	-0.494077000
C	3.601841000	-1.209514000	-1.156382000
H	4.525027000	-0.913921000	-0.647983000
H	3.631214000	-2.302036000	-1.280881000
H	3.580150000	-0.762611000	-2.154664000
H	2.890949000	-1.227724000	1.799316000

C-DR5-T1-TS2

C	0.985220000	-0.507873000	-1.032293000
C	2.388319000	-0.398971000	-0.406164000
C	2.078139000	-0.409809000	1.082597000
C	0.696316000	-0.791862000	1.283814000
N	0.064462000	-0.695782000	-0.018737000
O	0.719817000	-0.356386000	-2.216355000
O	0.363739000	-1.681561000	2.164471000
C	-1.269921000	-0.179107000	-0.115484000
C	-2.357877000	-1.061064000	-0.088611000

C	-1.420854000	1.220214000	-0.170498000
C	-3.645377000	-0.511309000	-0.128203000
C	-2.724932000	1.726867000	-0.212891000
C	-3.827350000	0.869894000	-0.190609000
H	-4.507131000	-1.173335000	-0.108440000
H	-2.877297000	2.802026000	-0.260571000
H	-4.832163000	1.282508000	-0.219040000
C	-0.226783000	2.163547000	-0.228226000
H	-0.623762000	3.178085000	-0.326170000
H	0.319786000	1.978909000	-1.159418000
C	0.754982000	2.159476000	0.986593000
H	0.930998000	3.203043000	1.282052000
H	0.257551000	1.697431000	1.853527000
C	2.122155000	1.521834000	0.865884000
H	2.798140000	1.835823000	1.660972000
C	2.778990000	1.119869000	-0.442963000
H	2.421280000	1.632760000	-1.341927000
H	3.866901000	1.215219000	-0.383351000
C	-2.128312000	-2.550723000	-0.017409000
H	-3.075164000	-3.091876000	0.066713000
H	-1.496813000	-2.804782000	0.841188000
H	-1.605529000	-2.909867000	-0.912285000
C	3.389514000	-1.385348000	-0.991279000
H	3.460167000	-1.244304000	-2.074536000
H	4.380382000	-1.235048000	-0.551532000
H	3.075534000	-2.417031000	-0.797913000
H	2.834069000	-0.689323000	1.811396000

C-DR6-T1-TS1

C	0.938140000	-1.086662000	-0.856473000
C	2.266360000	-1.050073000	-0.264855000
C	2.123159000	-0.502158000	1.076376000
C	0.703433000	-0.498211000	1.400117000
N	0.035500000	-0.728396000	0.173516000
O	0.607868000	-1.341149000	-2.016323000
O	0.134364000	-0.251650000	2.461737000
C	-1.272467000	-0.206092000	-0.066991000
C	-2.397861000	-1.014664000	0.130359000
C	-1.363570000	1.140679000	-0.462864000
C	-3.657967000	-0.442532000	-0.083681000
C	-2.639531000	1.676446000	-0.666402000
C	-3.778104000	0.890569000	-0.477368000
H	-4.548470000	-1.048171000	0.062900000
H	-2.740140000	2.714019000	-0.974252000
H	-4.763291000	1.320011000	-0.637691000
C	-0.111789000	1.971493000	-0.687877000

H	-0.413630000	2.928387000	-1.122638000
H	0.495374000	1.478281000	-1.454915000
C	0.746623000	2.247106000	0.587289000
H	0.893652000	3.333039000	0.680615000
H	0.195618000	1.958981000	1.486569000
C	2.151760000	1.675889000	0.654658000
H	2.630037000	1.814148000	1.622272000
C	2.989630000	1.641731000	-0.466785000
H	2.610059000	1.771095000	-1.474390000
H	4.048138000	1.432869000	-0.358399000
C	-2.233918000	-2.448899000	0.568106000
H	-3.202490000	-2.949808000	0.652405000
H	-1.730606000	-2.501912000	1.540481000
H	-1.615903000	-3.008488000	-0.143542000
C	3.481929000	-1.591578000	-0.921513000
H	4.375485000	-1.011987000	-0.670170000
H	3.668541000	-2.626950000	-0.595728000
H	3.352036000	-1.607076000	-2.007803000
H	2.884263000	-0.573541000	1.843784000

C-DR6-T1-TS2

C	1.006222000	-0.971135000	-0.824510000
C	2.328542000	-0.646250000	-0.302522000
C	2.087970000	-0.010169000	1.053374000
C	0.639695000	-0.289076000	1.400297000
N	0.033005000	-0.694760000	0.226339000
O	0.784162000	-1.905301000	-1.691388000
O	0.071632000	-0.043705000	2.451582000
C	-1.284632000	-0.207082000	-0.055018000
C	-2.390426000	-1.046986000	0.120720000
C	-1.397575000	1.138786000	-0.449755000
C	-3.662421000	-0.505624000	-0.101346000
C	-2.687065000	1.641907000	-0.657553000
C	-3.809169000	0.828970000	-0.480291000
H	-4.539287000	-1.134818000	0.027196000
H	-2.812707000	2.676907000	-0.965345000
H	-4.802348000	1.238056000	-0.644711000
C	-0.177332000	2.002397000	-0.737629000
H	-0.551170000	2.965582000	-1.098166000
H	0.351544000	1.557525000	-1.588682000
C	0.844987000	2.313200000	0.403378000
H	1.180114000	3.344419000	0.243510000
H	0.335462000	2.308489000	1.372725000
C	2.161498000	1.497133000	0.521618000
H	2.826808000	2.049398000	1.195347000
C	2.847523000	1.146366000	-0.783818000

H	2.412209000	1.441659000	-1.734827000
H	3.936056000	1.142709000	-0.777286000
C	-2.188445000	-2.481281000	0.541529000
H	-3.125769000	-3.043286000	0.496250000
H	-1.803589000	-2.536135000	1.567135000
H	-1.449636000	-2.970679000	-0.102842000
C	3.487653000	-1.564066000	-0.578213000
H	3.560538000	-1.783445000	-1.647690000
H	4.430832000	-1.137812000	-0.226281000
H	3.329840000	-2.515342000	-0.051568000
H	2.801572000	-0.230402000	1.847753000

D-DR7-T1-TS1

C	-1.029818000	-0.597136000	1.140216000
C	-2.334653000	-0.912398000	0.605499000
C	-2.189477000	-1.065183000	-0.847828000
C	-0.788331000	-0.925042000	-1.179005000
N	-0.139830000	-0.601794000	0.036978000
O	-0.703136000	-0.347268000	2.307190000
O	-0.221435000	-0.994970000	-2.274345000
C	1.223775000	-0.187615000	0.113980000
C	2.237573000	-1.143501000	-0.065033000
C	1.506265000	1.171231000	0.347569000
C	3.567634000	-0.708979000	-0.012217000
C	2.848760000	1.561789000	0.400287000
C	3.873012000	0.631600000	0.219234000
H	4.366664000	-1.432784000	-0.151292000
H	3.090056000	2.607038000	0.576202000
H	4.910128000	0.953619000	0.256823000
C	0.402499000	2.193686000	0.539997000
H	0.867639000	3.159538000	0.755632000
H	-0.173765000	1.926400000	1.432889000
C	-0.562304000	2.349345000	-0.679362000
H	-0.569029000	3.408815000	-0.978502000
H	-0.183783000	1.798774000	-1.548487000
C	-1.984993000	1.958990000	-0.412317000
H	-2.395384000	2.226938000	0.561083000
C	-2.781775000	1.307842000	-1.307767000
H	-2.443986000	1.117313000	-2.323224000
H	-3.833036000	1.133833000	-1.096936000
C	1.897600000	-2.593105000	-0.309568000
H	2.794677000	-3.217875000	-0.276271000
H	1.423935000	-2.715389000	-1.290432000
H	1.188775000	-2.966725000	0.438711000
C	-3.562753000	-1.075617000	1.412483000
H	-3.952486000	-2.102340000	1.327971000

H	-3.359179000	-0.861710000	2.465162000
H	-4.364257000	-0.411629000	1.058351000
H	-2.929667000	-1.468797000	-1.526294000

D-DR7-T1-TS2

C	-0.947996000	-0.220608000	1.277299000
C	-2.249248000	-0.143639000	0.634035000
C	-2.189622000	-1.150226000	-0.510964000
C	-0.679865000	-1.341333000	-0.731484000
N	-0.008689000	-0.727300000	0.324085000
O	-0.602225000	0.287535000	2.416555000
O	-0.140095000	-1.848801000	-1.701908000
C	1.284298000	-0.130888000	0.165941000
C	2.430184000	-0.941017000	0.194982000
C	1.342083000	1.268077000	-0.014120000
C	3.672707000	-0.318325000	0.032352000
C	2.608032000	1.845877000	-0.162196000
C	3.763530000	1.063541000	-0.138816000
H	4.574697000	-0.924590000	0.047264000
H	2.685595000	2.920498000	-0.307092000
H	4.736701000	1.532431000	-0.255883000
C	0.092934000	2.134841000	-0.073797000
H	0.416839000	3.161693000	-0.266277000
H	-0.400161000	2.152278000	0.903157000
C	-0.940833000	1.723108000	-1.183391000
H	-1.182074000	2.631672000	-1.751396000
H	-0.434961000	1.060732000	-1.894519000
C	-2.269983000	1.108308000	-0.764786000
H	-3.030282000	1.844022000	-0.500017000
C	-2.728277000	-0.125820000	-1.549735000
H	-2.294743000	-0.237518000	-2.549900000
H	-3.817286000	-0.197395000	-1.611967000
C	2.312605000	-2.431469000	0.392325000
H	3.297832000	-2.891537000	0.510731000
H	1.810420000	-2.895016000	-0.463832000
H	1.711709000	-2.664058000	1.279244000
C	-3.489208000	0.005599000	1.470243000
H	-3.650501000	-0.893115000	2.077956000
H	-3.397536000	0.863309000	2.144433000
H	-4.372212000	0.143532000	0.838612000
H	-2.722704000	-2.101862000	-0.413604000

D-DR8-T1-TS1

C	-0.929004000	-0.405903000	1.140085000
C	-2.237036000	-0.669815000	0.545021000

C	-1.989616000	-1.391849000	-0.689815000
C	-0.573831000	-1.343217000	-0.978325000
N	0.028421000	-0.722176000	0.151102000
O	-0.669409000	0.063456000	2.247348000
O	0.040738000	-1.704622000	-1.984028000
C	1.317939000	-0.113435000	0.121706000
C	2.467861000	-0.918401000	0.104308000
C	1.377644000	1.294242000	0.090029000
C	3.712669000	-0.280199000	0.047068000
C	2.643594000	1.888739000	0.041018000
C	3.801733000	1.110855000	0.016690000
H	4.616663000	-0.883458000	0.031848000
H	2.719623000	2.972704000	0.011619000
H	4.775327000	1.591291000	-0.027738000
C	0.131817000	2.166513000	0.133440000
H	0.449673000	3.198792000	-0.038755000
H	-0.277564000	2.145183000	1.149474000
C	-0.992448000	1.825095000	-0.886891000
H	-1.223636000	2.738615000	-1.452496000
H	-0.632845000	1.119888000	-1.644825000
C	-2.339846000	1.363094000	-0.357342000
H	-2.632264000	1.742890000	0.620610000
C	-3.350547000	1.091068000	-1.292287000
H	-3.111522000	0.962677000	-2.343612000
H	-4.378552000	0.932049000	-0.986388000
C	2.358186000	-2.421727000	0.155641000
H	3.341080000	-2.883064000	0.287584000
H	1.911421000	-2.805926000	-0.767611000
H	1.711997000	-2.741314000	0.981422000
C	-3.463368000	-0.788654000	1.391895000
H	-4.374688000	-0.633766000	0.806986000
H	-3.522056000	-1.791127000	1.836347000
H	-3.431943000	-0.062825000	2.209494000
H	-2.724770000	-1.856493000	-1.331684000

D-DR8-T1-TS2

C	0.867912000	0.135403000	1.191667000
C	2.236714000	0.133746000	0.547789000
C	2.151961000	1.120886000	-0.595109000
C	0.749136000	1.371706000	-0.800504000
N	-0.010854000	0.694852000	0.271618000
O	0.560517000	-0.355883000	2.263717000
O	0.266801000	2.386392000	-1.436957000
C	-1.303634000	0.110906000	0.112131000
C	-2.447701000	0.929985000	0.149248000
C	-1.383642000	-1.291808000	-0.061725000

C	-3.696981000	0.322184000	-0.012598000
C	-2.656349000	-1.854029000	-0.204433000
C	-3.802524000	-1.057649000	-0.186371000
H	-4.592802000	0.936844000	0.011549000
H	-2.748921000	-2.928058000	-0.343425000
H	-4.780440000	-1.515491000	-0.307323000
C	-0.156089000	-2.195495000	-0.093858000
H	-0.492260000	-3.181484000	-0.428327000
H	0.221664000	-2.344690000	0.924495000
C	0.985739000	-1.727629000	-1.036471000
H	1.322918000	-2.584456000	-1.632307000
H	0.563237000	-1.024975000	-1.762728000
C	2.297077000	-1.124111000	-0.473468000
H	2.913710000	-1.905392000	-0.008796000
C	2.962102000	-0.322646000	-1.571029000
H	2.609383000	-0.421700000	-2.595720000
H	4.028136000	-0.121107000	-1.475353000
C	-2.324095000	2.412788000	0.387031000
H	-3.309294000	2.883386000	0.451871000
H	-1.751065000	2.891653000	-0.413759000
H	-1.780433000	2.611885000	1.318420000
C	3.403834000	0.202272000	1.511789000
H	3.417916000	1.168139000	2.027835000
H	3.311957000	-0.587811000	2.263113000
H	4.357009000	0.079438000	0.988619000
H	2.865966000	1.936739000	-0.718097000

A-DR1-T1S0

C	-0.956286300	0.074888000	1.420150400
C	-2.388000700	0.041236000	0.905367300
C	-2.356164700	-1.059149300	-0.099347000
C	-0.973923300	-1.255217400	-0.499108100
N	-0.172537000	-0.516530100	0.426284100
H	-3.120045900	-0.063869000	1.711147500
O	-0.548329200	0.618613200	2.425819700
O	-0.537936200	-1.902824500	-1.440101400
C	1.201932300	-0.204596100	0.190159100
C	2.142811600	-1.248320300	0.177122000
C	1.557187400	1.136492300	-0.071373000
C	3.467359000	-0.936586300	-0.146957000
C	2.897260800	1.393929400	-0.385819100
C	3.842636100	0.371804100	-0.436942100
H	4.207692200	-1.732263500	-0.163626000
H	3.201075900	2.417539700	-0.590385200
H	4.875088400	0.599733200	-0.688010200
C	0.599633200	2.315440600	0.026710000

H	1.212674300	3.222602900	-0.015762000
H	0.128317000	2.328695700	1.013299300
C	-0.493582100	2.483987700	-1.075177300
H	-0.813953200	3.539143000	-1.000705300
H	-0.019930000	2.382265700	-2.058227600
C	-1.715284500	1.618660500	-1.025493300
H	-1.991248600	1.074019300	-1.924625500
C	-2.595400700	1.442375400	0.175439000
H	-2.426032700	2.225499600	0.924283300
H	-3.652961000	1.485887400	-0.118766000
C	-3.507522000	-1.675917500	-0.797356200
H	-4.182619200	-2.179962600	-0.091550000
H	-3.156821900	-2.401049700	-1.536836400
H	-4.112035200	-0.915372300	-1.315765400
C	1.748030500	-2.665634700	0.509665100
H	2.628740700	-3.266219900	0.756457200
H	1.233218300	-3.131519900	-0.336812100
H	1.062601300	-2.696084800	1.363919400

A-DR2-T1S0

C	-0.583657200	-0.828136200	1.520443400
C	-1.999330600	-0.798831200	1.221011300
C	-2.206383600	-0.572848200	-0.235073100
C	-0.829866200	-0.913911300	-0.805068200
N	0.083416000	-0.831514200	0.257902100
H	-2.767800800	-0.829352200	1.981901600
O	-0.015001000	-0.802016200	2.600200700
O	-0.546507200	-1.099388300	-1.969000600
C	1.338410400	-0.161787000	0.081925000
C	2.511575700	-0.885083200	-0.142082000
C	1.294254400	1.243587300	0.120669000
C	3.693333000	-0.157598000	-0.323757100
C	2.496701700	1.932248500	-0.063585000
C	3.686472000	1.236153300	-0.282454100
H	4.623533300	-0.691565200	-0.499997100
H	2.499767700	3.019145800	-0.038626000
H	4.613644300	1.784803500	-0.425073100
C	-0.017644000	1.983627600	0.344315100
H	0.220311100	3.045660900	0.460252100
H	-0.456662100	1.679865500	1.302588400
C	-1.068364300	1.833979500	-0.805837200
H	-1.415748400	2.836927800	-1.080331300
H	-0.570510200	1.439951400	-1.696482500
C	-2.373402700	1.020536300	-0.563075200
H	-2.882494800	1.002160300	-1.537972400
C	-3.267645900	1.662165500	0.438377100

H	-2.875689800	2.348320700	1.182205300
H	-4.299054200	1.340410400	0.545014200
C	-3.353930900	-1.358485400	-0.870309200
H	-3.310475900	-2.414341700	-0.584188200
H	-3.281667900	-1.296495400	-1.960339500
H	-4.323662200	-0.958244300	-0.555686200
C	2.473870700	-2.391266700	-0.191601100
H	3.468382000	-2.806421800	-0.380061100
H	1.798868500	-2.731927800	-0.984926300
H	2.101068600	-2.803175800	0.753417200

B-DR3-T1S0

C	-0.807739200	-0.385625100	1.604968400
C	-2.222378600	-0.547593200	1.323035400
C	-2.450641700	-0.505235100	-0.138423000
C	-1.041758300	-0.735941200	-0.693930200
N	-0.148122000	-0.491647100	0.344744100
H	-2.978611800	-0.563272200	2.097475600
O	-0.238454100	-0.180047100	2.665115700
O	-0.747360200	-0.980962300	-1.846482500
C	1.236176300	-0.206301100	0.120863000
C	2.125502600	-1.267878400	-0.090178000
C	1.632281500	1.140366300	0.067028000
C	3.463796000	-0.956174300	-0.350194100
C	2.980373800	1.407705400	-0.195251100
C	3.888763100	0.370226100	-0.401151100
H	4.173764200	-1.762385500	-0.515423100
H	3.317669900	2.440163700	-0.239210100
H	4.931819400	0.597247200	-0.604871200
C	0.649051200	2.272299600	0.292225100
H	1.209838300	3.212312900	0.284617100
H	0.228552100	2.178139600	1.300522400
C	-0.528955100	2.367812700	-0.750529200
H	-0.528727100	3.394327900	-1.150330300
H	-0.326507100	1.714486500	-1.606622400
C	-3.491255000	-1.474292400	-0.700357200
H	-3.280984900	-2.500744700	-0.383403100
H	-3.472107000	-1.444841400	-1.793721500
H	-4.495997300	-1.206144300	-0.356538100
C	-1.878518500	2.072561600	-0.169070000
H	-2.124929600	2.572212700	0.766858200
C	-2.796119800	1.002229300	-0.636448200
H	-2.795643800	0.927301300	-1.731755500
H	-3.822227100	1.197161300	-0.304644100
C	1.636719500	-2.694058800	-0.049676000
H	2.468020700	-3.397741000	-0.151492000

H	0.927189300	-2.879656800	-0.864334200
H	1.120459300	-2.909570800	0.893125200

B-DR4-T1S0

C	0.755477200	0.009702000	1.421525400
C	2.162248600	0.085910000	0.850587200
C	2.073262600	1.217584300	-0.118136000
C	0.673375200	1.440588400	-0.424098100
N	-0.078194000	0.635619200	0.486918100
H	2.934425800	0.194602100	1.618254500
O	0.391437100	-0.611528200	2.396760700
O	0.184400100	2.141359600	-1.299664400
C	-1.353622400	0.085576000	0.149868000
C	-2.493791700	0.900939300	0.158584000
C	-1.383015400	-1.270082400	-0.234321100
C	-3.706657000	0.327200100	-0.235817100
C	-2.621770700	-1.798453500	-0.616477200
C	-3.771467100	-1.010435300	-0.620369200
H	-4.605479300	0.938314300	-0.237566100
H	-2.682311800	-2.840877800	-0.919549300
H	-4.721155300	-1.441672400	-0.925490300
C	-0.166422000	-2.190958600	-0.200106100
H	-0.460734100	-3.107708900	-0.720901200
H	0.009630000	-2.490271700	0.841235200
C	1.185975300	-1.716336500	-0.827253200
H	1.571519400	-2.555149700	-1.417867400
H	1.012223300	-0.910108300	-1.549081400
C	3.181521900	1.950716500	-0.773760200
H	3.853092100	2.405592700	-0.031373000
H	2.781667800	2.734983800	-1.422519400
H	3.798488100	1.271992400	-1.379264400
C	2.342907700	-1.326815400	0.142738000
H	2.320277600	-2.049289600	0.980054300
C	3.674165000	-1.390223400	-0.527642100
H	3.827003100	-1.992888600	-1.417331400
H	4.548903300	-0.955865300	-0.052940000
C	-2.405532700	2.345000700	0.583288200
H	-3.402116000	2.782846800	0.693708200
H	-1.845613500	2.926888800	-0.156086000
H	-1.879079500	2.441152700	1.539858400

C-DR5-T1S0

C	1.143518900	-0.314328300	-1.021280600
C	2.475301800	-0.419313900	-0.274273600
C	2.124099600	-1.312730300	0.856692400
C	0.688658100	-1.299247500	1.048567400

N	0.145561800	-0.647122100	-0.107309700
O	0.978757000	0.087893700	-2.155337400
O	0.023500400	-1.721398300	1.979940900
C	-1.202900100	-0.179722000	-0.179039200
C	-2.248962700	-1.118207000	-0.188709300
C	-1.436374400	1.212111200	-0.192975700
C	-3.563006600	-0.638573800	-0.173484100
C	-2.769876300	1.638636700	-0.182106300
C	-3.824455600	0.728417700	-0.160570900
H	-4.384611500	-1.350400900	-0.179294400
H	-2.980232700	2.705136100	-0.194789900
H	-4.850301700	1.086808800	-0.148839600
C	-0.340279800	2.264012200	-0.277177100
H	-0.834588200	3.220869100	-0.477891300
H	0.291310100	2.072628700	-1.149486800
C	0.560858000	2.499272700	0.976503200
H	1.018184800	3.492872000	0.819402400
H	-0.082151000	2.599187900	1.858371600
C	1.656198400	1.522688200	1.272320500
H	1.713667900	1.112297300	2.275661100
C	2.692287300	1.078618800	0.297612600
H	2.744464600	1.737776700	-0.577555400
H	3.684785400	1.065351300	0.767711600
C	-1.974971900	-2.601075500	-0.225208900
H	-2.863755400	-3.152071200	-0.547348500
H	-1.678793900	-2.963548800	0.764543000
H	-1.157685600	-2.836476600	-0.915903100
C	3.644593300	-0.831690100	-1.162617400
H	4.588514300	-0.792591500	-0.608449500
H	3.505454100	-1.850963000	-1.536435300
H	3.712555600	-0.161688900	-2.025336900
H	2.805744300	-1.760311000	1.565900000

C-DR6-T1S0

C	0.783317200	-1.236103300	-0.859687200
C	2.142994600	-1.056916300	-0.385482100
C	2.094559600	-0.337094100	0.921851300
C	0.653054200	-0.544099200	1.370383400
N	-0.077098000	-0.841112200	0.206595100
O	0.397991100	-1.614833500	-1.956042500
O	0.180722100	-0.349765100	2.468947700
C	-1.323967400	-0.183153100	-0.051251000
C	-2.538580700	-0.824484200	0.200267100
C	-1.234066300	1.133505300	-0.538991200
C	-3.712917000	-0.110380000	-0.064089000
C	-2.430342700	1.810894500	-0.792326200

C	-3.659438000	1.192210300	-0.558487200
H	-4.674368300	-0.582457200	0.120860000
H	-2.398145700	2.829569800	-1.170915300
H	-4.581289300	1.731439500	-0.759670200
C	0.116944000	1.800472500	-0.762769200
H	-0.068072000	2.756069800	-1.263554400
H	0.711891200	1.212550300	-1.472559400
C	0.940867300	2.072128600	0.540162200
H	1.254502400	3.122659900	0.534639100
H	0.281389100	1.965309600	1.405968400
C	2.247763600	1.268786400	0.807601200
H	2.551462700	1.553909400	1.826051500
C	3.339301900	1.630021500	-0.139668000
H	3.128842900	2.130939600	-1.079016300
H	4.361967200	1.318762400	0.050665000
C	-2.552217700	-2.229193600	0.746949200
H	-3.575417000	-2.591814700	0.882933200
H	-2.037780600	-2.268622600	1.713873500
H	-2.028787600	-2.915189800	0.070993000
C	3.333451900	-1.544691400	-1.121779300
H	3.928296100	-2.232524600	-0.502643100
H	3.020642800	-2.065904600	-2.030921600
H	4.000915100	-0.719006200	-1.402208400
H	2.829569800	-0.692538200	1.649982500

D-DR7-T1S0

C	1.004341300	-0.782774200	-1.100826300
C	2.343279700	-0.895700300	-0.548219200
C	2.283239600	-0.582422200	0.907849300
C	0.793146200	-0.662875200	1.225046300
N	0.120810000	-0.625545200	0.005160000
O	0.654781200	-0.791926200	-2.272508600
O	0.274597100	-0.640103200	2.323113700
C	-1.244320300	-0.211495100	-0.110437000
C	-2.267393600	-1.131062300	0.151147000
C	-1.492770400	1.133046300	-0.435444100
C	-3.588204000	-0.678511200	0.063813000
C	-2.827863800	1.542770400	-0.514897100
C	-3.866903100	0.645723200	-0.269277100
H	-4.400805200	-1.372881400	0.261206100
H	-3.051755900	2.576035700	-0.767794200
H	-4.898250400	0.982235300	-0.333594100
C	-0.364157100	2.114103600	-0.692925200
H	-0.808357200	3.062486900	-1.011424300
H	0.230238100	1.758711500	-1.542486400
C	0.590843200	2.380515700	0.533287100

H	0.594723200	3.467188000	0.713869200
H	0.166749000	1.932061500	1.438330400
C	2.004550600	1.921309500	0.333186100
H	2.512274700	2.256429600	-0.569590200
C	2.703205800	0.921982300	1.201419300
H	2.484449700	1.092218300	2.264096600
H	3.788616100	0.988835300	1.065410300
C	-1.938159500	-2.552874700	0.530221100
H	-2.846505800	-3.154211900	0.630274200
H	-1.400229400	-2.578475700	1.484818400
H	-1.296288400	-3.025520800	-0.222461100
C	3.555441000	-1.083096300	-1.377894400
H	4.169490200	-1.918279500	-1.013038300
H	3.275147900	-1.270865400	-2.417980700
H	4.197271200	-0.188769100	-1.348662400
H	2.872884800	-1.243978300	1.551751400

D-DR8-T1S0

C	-0.893243200	-0.376930100	1.098719300
C	-2.226710600	-0.460080100	0.364914100
C	-1.900094500	-1.368805400	-0.768295200
C	-0.464272100	-1.433462400	-0.942879300
N	0.098066000	-0.765752200	0.189504100
O	-0.705217200	0.071389000	2.209994600
O	0.186126100	-1.902820500	-1.864592500
C	1.356168400	-0.090340000	0.136005000
C	2.550371700	-0.823626200	0.152644000
C	1.319200400	1.313136400	0.020043000
C	3.750322000	-0.112541000	0.049499000
C	2.546057700	1.979465600	-0.075415000
C	3.749752000	1.276287400	-0.063033000
H	4.690691300	-0.657538200	0.060543000
H	2.555380700	3.062789900	-0.166781000
H	4.690622300	1.814123500	-0.143226000
C	0.028930000	2.126974600	0.042454000
H	0.299978100	3.144788900	-0.255608100
H	-0.312584100	2.207726600	1.082096300
C	-1.169467300	1.683296500	-0.858174200
H	-1.547249400	2.585362700	-1.351820400
H	-0.816985200	1.037622300	-1.671196500
C	-2.421207700	1.051585300	-0.175763000
H	-2.637502700	1.627008500	0.736385200
C	-3.593581000	1.111466300	-1.097872300
H	-3.449138000	1.063434300	-2.172968600
H	-4.609965300	1.082716300	-0.720442200
C	2.532658700	-2.325770700	0.279955100

H	3.538609000	-2.715873800	0.461341100
H	2.138698600	-2.782457800	-0.634134200
H	1.886277500	-2.642410700	1.106560300
C	-3.387686900	-0.885887200	1.262686400
H	-3.452468000	-0.216832100	2.125977600
H	-4.336798200	-0.860907200	0.719652200
H	-3.231654900	-1.903349500	1.635123500
H	-2.602821700	-1.823113500	-1.454174400

**Minimum-energy path connecting the T₁/S₀ crossing point (A-DR1-T1S0)
and its corresponding ground-state S0 product (A-S0-P)**

C2-C3 distance: 3.0

C	-0.913846000	0.168186000	1.368676000
C	-2.320792000	0.250445000	0.815271000
C	-2.421879000	-0.972616000	-0.010957000
C	-1.076042000	-1.368348000	-0.369347000
N	-0.192079000	-0.604165000	0.455403000
H	-3.086542000	0.383827000	1.581580000
O	-0.451410000	0.738656000	2.339313000
O	-0.707110000	-2.163522000	-1.227905000
C	1.218002000	-0.509558000	0.246240000
C	2.000236000	-1.673849000	0.364540000
C	1.776278000	0.742266000	-0.104495000
C	3.363886000	-1.586613000	0.061024000
C	3.147515000	0.772277000	-0.392935000
C	3.933141000	-0.377350000	-0.329604000
H	3.981355000	-2.477026000	0.145820000
H	3.604549000	1.719801000	-0.666060000
H	4.992916000	-0.323901000	-0.563147000
C	1.014838000	2.059794000	-0.112801000
H	1.760026000	2.857977000	-0.197787000
H	0.529467000	2.210955000	0.854915000
C	-0.029784000	2.325882000	-1.245319000
H	-0.261765000	3.400535000	-1.168404000
H	0.461975000	2.181158000	-2.213554000
C	-1.304473000	1.544606000	-1.216404000
H	-1.471206000	0.819977000	-2.009844000
C	-2.304372000	1.583214000	-0.119734000
H	-2.141088000	2.431657000	0.553933000
H	-3.325416000	1.651858000	-0.516200000
C	-3.644766000	-1.530968000	-0.632237000
H	-4.388613000	-1.806133000	0.126903000
H	-3.404095000	-2.411625000	-1.233589000
H	-4.126814000	-0.787163000	-1.285769000
C	1.409057000	-2.982935000	0.828806000

H	2.190625000	-3.640778000	1.220067000
H	0.902203000	-3.497558000	0.006471000
H	0.664093000	-2.826206000	1.616403000

C2-C3 distance: 2.9

C	-0.900788000	0.144667000	1.394543000
C	-2.309208000	0.245822000	0.842723000
C	-2.404807000	-0.938117000	-0.046702000
C	-1.058066000	-1.346668000	-0.386622000
N	-0.180880000	-0.621594000	0.476711000
H	-3.073040000	0.331011000	1.618526000
O	-0.434948000	0.707839000	2.368454000
O	-0.684679000	-2.129307000	-1.254407000
C	1.228677000	-0.519746000	0.265300000
C	2.019543000	-1.675924000	0.392525000
C	1.770556000	0.731926000	-0.104481000
C	3.382717000	-1.577962000	0.090534000
C	3.141821000	0.774645000	-0.391263000
C	3.939504000	-0.365861000	-0.310714000
H	4.009010000	-2.461499000	0.181891000
H	3.588314000	1.722949000	-0.678798000
H	4.999059000	-0.303866000	-0.543227000
C	0.984309000	2.034655000	-0.143256000
H	1.716050000	2.843007000	-0.245841000
H	0.496657000	2.200811000	0.821436000
C	-0.060646000	2.249684000	-1.284290000
H	-0.261164000	3.334800000	-1.282291000
H	0.418173000	2.029005000	-2.244770000
C	-1.364743000	1.518692000	-1.199607000
H	-1.633387000	0.859966000	-2.021267000
C	-2.305613000	1.586363000	-0.045495000
H	-2.073966000	2.420102000	0.626947000
H	-3.340001000	1.708254000	-0.391749000
C	-3.623973000	-1.464368000	-0.700643000
H	-4.369100000	-1.778665000	0.042331000
H	-3.380676000	-2.313101000	-1.345194000
H	-4.106080000	-0.688227000	-1.314686000
C	1.430308000	-2.985478000	0.856887000
H	2.216048000	-3.660542000	1.208117000
H	0.886913000	-3.478269000	0.044241000
H	0.716177000	-2.832247000	1.673411000

C2-C3 distance: 2.8

C	-0.877066000	0.102354000	1.421287000
C	-2.288002000	0.230967000	0.876997000
C	-2.377279000	-0.898129000	-0.101599000

C	-1.029677000	-1.318197000	-0.423575000
N	-0.162312000	-0.653948000	0.495891000
H	-3.044282000	0.238942000	1.665981000
O	-0.405072000	0.652031000	2.401658000
O	-0.646666000	-2.081819000	-1.304350000
C	1.246740000	-0.540369000	0.288474000
C	2.053518000	-1.680628000	0.437603000
C	1.763728000	0.711449000	-0.105460000
C	3.418092000	-1.561640000	0.150286000
C	3.136926000	0.779146000	-0.376768000
C	3.955731000	-0.343850000	-0.261965000
H	4.059809000	-2.432141000	0.257903000
H	3.567070000	1.729388000	-0.682380000
H	5.016672000	-0.265158000	-0.482939000
C	0.934615000	1.985534000	-0.198552000
H	1.643265000	2.808991000	-0.332422000
H	0.443403000	2.178557000	0.759912000
C	-0.105285000	2.107227000	-1.352410000
H	-0.218124000	3.192777000	-1.532412000
H	0.335028000	1.708160000	-2.274415000
C	-1.480240000	1.534119000	-1.176334000
H	-1.978049000	1.171760000	-2.071994000
C	-2.308282000	1.601664000	0.078420000
H	-1.974578000	2.394372000	0.759004000
H	-3.355296000	1.804053000	-0.176015000
C	-3.591564000	-1.378888000	-0.796652000
H	-4.331432000	-1.759579000	-0.079146000
H	-3.340839000	-2.172087000	-1.505816000
H	-4.082601000	-0.560685000	-1.343908000
C	1.468165000	-2.991978000	0.900375000
H	2.258188000	-3.695765000	1.177607000
H	0.860573000	-3.444728000	0.109729000
H	0.813194000	-2.849142000	1.767262000

C2-C3 distance: 2.7

C	-0.832838000	0.065086000	1.415401000
C	-2.251377000	0.233857000	0.901768000
C	-2.338580000	-0.784872000	-0.212211000
C	-1.002042000	-1.228959000	-0.526458000
N	-0.134935000	-0.660992000	0.457082000
H	-2.986133000	0.118707000	1.704560000
O	-0.343136000	0.576353000	2.408646000
O	-0.605686000	-1.927396000	-1.457164000
C	1.279170000	-0.547725000	0.284204000
C	2.098410000	-1.669721000	0.470087000
C	1.781954000	0.711135000	-0.096729000

C	3.474432000	-1.512164000	0.265408000
C	3.164376000	0.824766000	-0.282927000
C	4.003548000	-0.276228000	-0.105464000
H	4.132129000	-2.366498000	0.402331000
H	3.583598000	1.783494000	-0.576809000
H	5.073968000	-0.169922000	-0.258972000
C	0.873077000	1.912422000	-0.304701000
H	1.509899000	2.768182000	-0.546262000
H	0.388280000	2.170991000	0.642322000
C	-0.189733000	1.761140000	-1.437469000
H	-0.072971000	2.609928000	-2.129105000
H	0.066749000	0.884617000	-2.056421000
C	-1.652742000	1.679038000	-1.097125000
H	-2.316772000	1.740515000	-1.956001000
C	-2.324032000	1.662403000	0.263551000
H	-1.900165000	2.395271000	0.964311000
H	-3.379987000	1.918229000	0.133376000
C	-3.566900000	-1.247536000	-0.898151000
H	-4.176438000	-1.870478000	-0.226070000
H	-3.312522000	-1.841119000	-1.780628000
H	-4.198984000	-0.403834000	-1.202371000
C	1.504498000	-2.995807000	0.874900000
H	2.287236000	-3.732098000	1.077883000
H	0.857469000	-3.384524000	0.080812000
H	0.885249000	-2.893505000	1.773673000

C2-C3 distance: 2.6

C	-0.831541000	0.059745000	1.422711000
C	-2.249600000	0.237717000	0.907547000
C	-2.327776000	-0.749815000	-0.244280000
C	-0.996286000	-1.214144000	-0.537195000
N	-0.134600000	-0.667553000	0.466863000
H	-2.985741000	0.097537000	1.705396000
O	-0.342061000	0.569647000	2.417719000
O	-0.590042000	-1.909954000	-1.466327000
C	1.279014000	-0.553174000	0.292632000
C	2.100246000	-1.672261000	0.484682000
C	1.778129000	0.702012000	-0.103252000
C	3.475340000	-1.514926000	0.273852000
C	3.159689000	0.816183000	-0.296269000
C	4.001195000	-0.281751000	-0.110855000
H	4.134723000	-2.367204000	0.415542000
H	3.576572000	1.772514000	-0.601140000
H	5.070843000	-0.175345000	-0.269592000
C	0.867625000	1.901838000	-0.313726000
H	1.504184000	2.754633000	-0.566149000

H	0.390832000	2.167759000	0.635487000
C	-0.204740000	1.754283000	-1.437391000
H	-0.123468000	2.631112000	-2.099387000
H	0.065405000	0.908398000	-2.091012000
C	-1.661636000	1.623996000	-1.089448000
H	-2.331544000	1.694856000	-1.942944000
C	-2.322050000	1.663603000	0.282472000
H	-1.879033000	2.405595000	0.960879000
H	-3.375224000	1.932128000	0.155515000
C	-3.557968000	-1.223187000	-0.922699000
H	-4.126594000	-1.900670000	-0.267114000
H	-3.304741000	-1.767382000	-1.837002000
H	-4.227488000	-0.391548000	-1.172995000
C	1.507385000	-2.995526000	0.900245000
H	2.289936000	-3.735563000	1.090007000
H	0.845086000	-3.380681000	0.117087000
H	0.904002000	-2.890115000	1.809414000

C2-C3 distance: 2.5

C	-0.830136000	0.052324000	1.428554000
C	-2.247023000	0.241113000	0.911490000
C	-2.314096000	-0.707883000	-0.282815000
C	-0.988452000	-1.198089000	-0.550769000
N	-0.133701000	-0.675526000	0.474442000
H	-2.985184000	0.072625000	1.702277000
O	-0.340893000	0.558472000	2.426418000
O	-0.572487000	-1.890175000	-1.478674000
C	1.279671000	-0.559764000	0.300262000
C	2.103616000	-1.674959000	0.500225000
C	1.774243000	0.691726000	-0.111262000
C	3.477826000	-1.516572000	0.284746000
C	3.154940000	0.807707000	-0.309811000
C	3.999604000	-0.286093000	-0.114312000
H	4.139667000	-2.365895000	0.432670000
H	3.568806000	1.761587000	-0.626268000
H	5.068564000	-0.178834000	-0.277070000
C	0.860181000	1.888273000	-0.325651000
H	1.494163000	2.738712000	-0.592132000
H	0.392890000	2.162747000	0.625994000
C	-0.224324000	1.739394000	-1.437162000
H	-0.172270000	2.633446000	-2.079267000
H	0.049517000	0.914492000	-2.114583000
C	-1.675419000	1.581623000	-1.077808000
H	-2.352418000	1.673743000	-1.923680000
C	-2.320518000	1.668822000	0.306034000
H	-1.857788000	2.415342000	0.965546000

H	-3.371131000	1.949872000	0.185926000
C	-3.546448000	-1.196847000	-0.950473000
H	-4.074081000	-1.920042000	-0.309215000
H	-3.297725000	-1.697689000	-1.890621000
H	-4.249728000	-0.381102000	-1.153823000
C	1.512567000	-2.995620000	0.926555000
H	2.295079000	-3.738708000	1.104309000
H	0.836388000	-3.378180000	0.154045000
H	0.924176000	-2.887284000	1.845178000

C2-C3 distance: 2.4

C	-0.830142000	0.043452000	1.433757000
C	-2.244654000	0.245052000	0.913544000
C	-2.298815000	-0.660564000	-0.325425000
C	-0.978831000	-1.181833000	-0.565171000
N	-0.133307000	-0.684904000	0.480737000
H	-2.985784000	0.047926000	1.695179000
O	-0.341204000	0.542940000	2.435595000
O	-0.554116000	-1.869740000	-1.491686000
C	1.280142000	-0.567461000	0.307741000
C	2.107154000	-1.678236000	0.516262000
C	1.769470000	0.680288000	-0.119995000
C	3.480419000	-1.518313000	0.296027000
C	3.149215000	0.798319000	-0.324356000
C	3.997498000	-0.290797000	-0.118303000
H	4.145116000	-2.364192000	0.450761000
H	3.559619000	1.749614000	-0.652869000
H	5.065680000	-0.182418000	-0.285335000
C	0.851413000	1.873189000	-0.337899000
H	1.482542000	2.721600000	-0.617301000
H	0.393364000	2.155368000	0.616098000
C	-0.244938000	1.723772000	-1.437639000
H	-0.218637000	2.632831000	-2.060154000
H	0.029445000	0.917843000	-2.136207000
C	-1.691530000	1.546671000	-1.066917000
H	-2.374544000	1.671640000	-1.903771000
C	-2.318454000	1.677095000	0.329795000
H	-1.836536000	2.425660000	0.972577000
H	-3.366658000	1.970174000	0.218704000
C	-3.532902000	-1.172898000	-0.977698000
H	-4.014885000	-1.937211000	-0.348214000
H	-3.292086000	-1.633504000	-1.940376000
H	-4.269873000	-0.377960000	-1.136529000
C	1.518774000	-2.996360000	0.954000000
H	2.301707000	-3.740967000	1.123433000
H	0.831813000	-3.378895000	0.191006000

H	0.942594000	-2.884422000	1.879902000
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C2-C3 distance: 2.3

C	-0.831779000	0.032214000	1.440740000
C	-2.243119000	0.246453000	0.917021000
C	-2.283248000	-0.613659000	-0.361991000
C	-0.968109000	-1.169930000	-0.574452000
N	-0.132998000	-0.696388000	0.487435000
H	-2.988928000	0.023722000	1.687284000
O	-0.343146000	0.521264000	2.447580000
O	-0.540510000	-1.856066000	-1.498869000
C	1.280709000	-0.576242000	0.315026000
C	2.111629000	-1.681906000	0.531945000
C	1.763064000	0.668142000	-0.129479000
C	3.483533000	-1.519705000	0.304903000
C	3.141500000	0.788477000	-0.341557000
C	3.994370000	-0.295284000	-0.126103000
H	4.151822000	-2.361511000	0.466122000
H	3.547465000	1.737202000	-0.682737000
H	5.061408000	-0.185134000	-0.299107000
C	0.840935000	1.857750000	-0.349302000
H	1.470152000	2.704522000	-0.637987000
H	0.391175000	2.145483000	0.607112000
C	-0.266103000	1.711829000	-1.439123000
H	-0.264856000	2.639264000	-2.034263000
H	0.012301000	0.929764000	-2.161286000
C	-1.709448000	1.509196000	-1.057305000
H	-2.396992000	1.662820000	-1.885984000
C	-2.316441000	1.683219000	0.349884000
H	-1.816343000	2.432307000	0.977252000
H	-3.362685000	1.986822000	0.249916000
C	-3.517426000	-1.143907000	-1.005641000
H	-3.967406000	-1.934740000	-0.385909000
H	-3.282072000	-1.575797000	-1.982936000
H	-4.275083000	-0.363738000	-1.134850000
C	1.527836000	-2.997497000	0.983296000
H	2.312422000	-3.741280000	1.148650000
H	0.833122000	-3.384372000	0.229479000
H	0.961321000	-2.880537000	1.914511000

C2-C3 distance: 2.2

C	-0.833370000	0.020069000	1.450071000
C	-2.241940000	0.245051000	0.923459000
C	-2.268141000	-0.569562000	-0.385466000
C	-0.958875000	-1.163528000	-0.575630000
N	-0.131911000	-0.708312000	0.494668000

H	-2.993793000	0.001008000	1.680867000
O	-0.345303000	0.495721000	2.462526000
O	-0.537333000	-1.853149000	-1.497348000
C	1.282133000	-0.584744000	0.321451000
C	2.117781000	-1.684925000	0.545308000
C	1.755819000	0.657497000	-0.137866000
C	3.488093000	-1.518784000	0.311433000
C	3.132856000	0.781392000	-0.357167000
C	3.991357000	-0.296440000	-0.134197000
H	4.160839000	-2.355965000	0.477893000
H	3.533446000	1.728381000	-0.709329000
H	5.057144000	-0.183229000	-0.312839000
C	0.828377000	1.842852000	-0.360495000
H	1.455430000	2.688587000	-0.657033000
H	0.385725000	2.135760000	0.597832000
C	-0.288017000	1.697200000	-1.442040000
H	-0.306768000	2.638109000	-2.013853000
H	-0.003254000	0.933580000	-2.179760000
C	-1.729643000	1.465327000	-1.046674000
H	-2.421441000	1.633473000	-1.869722000
C	-2.314766000	1.685760000	0.365146000
H	-1.795511000	2.433316000	0.977179000
H	-3.359374000	1.999085000	0.279942000
C	-3.501392000	-1.102773000	-1.034146000
H	-3.937264000	-1.911613000	-0.428936000
H	-3.266172000	-1.509991000	-2.022014000
H	-4.266599000	-0.327291000	-1.143301000
C	1.540347000	-2.998948000	1.009206000
H	2.327957000	-3.739615000	1.174100000
H	0.841837000	-3.393101000	0.262600000
H	0.979800000	-2.877438000	1.943409000

C2-C3 distance: 2.1

C	-0.834868000	0.007139000	1.457836000
C	-2.240454000	0.243526000	0.928407000
C	-2.252317000	-0.522986000	-0.409810000
C	-0.950278000	-1.154968000	-0.579633000
N	-0.131049000	-0.718991000	0.498736000
H	-2.998515000	-0.021510000	1.671967000
O	-0.347627000	0.466878000	2.476900000
O	-0.535405000	-1.847596000	-1.499355000
C	1.283499000	-0.593022000	0.325943000
C	2.123407000	-1.687762000	0.558015000
C	1.749104000	0.647016000	-0.146874000
C	3.492386000	-1.517670000	0.319468000
C	3.125144000	0.774518000	-0.371299000

C	3.988785000	-0.297391000	-0.139755000
H	4.169484000	-2.350036000	0.492157000
H	3.520856000	1.719745000	-0.733549000
H	5.053612000	-0.181275000	-0.322209000
C	0.816556000	1.828224000	-0.373003000
H	1.441308000	2.672562000	-0.678532000
H	0.381451000	2.127192000	0.587090000
C	-0.310171000	1.682250000	-1.445142000
H	-0.346008000	2.633448000	-1.996974000
H	-0.021391000	0.933835000	-2.195646000
C	-1.750345000	1.424538000	-1.035796000
H	-2.445330000	1.612971000	-1.852683000
C	-2.312483000	1.688992000	0.379942000
H	-1.773860000	2.433677000	0.977272000
H	-3.354943000	2.012682000	0.310153000
C	-3.485183000	-1.064542000	-1.059131000
H	-3.899118000	-1.894940000	-0.469280000
H	-3.253304000	-1.442672000	-2.059298000
H	-4.262937000	-0.298676000	-1.142327000
C	1.551346000	-2.999914000	1.033548000
H	2.341595000	-3.737031000	1.201659000
H	0.851974000	-3.402327000	0.292054000
H	0.993153000	-2.873124000	1.968420000

C2-C3 distance: 2.0

C	-0.836770000	-0.007065000	1.464529000
C	-2.238866000	0.240952000	0.932501000
C	-2.235718000	-0.474565000	-0.434466000
C	-0.941456000	-1.142853000	-0.587091000
N	-0.130288000	-0.728303000	0.500150000
H	-3.003409000	-0.045018000	1.660925000
O	-0.350653000	0.434370000	2.491222000
O	-0.533274000	-1.836602000	-1.506406000
C	1.284854000	-0.600867000	0.329052000
C	2.128381000	-1.690233000	0.570632000
C	1.743145000	0.636574000	-0.157159000
C	3.496198000	-1.517031000	0.327629000
C	3.118163000	0.766781000	-0.386557000
C	3.986304000	-0.299614000	-0.145977000
H	4.177111000	-2.344726000	0.507462000
H	3.509724000	1.709807000	-0.758903000
H	5.050216000	-0.181283000	-0.332280000
C	0.805521000	1.813927000	-0.385829000
H	1.427863000	2.656691000	-0.700716000
H	0.378913000	2.118726000	0.576466000
C	-0.332559000	1.667865000	-1.447248000

H	-0.383998000	2.627226000	-1.981461000
H	-0.042049000	0.932621000	-2.209250000
C	-1.771090000	1.386294000	-1.023311000
H	-2.467910000	1.596928000	-1.834234000
C	-2.310753000	1.691828000	0.395144000
H	-1.753892000	2.433042000	0.978620000
H	-3.351001000	2.024868000	0.340335000
C	-3.467847000	-1.027838000	-1.082947000
H	-3.853125000	-1.883832000	-0.512030000
H	-3.241884000	-1.370764000	-2.097135000
H	-4.262171000	-0.276503000	-1.133941000
C	1.561035000	-2.999370000	1.059811000
H	2.353686000	-3.732382000	1.234336000
H	0.862127000	-3.412016000	0.323405000
H	1.003542000	-2.864880000	1.993996000

C2-C3 distance: 1.9

C	-0.838702000	-0.021461000	1.471064000
C	-2.237146000	0.238300000	0.936141000
C	-2.219052000	-0.425853000	-0.457788000
C	-0.933045000	-1.129229000	-0.595611000
N	-0.129614000	-0.736711000	0.500969000
H	-3.008332000	-0.067070000	1.648919000
O	-0.354379000	0.400473000	2.505888000
O	-0.531241000	-1.823670000	-1.514872000
C	1.286167000	-0.608211000	0.331850000
C	2.133010000	-1.692417000	0.582636000
C	1.737606000	0.626636000	-0.166888000
C	3.499670000	-1.516446000	0.335162000
C	3.111571000	0.759206000	-0.401308000
C	3.983816000	-0.302018000	-0.152308000
H	4.184209000	-2.339629000	0.521720000
H	3.499210000	1.699950000	-0.783389000
H	5.046828000	-0.181893000	-0.342547000
C	0.794919000	1.800195000	-0.397710000
H	1.414382000	2.641598000	-0.721987000
H	0.376658000	2.110457000	0.566726000
C	-0.354365000	1.653557000	-1.448160000
H	-0.420822000	2.619987000	-1.965680000
H	-0.062217000	0.931248000	-2.221274000
C	-1.790816000	1.347609000	-1.010590000
H	-2.487549000	1.580328000	-1.816721000
C	-2.309042000	1.694263000	0.408640000
H	-1.735421000	2.432527000	0.978233000
H	-3.347050000	2.035559000	0.367369000
C	-3.450544000	-0.992529000	-1.104505000

H	-3.806335000	-1.872664000	-0.553119000
H	-3.231960000	-1.299803000	-2.131757000
H	-4.261102000	-0.257274000	-1.123242000
C	1.569876000	-2.998256000	1.085120000
H	2.364688000	-3.727069000	1.267162000
H	0.872216000	-3.421233000	0.353292000
H	1.011981000	-2.855700000	2.017839000

C2-C3 distance: 1.8

C	-0.840257000	-0.035649000	1.476887000
C	-2.234842000	0.235785000	0.939302000
C	-2.202346000	-0.376459000	-0.479831000
C	-0.924966000	-1.113842000	-0.605458000
N	-0.128923000	-0.744479000	0.500913000
H	-3.012582000	-0.087828000	1.636134000
O	-0.358100000	0.366157000	2.519962000
O	-0.529458000	-1.808615000	-1.525111000
C	1.287463000	-0.615302000	0.334079000
C	2.137337000	-1.694636000	0.593416000
C	1.732621000	0.617166000	-0.175823000
C	3.502979000	-1.515913000	0.342217000
C	3.105626000	0.752164000	-0.414413000
C	3.981647000	-0.304228000	-0.157647000
H	4.190885000	-2.334829000	0.535019000
H	3.489685000	1.690888000	-0.804999000
H	5.043873000	-0.182328000	-0.351127000
C	0.784859000	1.786921000	-0.408632000
H	1.401181000	2.626970000	-0.742487000
H	0.374899000	2.102690000	0.557812000
C	-0.375468000	1.638915000	-1.447993000
H	-0.456579000	2.611376000	-1.949927000
H	-0.081902000	0.929100000	-2.231723000
C	-1.810060000	1.308922000	-0.997979000
H	-2.504189000	1.563879000	-1.801036000
C	-2.308406000	1.696397000	0.420207000
H	-1.719920000	2.432858000	0.975677000
H	-3.344584000	2.043798000	0.391135000
C	-3.433467000	-0.958512000	-1.123046000
H	-3.762327000	-1.857713000	-0.587561000
H	-3.222588000	-1.236276000	-2.160416000
H	-4.258039000	-0.238773000	-1.114868000
C	1.578027000	-2.997192000	1.108349000
H	2.374582000	-3.722883000	1.295129000
H	0.879507000	-3.428526000	0.382157000
H	1.021902000	-2.847247000	2.040957000

C2-C3 distance: 1.7

C	-0.841283000	-0.048394000	1.482045000
C	-2.232155000	0.234236000	0.942349000
C	-2.186119000	-0.326243000	-0.499782000
C	-0.918094000	-1.097183000	-0.615410000
N	-0.128553000	-0.751886000	0.500790000
H	-3.016059000	-0.106215000	1.623462000
O	-0.361308000	0.334380000	2.532637000
O	-0.529463000	-1.793076000	-1.535382000
C	1.288459000	-0.622293000	0.335986000
C	2.141261000	-1.697036000	0.602945000
C	1.727950000	0.608159000	-0.183475000
C	3.506024000	-1.515402000	0.348894000
C	3.100115000	0.745779000	-0.425285000
C	3.979701000	-0.306015000	-0.161464000
H	4.197115000	-2.330299000	0.547233000
H	3.480802000	1.682820000	-0.823152000
H	5.041259000	-0.182229000	-0.357402000
C	0.775454000	1.774206000	-0.418661000
H	1.388444000	2.612547000	-0.762965000
H	0.373809000	2.096382000	0.549414000
C	-0.395536000	1.623577000	-1.446827000
H	-0.491111000	2.600962000	-1.934615000
H	-0.100819000	0.925543000	-2.240415000
C	-1.828288000	1.269958000	-0.985280000
H	-2.517730000	1.545832000	-1.787006000
C	-2.308645000	1.698836000	0.429692000
H	-1.707262000	2.434821000	0.970778000
H	-3.343428000	2.050360000	0.410886000
C	-3.416626000	-0.925737000	-1.138629000
H	-3.718431000	-1.842164000	-0.618178000
H	-3.213908000	-1.175890000	-2.184811000
H	-4.255025000	-0.222731000	-1.105274000
C	1.585736000	-2.996890000	1.128511000
H	2.384059000	-3.719693000	1.318859000
H	0.886202000	-3.435427000	0.407554000
H	1.031525000	-2.840838000	2.061250000

C2-C3 distance: 1.6

C	-0.842532000	-0.060811000	1.486240000
C	-2.229804000	0.232385000	0.944786000
C	-2.170449000	-0.275128000	-0.519073000
C	-0.911930000	-1.078141000	-0.626903000
N	-0.128703000	-0.759005000	0.500093000
H	-3.019704000	-0.124314000	1.609851000
O	-0.365126000	0.303854000	2.543973000

O	-0.530025000	-1.775020000	-1.547421000
C	1.289023000	-0.629133000	0.337422000
C	2.144603000	-1.699350000	0.612198000
C	1.723608000	0.599141000	-0.191054000
C	3.508549000	-1.515321000	0.355152000
C	3.094877000	0.738851000	-0.436407000
C	3.977667000	-0.308637000	-0.165931000
H	4.202537000	-2.326361000	0.559109000
H	3.472423000	1.674063000	-0.841514000
H	5.038549000	-0.183435000	-0.364619000
C	0.767097000	1.762102000	-0.427951000
H	1.376955000	2.598170000	-0.783362000
H	0.374562000	2.091176000	0.541840000
C	-0.414702000	1.609076000	-1.444143000
H	-0.525272000	2.590957000	-1.917841000
H	-0.119774000	0.923105000	-2.247983000
C	-1.845416000	1.231588000	-0.971292000
H	-2.528235000	1.527887000	-1.773150000
C	-2.309544000	1.701204000	0.438521000
H	-1.696378000	2.436676000	0.965993000
H	-3.343067000	2.056009000	0.428342000
C	-3.399579000	-0.894709000	-1.153136000
H	-3.670593000	-1.829334000	-0.649819000
H	-3.206823000	-1.114771000	-2.208164000
H	-4.253415000	-0.212160000	-1.091985000
C	1.592849000	-2.996169000	1.148981000
H	2.393037000	-3.715688000	1.343820000
H	0.892785000	-3.442551000	0.433311000
H	1.040021000	-2.833448000	2.081391000

UB3LYP-D3/6-31G*/PCM level in toluene solution

S0-D(C-N-C-C): -70 (degree)

C	-0.980349000	-0.688672000	1.639772000
C	-2.450187000	-0.791273000	1.405880000
C	-2.695029000	-0.752899000	0.089072000
C	-1.369238000	-0.645497000	-0.623578000
N	-0.382726000	-0.582802000	0.365967000
H	-3.153502000	-0.870541000	2.225192000
O	-0.382622000	-0.679551000	2.696369000
O	-1.186702000	-0.634530000	-1.825286000
C	1.023314000	-0.456543000	0.122223000
C	1.703348000	-1.552583000	-0.440154000
C	1.680504000	0.742480000	0.449868000
C	3.070755000	-1.417786000	-0.698093000
C	3.053378000	0.827743000	0.184311000

C	3.743533000	-0.236150000	-0.390063000
H	3.611278000	-2.252988000	-1.135635000
H	3.580295000	1.745449000	0.434563000
H	4.808261000	-0.149588000	-0.589088000
C	0.970660000	1.944398000	1.039456000
H	1.655863000	2.442526000	1.735603000
H	0.102941000	1.639390000	1.627421000
C	0.520292000	2.984204000	-0.021517000
H	0.091333000	3.848220000	0.501218000
H	1.412031000	3.338593000	-0.557952000
C	-0.471673000	2.428891000	-1.004224000
H	-0.098786000	1.653094000	-1.671015000
C	-1.756293000	2.782626000	-1.081031000
H	-2.182345000	3.544518000	-0.430195000
H	-2.427755000	2.323319000	-1.802264000
C	-3.967226000	-0.793124000	-0.681728000
H	-3.937230000	-1.595577000	-1.427676000
H	-4.099695000	0.144155000	-1.236029000
H	-4.829210000	-0.941516000	-0.026715000
C	0.980015000	-2.837063000	-0.762658000
H	1.689287000	-3.634166000	-1.002794000
H	0.311629000	-2.703688000	-1.620680000
H	0.364472000	-3.171456000	0.080388000

S0-D(C-N-C-C): 20 (degree)

C	-1.309150000	-0.851515000	-1.257614000
C	-2.728553000	-1.213280000	-1.097226000
C	-3.228289000	-0.522374000	-0.071713000
C	-2.104623000	0.242015000	0.555608000
N	-0.850609000	-0.137636000	-0.036242000
H	-3.226730000	-1.876663000	-1.792903000
O	-0.661866000	-1.040611000	-2.260743000
O	-2.262745000	0.941280000	1.534560000
C	0.307691000	0.709758000	-0.344488000
C	0.594155000	1.979436000	0.227762000
C	1.417678000	-0.028446000	-0.864676000
C	1.801524000	2.606224000	-0.128327000
C	2.570445000	0.657931000	-1.258732000
C	2.760455000	1.990173000	-0.920046000
H	1.974888000	3.616358000	0.231261000
H	3.366464000	0.102460000	-1.748284000
H	3.665374000	2.518058000	-1.207834000
C	1.553837000	-1.547662000	-0.810267000
H	1.753909000	-1.946486000	-1.810873000
H	0.644666000	-2.027978000	-0.454073000
C	2.689596000	-1.980757000	0.155719000

H	2.762785000	-3.075828000	0.132984000
H	3.650520000	-1.591011000	-0.206435000
C	2.457054000	-1.510729000	1.566236000
H	2.416757000	-0.429510000	1.702548000
C	2.277808000	-2.309597000	2.619292000
H	2.303817000	-3.394132000	2.524482000
H	2.100255000	-1.913885000	3.616204000
C	-4.600808000	-0.436700000	0.496070000
H	-4.934572000	0.606508000	0.528782000
H	-4.604659000	-0.797115000	1.531417000
H	-5.310525000	-1.024896000	-0.090416000
C	-0.358701000	2.842972000	1.031053000
H	0.088232000	3.829299000	1.186056000
H	-0.585197000	2.409307000	2.005548000
H	-1.315551000	2.988927000	0.522802000

S0-D(C-N-C-C): 110 (degree)

C	1.164171000	-0.471335000	1.247477000
C	2.613930000	-0.587174000	0.917786000
C	2.759737000	-0.752536000	-0.403710000
C	1.382934000	-0.746664000	-1.022326000
N	0.470106000	-0.559368000	0.023068000
H	3.376931000	-0.538540000	1.684301000
O	0.651178000	-0.340512000	2.340780000
O	1.109363000	-0.869300000	-2.199500000
C	-0.953985000	-0.500016000	-0.124257000
C	-1.720669000	-1.566456000	0.382046000
C	-1.543340000	0.605911000	-0.762529000
C	-3.111314000	-1.496099000	0.256690000
C	-2.939428000	0.626073000	-0.876977000
C	-3.719561000	-0.408346000	-0.367878000
H	-3.718711000	-2.309690000	0.644425000
H	-3.413108000	1.470805000	-1.371376000
H	-4.801229000	-0.372760000	-0.465211000
C	-0.749325000	1.785422000	-1.286127000
H	-1.239754000	2.156934000	-2.193754000
H	0.257680000	1.484731000	-1.581153000
C	-0.648675000	2.958440000	-0.274524000
H	-0.137714000	3.796681000	-0.764732000
H	-1.667205000	3.294769000	-0.033522000
C	0.071793000	2.579999000	0.988719000
H	-0.424030000	1.842230000	1.617491000
C	1.268980000	3.041141000	1.355906000
H	1.811476000	3.770641000	0.756391000
H	1.749466000	2.704873000	2.271059000
C	3.972976000	-0.918132000	-1.249758000

H	4.019333000	-0.126432000	-2.006928000
H	3.931335000	-1.868307000	-1.795430000
H	4.885687000	-0.891526000	-0.649443000
C	-1.068033000	-2.755460000	1.043508000
H	-1.783576000	-3.573206000	1.167536000
H	-0.679062000	-2.487490000	2.031998000
H	-0.223745000	-3.128242000	0.452363000

T1-D(C-N-C-C): -60 (degree)

C	-0.978555000	-0.421369000	1.729346000
C	-2.377251000	-0.638162000	1.520938000
C	-2.639127000	-0.822569000	0.087166000
C	-1.385428000	-0.803379000	-0.603101000
N	-0.394536000	-0.545581000	0.412550000
H	-3.090787000	-0.746989000	2.326451000
O	-0.328636000	-0.230696000	2.753273000
O	-1.135957000	-0.896928000	-1.805107000
C	0.986798000	-0.447215000	0.150041000
C	1.654008000	-1.581432000	-0.380425000
C	1.677064000	0.757056000	0.435684000
C	3.023242000	-1.481370000	-0.626353000
C	3.046588000	0.802131000	0.164028000
C	3.717836000	-0.300653000	-0.361595000
H	3.553106000	-2.345855000	-1.016682000
H	3.589756000	1.722752000	0.361067000
H	4.784439000	-0.243030000	-0.559896000
C	0.988305000	2.018974000	0.906470000
H	1.694584000	2.581669000	1.528009000
H	0.131714000	1.791311000	1.541095000
C	0.532847000	2.940767000	-0.259240000
H	0.137037000	3.867469000	0.174612000
H	1.419609000	3.212374000	-0.849811000
C	-0.496990000	2.309399000	-1.154265000
H	-0.171738000	1.444111000	-1.729885000
C	-1.766028000	2.708538000	-1.258612000
H	-2.148700000	3.560722000	-0.698950000
H	-2.468438000	2.194714000	-1.910094000
C	-3.953705000	-0.840038000	-0.588244000
H	-3.827786000	-1.044951000	-1.654437000
H	-4.465966000	0.129066000	-0.478203000
H	-4.620119000	-1.593473000	-0.145365000
C	0.928995000	-2.877298000	-0.636285000
H	1.639009000	-3.697246000	-0.774857000
H	0.307399000	-2.796281000	-1.534360000
H	0.263781000	-3.136578000	0.194797000

T1-D(C-N-C-C): 10 (degree)

C	-1.086019000	-0.599813000	-1.637836000
C	-2.460388000	-0.346881000	-1.592824000
C	-2.884261000	0.224422000	-0.382246000
C	-1.784119000	0.411481000	0.486642000
N	-0.553524000	-0.068811000	-0.181645000
H	-3.079026000	-0.548631000	-2.458551000
O	-0.322727000	-0.969370000	-2.511757000
O	-1.766752000	0.712712000	1.689300000
C	0.639578000	0.602794000	-0.279721000
C	0.966731000	1.841391000	0.400296000
C	1.760199000	-0.239573000	-0.701131000
C	2.270909000	2.311595000	0.307105000
C	3.029989000	0.319294000	-0.819409000
C	3.290807000	1.595901000	-0.334640000
H	2.499547000	3.283760000	0.733303000
H	3.844708000	-0.297043000	-1.188650000
H	4.289818000	2.017242000	-0.399773000
C	1.683355000	-1.745702000	-0.689523000
H	2.497995000	-2.142212000	-1.305497000
H	0.753228000	-2.130109000	-1.094405000
C	1.856304000	-2.315209000	0.760744000
H	1.926855000	-3.405495000	0.665168000
H	2.812360000	-1.957647000	1.165624000
C	0.730576000	-1.958885000	1.690481000
H	0.698414000	-0.935716000	2.060111000
C	-0.240982000	-2.799671000	2.059624000
H	-0.268498000	-3.830868000	1.711644000
H	-1.048593000	-2.478691000	2.711466000
C	-4.281573000	0.554849000	0.025076000
H	-4.289666000	0.957957000	1.041142000
H	-4.923315000	-0.336352000	0.001208000
H	-4.734888000	1.293246000	-0.649546000
C	-0.058608000	2.796536000	0.964818000
H	0.383237000	3.790376000	1.077485000
H	-0.438131000	2.455728000	1.929205000
H	-0.928545000	2.884212000	0.306511000

T1-D(C-N-C-C): 120 (degree)

C	1.414667000	-0.541794000	-1.120247000
C	2.710444000	-0.688277000	-0.528647000
C	2.553498000	-0.710858000	0.929818000
C	1.167653000	-0.644558000	1.265443000
N	0.490003000	-0.535650000	-0.007628000
O	1.073938000	-0.491679000	-2.300726000
O	0.593961000	-0.603288000	2.352236000

C	-0.909515000	-0.488225000	-0.147352000
C	-1.676504000	-1.578914000	0.342445000
C	-1.519056000	0.625701000	-0.779509000
C	-3.061382000	-1.528339000	0.185945000
C	-2.909834000	0.623508000	-0.903748000
C	-3.678335000	-0.438235000	-0.428447000
H	-3.661598000	-2.363304000	0.536627000
H	-3.395708000	1.476570000	-1.370117000
H	-4.758749000	-0.419271000	-0.540639000
C	-0.755282000	1.860732000	-1.202345000
H	-1.264069000	2.298138000	-2.069337000
H	0.254715000	1.612880000	-1.528093000
C	-0.685642000	2.941698000	-0.087620000
H	-0.214884000	3.837804000	-0.510771000
H	-1.713564000	3.215990000	0.190042000
C	0.067231000	2.493066000	1.133890000
H	-0.369673000	1.669814000	1.697493000
C	1.229813000	3.004653000	1.542603000
H	1.716409000	3.821441000	1.011544000
H	1.737531000	2.622747000	2.424607000
C	-1.030234000	-2.788251000	0.966064000
H	-1.728699000	-3.629124000	0.992178000
H	-0.710167000	-2.565438000	1.989457000
H	-0.138821000	-3.099851000	0.410617000
C	3.957405000	-0.888059000	-1.298023000
H	4.721727000	-0.153796000	-1.003719000
H	4.394170000	-1.879723000	-1.104523000
H	3.761648000	-0.793545000	-2.369005000
H	3.346946000	-0.665138000	1.663334000

S0-D(C-C-C-C): 110 (degree)

C	-0.982810000	-0.677472000	1.641716000
C	-2.452446000	-0.781078000	1.407334000
C	-2.696320000	-0.749883000	0.090166000
C	-1.370038000	-0.646043000	-0.622040000
N	-0.384260000	-0.577278000	0.367862000
H	-3.156361000	-0.855883000	2.226567000
O	-0.385825000	-0.663876000	2.698715000
O	-1.186771000	-0.640984000	-1.823655000
C	1.022335000	-0.457039000	0.124413000
C	1.698600000	-1.556201000	-0.436453000
C	1.683394000	0.740761000	0.448775000
C	3.066367000	-1.426117000	-0.695213000
C	3.056394000	0.821188000	0.182634000
C	3.743033000	-0.246039000	-0.389834000
H	3.604078000	-2.263908000	-1.131296000

H	3.586217000	1.737859000	0.430528000
H	4.807954000	-0.163238000	-0.589482000
C	0.977182000	1.946664000	1.034520000
H	1.664630000	2.446263000	1.727385000
H	0.109793000	1.646115000	1.625229000
C	0.527589000	2.983013000	-0.030219000
H	0.101039000	3.849990000	0.489591000
H	1.419399000	3.333468000	-0.569117000
C	-0.466700000	2.426048000	-1.009677000
H	-0.095986000	1.647526000	-1.674511000
C	-1.750914000	2.781397000	-1.085687000
H	-2.174883000	3.546011000	-0.436696000
H	-2.424101000	2.320865000	-1.804514000
C	-3.967946000	-0.794367000	-0.681305000
H	-3.937438000	-1.600965000	-1.422741000
H	-4.100079000	0.139782000	-1.240922000
H	-4.830392000	-0.939122000	-0.026081000
C	0.971947000	-2.839618000	-0.755732000
H	1.679416000	-3.640464000	-0.988645000
H	0.307878000	-2.708206000	-1.617379000
H	0.351418000	-3.167543000	0.086177000

S0-D(C-C-C-C): 40 (degree)

C	-0.993213000	-0.491792000	1.589977000
C	-2.443255000	-0.714817000	1.317060000
C	-2.632028000	-0.850752000	-0.002543000
C	-1.284715000	-0.740891000	-0.674746000
N	-0.347412000	-0.516996000	0.339553000
H	-3.176707000	-0.736200000	2.113301000
O	-0.447118000	-0.305883000	2.659308000
O	-1.047721000	-0.850743000	-1.860679000
C	1.063703000	-0.400909000	0.133072000
C	1.773676000	-1.557142000	-0.242721000
C	1.696810000	0.840472000	0.306749000
C	3.148394000	-1.444545000	-0.467980000
C	3.079121000	0.902898000	0.082471000
C	3.799513000	-0.222425000	-0.307625000
H	3.710969000	-2.326673000	-0.762263000
H	3.590566000	1.853106000	0.216246000
H	4.870357000	-0.150423000	-0.477870000
C	0.964297000	2.113529000	0.684906000
H	1.662129000	2.737672000	1.253781000
H	0.133348000	1.902666000	1.360863000
C	0.479372000	2.927973000	-0.545837000
H	0.510573000	3.995763000	-0.283760000
H	1.204001000	2.803420000	-1.358198000

C	-0.913190000	2.622999000	-1.059707000
H	-1.027482000	2.621560000	-2.143367000
C	-1.994254000	2.398655000	-0.310419000
H	-1.960302000	2.383359000	0.776664000
H	-2.968270000	2.223914000	-0.759520000
C	-3.865564000	-1.065541000	-0.806219000
H	-3.772548000	-1.972895000	-1.414367000
H	-4.007773000	-0.234127000	-1.507159000
H	-4.749855000	-1.149456000	-0.169694000
C	1.072906000	-2.883755000	-0.406195000
H	1.796963000	-3.697943000	-0.500734000
H	0.440676000	-2.883005000	-1.301261000
H	0.424521000	-3.102524000	0.449993000

S0-D(C-C-C-C): 0 (degree)

C	1.551164000	0.178407000	1.540644000
C	2.894595000	-0.392780000	1.228643000
C	3.007488000	-0.569997000	-0.095291000
C	1.715618000	-0.114888000	-0.732315000
N	0.891331000	0.331534000	0.303096000
H	3.617080000	-0.609794000	2.005290000
O	1.079005000	0.456202000	2.623485000
O	1.433997000	-0.135216000	-1.915151000
C	-0.438403000	0.837480000	0.142314000
C	-0.598162000	2.121765000	-0.407081000
C	-1.527767000	0.040923000	0.533412000
C	-1.897196000	2.613712000	-0.555180000
C	-2.810633000	0.580496000	0.380759000
C	-2.995126000	1.850872000	-0.158469000
H	-2.045619000	3.603472000	-0.978805000
H	-3.676614000	-0.002726000	0.677141000
H	-4.000098000	2.248389000	-0.272293000
C	-1.317322000	-1.341390000	1.125045000
H	-1.323029000	-1.254119000	2.219336000
H	-0.317858000	-1.701737000	0.862257000
C	-2.335739000	-2.414132000	0.710439000
H	-2.136409000	-3.315721000	1.308916000
H	-3.352597000	-2.113054000	1.000543000
C	-2.340370000	-2.807468000	-0.746151000
H	-3.077252000	-3.571600000	-1.000233000
C	-1.546528000	-2.343177000	-1.713167000
H	-0.798700000	-1.572313000	-1.551834000
H	-1.631092000	-2.716611000	-2.730643000
C	4.118098000	-1.107893000	-0.927338000
H	4.439324000	-0.361488000	-1.663540000
H	3.777610000	-1.980475000	-1.497355000

H	4.975132000	-1.395063000	-0.313204000
C	0.598488000	2.937348000	-0.830586000
H	0.302713000	3.955036000	-1.100453000
H	1.091072000	2.483791000	-1.698461000
H	1.343789000	2.999721000	-0.029069000

S0-D(C-C-C-C): -50 (degree)

C	-1.388045000	-0.390607000	1.595100000
C	-2.809456000	-0.032822000	1.314607000
C	-2.974844000	0.133323000	-0.004992000
C	-1.644764000	-0.122882000	-0.673238000
N	-0.733403000	-0.416475000	0.345193000
H	-3.540780000	0.063990000	2.107156000
O	-0.859693000	-0.611014000	2.665161000
O	-1.409849000	-0.096862000	-1.865289000
C	0.649357000	-0.731968000	0.154389000
C	0.974914000	-1.964320000	-0.444046000
C	1.632267000	0.183513000	0.565740000
C	2.325308000	-2.266225000	-0.635771000
C	2.974250000	-0.172027000	0.373051000
C	3.320594000	-1.378728000	-0.226224000
H	2.596365000	-3.210907000	-1.099686000
H	3.753809000	0.512771000	0.696618000
H	4.367205000	-1.633011000	-0.370219000
C	1.304114000	1.514779000	1.213799000
H	1.751132000	1.518926000	2.216236000
H	0.227466000	1.622079000	1.357130000
C	1.817363000	2.762847000	0.453897000
H	1.764586000	3.610966000	1.146882000
H	2.884400000	2.638119000	0.222736000
C	1.057818000	3.124123000	-0.808028000
H	0.774468000	4.174117000	-0.894250000
C	0.725050000	2.300354000	-1.804375000
H	0.965288000	1.242696000	-1.802098000
H	0.174371000	2.661707000	-2.669302000
C	-4.171984000	0.496223000	-0.811278000
H	-4.379490000	-0.281282000	-1.555939000
H	-3.986994000	1.421055000	-1.370679000
H	-5.053783000	0.631617000	-0.180225000
C	-0.101284000	-2.931151000	-0.872975000
H	0.329911000	-3.898759000	-1.144811000
H	-0.649458000	-2.545190000	-1.739741000
H	-0.832291000	-3.097161000	-0.073057000

S0-D(C-C-C-C): -110 (degree)

C	-1.224914000	-0.464715000	1.639971000
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C	-2.685015000	-0.311936000	1.374440000
C	-2.890119000	-0.232613000	0.052852000
C	-1.548459000	-0.347424000	-0.631132000
N	-0.585693000	-0.442997000	0.381588000
H	-3.409950000	-0.279111000	2.178035000
O	-0.663419000	-0.576938000	2.710576000
O	-1.348211000	-0.375552000	-1.828317000
C	0.824395000	-0.589626000	0.174501000
C	1.291093000	-1.769728000	-0.435981000
C	1.698932000	0.428402000	0.593797000
C	2.665597000	-1.899045000	-0.656503000
C	3.068897000	0.247525000	0.363909000
C	3.551416000	-0.897589000	-0.262949000
H	3.041564000	-2.801973000	-1.130581000
H	3.760676000	1.023357000	0.683425000
H	4.617980000	-1.016898000	-0.433439000
C	1.239624000	1.716871000	1.243497000
H	1.976321000	2.000442000	2.004613000
H	0.295111000	1.581053000	1.774211000
C	1.103141000	2.891893000	0.238955000
H	0.935760000	3.810902000	0.818046000
H	2.052525000	3.015669000	-0.296967000
C	-0.017297000	2.691557000	-0.741770000
H	-1.024869000	2.720624000	-0.321343000
C	0.141658000	2.424212000	-2.037933000
H	1.131435000	2.362578000	-2.486178000
H	-0.702496000	2.232466000	-2.693257000
C	-4.135809000	-0.074339000	-0.746051000
H	-4.243350000	-0.906913000	-1.451167000
H	-4.086853000	0.839606000	-1.350176000
H	-5.020188000	-0.030593000	-0.105740000
C	0.346176000	-2.872791000	-0.845899000
H	0.893744000	-3.798109000	-1.046404000
H	-0.206657000	-2.597880000	-1.750671000
H	-0.393750000	-3.078246000	-0.063835000

T1-D(C-C-C-C): 110 (degree)

C	-0.991937000	-0.371439000	1.731466000
C	-2.389474000	-0.589510000	1.523452000
C	-2.649818000	-0.800810000	0.095331000
C	-1.396921000	-0.796359000	-0.595113000
N	-0.404704000	-0.519288000	0.416327000
H	-3.103954000	-0.682380000	2.330116000
O	-0.342453000	-0.167590000	2.753191000
O	-1.146597000	-0.909173000	-1.795451000
C	0.977948000	-0.453282000	0.158990000

C	1.623813000	-1.601820000	-0.369609000
C	1.691815000	0.740322000	0.436808000
C	2.994733000	-1.528091000	-0.614789000
C	3.061913000	0.757780000	0.166591000
C	3.712046000	-0.360026000	-0.354055000
H	3.508543000	-2.404129000	-1.000780000
H	3.622205000	1.669127000	0.358418000
H	4.779609000	-0.323896000	-0.552231000
C	1.025502000	2.020082000	0.890537000
H	1.742547000	2.580410000	1.501779000
H	0.166565000	1.816248000	1.529863000
C	0.583501000	2.931529000	-0.288903000
H	0.201349000	3.869998000	0.131624000
H	1.474456000	3.181461000	-0.882734000
C	-0.455179000	2.303203000	-1.175818000
H	-0.143085000	1.425005000	-1.739110000
C	-1.717446000	2.721141000	-1.288240000
H	-2.087440000	3.586982000	-0.741179000
H	-2.426988000	2.209108000	-1.933347000
C	-3.964530000	-0.836076000	-0.580033000
H	-3.837428000	-1.056400000	-1.642991000
H	-4.483015000	0.131061000	-0.484267000
H	-4.626196000	-1.587254000	-0.126250000
C	0.879290000	-2.888326000	-0.616281000
H	1.576888000	-3.722911000	-0.727977000
H	0.274725000	-2.811894000	-1.526116000
H	0.195009000	-3.121330000	0.206976000

T1-D(C-C-C-C): 40 (degree)

C	-1.109814000	-0.067492000	1.680299000
C	-2.516294000	-0.133392000	1.451679000
C	-2.783309000	-0.477821000	0.060698000
C	-1.537851000	-0.702954000	-0.603172000
N	-0.522346000	-0.432726000	0.400121000
H	-3.248245000	-0.041349000	2.242843000
O	-0.449813000	0.161765000	2.690345000
O	-1.290484000	-0.982223000	-1.774499000
C	0.853086000	-0.553791000	0.176528000
C	1.362182000	-1.811016000	-0.262342000
C	1.714948000	0.550302000	0.419535000
C	2.735555000	-1.929803000	-0.461060000
C	3.082182000	0.367393000	0.203614000
C	3.593818000	-0.852135000	-0.235318000
H	3.141167000	-2.887579000	-0.774684000
H	3.754347000	1.204795000	0.371884000
H	4.662489000	-0.967542000	-0.392922000

C	1.242309000	1.941797000	0.786796000
H	1.935323000	2.342159000	1.536215000
H	0.263946000	1.928677000	1.261819000
C	1.235001000	2.906529000	-0.426203000
H	1.168290000	3.933492000	-0.038471000
H	2.202661000	2.841853000	-0.937255000
C	0.119850000	2.683983000	-1.426928000
H	0.401095000	2.756329000	-2.477219000
C	-1.155062000	2.428323000	-1.129888000
H	-1.508807000	2.338850000	-0.105188000
H	-1.899182000	2.284316000	-1.907911000
C	-4.093070000	-0.467055000	-0.630229000
H	-3.980515000	-0.819635000	-1.658690000
H	-4.523286000	0.546062000	-0.654095000
H	-4.823374000	-1.100612000	-0.107261000
C	0.474574000	-3.015286000	-0.440793000
H	1.069552000	-3.932774000	-0.443803000
H	-0.077671000	-2.948911000	-1.383442000
H	-0.267612000	-3.090882000	0.361261000

T1-D(C-C-C-C): 0 (degree)

C	1.417344000	-0.231705000	1.617063000
C	2.752478000	-0.635924000	1.306409000
C	2.996920000	-0.485964000	-0.129510000
C	1.829498000	0.083293000	-0.730193000
N	0.886187000	0.242204000	0.351236000
H	3.481078000	-0.909914000	2.057434000
O	0.795103000	-0.188114000	2.673732000
O	1.567343000	0.323621000	-1.909500000
C	-0.398332000	0.786009000	0.214041000
C	-0.532027000	2.120659000	-0.255265000
C	-1.524259000	-0.004224000	0.565517000
C	-1.815463000	2.657096000	-0.330810000
C	-2.783498000	0.587405000	0.472970000
C	-2.931919000	1.903074000	0.034741000
H	-1.940519000	3.683653000	-0.663578000
H	-3.666305000	0.010305000	0.727318000
H	-3.923803000	2.342034000	-0.027060000
C	-1.375345000	-1.458179000	0.968663000
H	-1.422683000	-1.520516000	2.062443000
H	-0.379453000	-1.816525000	0.695544000
C	-2.407195000	-2.419316000	0.356945000
H	-2.263418000	-3.405754000	0.822495000
H	-3.427272000	-2.126995000	0.643954000
C	-2.352912000	-2.591669000	-1.141058000
H	-3.114721000	-3.264204000	-1.539451000

C	-1.484396000	-2.043334000	-1.993376000
H	-0.699522000	-1.354812000	-1.693159000
H	-1.537822000	-2.260386000	-3.057191000
C	4.172707000	-0.961236000	-0.892049000
H	4.076677000	-0.687052000	-1.945679000
H	4.280498000	-2.054433000	-0.821987000
H	5.102694000	-0.534085000	-0.489630000
C	0.667672000	2.960721000	-0.605520000
H	0.391103000	4.015348000	-0.687852000
H	1.097248000	2.633331000	-1.558170000
H	1.455702000	2.870284000	0.150655000

T1-D(C-C-C-C): -50 (degree)

C	-1.297016000	-0.031724000	1.690076000
C	-2.683806000	0.190759000	1.422861000
C	-2.937699000	0.070792000	-0.016990000
C	-1.715538000	-0.303035000	-0.661370000
N	-0.731278000	-0.351568000	0.393792000
H	-3.426379000	0.322532000	2.198226000
O	-0.652996000	-0.037289000	2.734540000
O	-1.460817000	-0.485819000	-1.851845000
C	0.614015000	-0.707573000	0.203504000
C	0.911308000	-1.991203000	-0.328980000
C	1.636728000	0.208321000	0.557566000
C	2.251726000	-2.337636000	-0.488366000
C	2.961771000	-0.197267000	0.383286000
C	3.272080000	-1.452636000	-0.134804000
H	2.499261000	-3.322111000	-0.875500000
H	3.761876000	0.488881000	0.646935000
H	4.310612000	-1.745717000	-0.260479000
C	1.363060000	1.615403000	1.047456000
H	1.846656000	1.724761000	2.026049000
H	0.299165000	1.779849000	1.210395000
C	1.886768000	2.739860000	0.116394000
H	1.924682000	3.659925000	0.711485000
H	2.927062000	2.530445000	-0.168853000
C	1.056702000	3.006730000	-1.123984000
H	0.853517000	4.059611000	-1.324625000
C	0.581534000	2.102117000	-1.983331000
H	0.729132000	1.033809000	-1.868670000
H	-0.003781000	2.406213000	-2.847508000
C	-4.188699000	0.397325000	-0.735182000
H	-4.077729000	0.188982000	-1.802224000
H	-4.456148000	1.457723000	-0.609391000
H	-5.035102000	-0.182080000	-0.338437000
C	-0.172150000	-2.984357000	-0.660268000

H	0.244067000	-3.990675000	-0.759120000
H	-0.666574000	-2.713791000	-1.599004000
H	-0.945580000	-3.007768000	0.115394000

T1-D(C-C-C-C): -110 (degree)

C	-1.145242000	-0.008099000	1.730622000
C	-2.548725000	-0.033884000	1.481680000
C	-2.804188000	-0.358637000	0.083672000
C	-1.556855000	-0.614706000	-0.562187000
N	-0.544985000	-0.359739000	0.452323000
H	-3.288726000	0.069330000	2.263883000
O	-0.499570000	0.181167000	2.758796000
O	-1.305749000	-0.911634000	-1.728982000
C	0.830508000	-0.517510000	0.240995000
C	1.308748000	-1.778544000	-0.218600000
C	1.720946000	0.561861000	0.501599000
C	2.677071000	-1.921344000	-0.438359000
C	3.079883000	0.357318000	0.256151000
C	3.559693000	-0.863646000	-0.214585000
H	3.058936000	-2.883240000	-0.768969000
H	3.771233000	1.177850000	0.429345000
H	4.622812000	-0.996830000	-0.394200000
C	1.275613000	1.945408000	0.915442000
H	2.081639000	2.394455000	1.507294000
H	0.404177000	1.905668000	1.568733000
C	0.987475000	2.885984000	-0.289960000
H	0.865321000	3.901245000	0.111566000
H	1.865320000	2.901467000	-0.948148000
C	-0.234120000	2.492071000	-1.069957000
H	-1.188678000	2.629748000	-0.558953000
C	-0.216020000	1.938797000	-2.283224000
H	0.719092000	1.759065000	-2.810273000
H	-1.123762000	1.619579000	-2.784723000
C	-4.107389000	-0.338052000	-0.619744000
H	-3.983745000	-0.670456000	-1.653595000
H	-4.543338000	0.672543000	-0.625943000
H	-4.839352000	-0.986570000	-0.117218000
C	0.398595000	-2.966528000	-0.395887000
H	0.975895000	-3.895306000	-0.383968000
H	-0.142591000	-2.898916000	-1.344686000
H	-0.352755000	-3.020653000	0.399135000

UB3LYP-D3/6-31G* level in vacuo

Minimum-energy path connecting the T₁/S₀ crossing point (A-DR1-T1S0) and its corresponding ground-state S0 product (A-S0-P)

C2-C3 distance: 3.0

C	-0.917355000	0.192953000	1.369187000
C	-2.327467000	0.263698000	0.810367000
C	-2.427659000	-0.974063000	0.009242000
C	-1.079005000	-1.375630000	-0.346572000
N	-0.194782000	-0.596732000	0.466319000
H	-3.089812000	0.413116000	1.578414000
O	-0.466095000	0.785188000	2.326459000
O	-0.721297000	-2.181131000	-1.194206000
C	1.214772000	-0.505378000	0.251216000
C	1.993352000	-1.672752000	0.355806000
C	1.777959000	0.744870000	-0.095695000
C	3.354779000	-1.588242000	0.045515000
C	3.146778000	0.771527000	-0.390470000
C	3.927984000	-0.380357000	-0.338764000
H	3.967815000	-2.482832000	0.119496000
H	3.605941000	1.719662000	-0.658858000
H	4.986990000	-0.329888000	-0.577128000
C	1.022763000	2.064976000	-0.097688000
H	1.770402000	2.861494000	-0.184868000
H	0.543003000	2.215964000	0.872571000
C	-0.022496000	2.335595000	-1.230028000
H	-0.269455000	3.406214000	-1.142094000
H	0.474762000	2.207419000	-2.198096000
C	-1.285572000	1.535978000	-1.217137000
H	-1.407587000	0.774095000	-1.983405000
C	-2.309357000	1.580812000	-0.143499000
H	-2.166095000	2.441332000	0.519839000
H	-3.323297000	1.636639000	-0.562838000
C	-3.642611000	-1.544282000	-0.619628000
H	-4.385694000	-1.844667000	0.131857000
H	-3.380229000	-2.413098000	-1.229523000
H	-4.137905000	-0.804111000	-1.268426000
C	1.402895000	-2.984991000	0.810050000
H	2.184457000	-3.642825000	1.202398000
H	0.900364000	-3.493779000	-0.018342000
H	0.656824000	-2.834016000	1.597806000

C2-C3 distance: 2.9

C	-0.905384000	0.172027000	1.394267000
C	-2.317386000	0.260228000	0.837156000
C	-2.412008000	-0.940763000	-0.023919000
C	-1.063457000	-1.357628000	-0.359526000
N	-0.184830000	-0.612509000	0.486866000
H	-3.078172000	0.364957000	1.614787000

O	-0.451160000	0.755332000	2.355967000
O	-0.702646000	-2.155000000	-1.213530000
C	1.224118000	-0.514139000	0.268862000
C	2.010765000	-1.674121000	0.380833000
C	1.771760000	0.736196000	-0.096330000
C	3.371500000	-1.579959000	0.070491000
C	3.140210000	0.774154000	-0.391396000
C	3.932711000	-0.369510000	-0.324525000
H	3.992787000	-2.468308000	0.150143000
H	3.589335000	1.722982000	-0.673989000
H	4.991255000	-0.311176000	-0.563236000
C	0.994289000	2.043306000	-0.125915000
H	1.729794000	2.849058000	-0.229329000
H	0.512215000	2.208432000	0.841385000
C	-0.052746000	2.268028000	-1.265225000
H	-0.274969000	3.348435000	-1.240037000
H	0.433095000	2.074749000	-2.228175000
C	-1.339179000	1.505644000	-1.198308000
H	-1.541161000	0.780269000	-1.981975000
C	-2.310524000	1.584890000	-0.073615000
H	-2.101661000	2.432489000	0.589325000
H	-3.338690000	1.691680000	-0.446787000
C	-3.622861000	-1.479806000	-0.686101000
H	-4.375261000	-1.802229000	0.047055000
H	-3.359267000	-2.327875000	-1.323986000
H	-4.107549000	-0.713483000	-1.311739000
C	1.422620000	-2.987083000	0.835066000
H	2.207631000	-3.656901000	1.199010000
H	0.895146000	-3.480581000	0.012651000
H	0.697751000	-2.839027000	1.643052000

C2-C3 distance: 2.8

C	-0.886648000	0.138078000	1.423775000
C	-2.301677000	0.246530000	0.872931000
C	-2.389410000	-0.908185000	-0.062573000
C	-1.040053000	-1.336853000	-0.380838000
N	-0.169563000	-0.639348000	0.510537000
H	-3.057200000	0.290129000	1.662402000
O	-0.427188000	0.713926000	2.388374000
O	-0.673822000	-2.119452000	-1.245906000
C	1.238298000	-0.530119000	0.290529000
C	2.038203000	-1.677720000	0.417358000
C	1.763741000	0.719884000	-0.099106000
C	3.398531000	-1.568012000	0.110995000
C	3.132345000	0.776281000	-0.390100000
C	3.942223000	-0.353805000	-0.298562000

H	4.032706000	-2.446083000	0.201936000
H	3.566920000	1.726201000	-0.691318000
H	5.000689000	-0.282953000	-0.534320000
C	0.953529000	2.006294000	-0.166863000
H	1.671544000	2.823782000	-0.295145000
H	0.471535000	2.191187000	0.797533000
C	-0.093890000	2.165067000	-1.313698000
H	-0.261620000	3.254300000	-1.401771000
H	0.368860000	1.856947000	-2.258283000
C	-1.428158000	1.495661000	-1.175664000
H	-1.799877000	0.926439000	-2.023358000
C	-2.314193000	1.592257000	0.027633000
H	-2.019733000	2.410613000	0.695091000
H	-3.355884000	1.765441000	-0.275043000
C	-3.592043000	-1.398021000	-0.774577000
H	-4.370132000	-1.727613000	-0.072110000
H	-3.328441000	-2.229187000	-1.434296000
H	-4.042950000	-0.600321000	-1.385863000
C	1.454433000	-2.991060000	0.874811000
H	2.244754000	-3.681432000	1.184582000
H	0.878788000	-3.457865000	0.068873000
H	0.773453000	-2.848230000	1.721309000

C2-C3 distance: 2.7

C	-0.829339000	0.084890000	1.422682000
C	-2.253368000	0.245623000	0.907004000
C	-2.340297000	-0.781696000	-0.193300000
C	-1.001608000	-1.240861000	-0.501532000
N	-0.132803000	-0.658815000	0.470382000
H	-2.982230000	0.136803000	1.717488000
O	-0.347601000	0.614668000	2.403504000
O	-0.623228000	-1.954311000	-1.421743000
C	1.280577000	-0.545421000	0.290228000
C	2.100762000	-1.667590000	0.462903000
C	1.782010000	0.713562000	-0.089367000
C	3.474915000	-1.507326000	0.254092000
C	3.162273000	0.829917000	-0.279641000
C	4.002670000	-0.270111000	-0.109792000
H	4.132858000	-2.363030000	0.382029000
H	3.579248000	1.790678000	-0.571136000
H	5.072774000	-0.162327000	-0.265632000
C	0.868266000	1.909857000	-0.301654000
H	1.500059000	2.768008000	-0.550868000
H	0.386169000	2.171701000	0.645572000
C	-0.193863000	1.737755000	-1.433641000
H	-0.060419000	2.557528000	-2.157248000

H	0.050128000	0.833152000	-2.016336000
C	-1.659359000	1.691352000	-1.092295000
H	-2.322878000	1.734307000	-1.953342000
C	-2.329008000	1.672320000	0.266437000
H	-1.901677000	2.400122000	0.970381000
H	-3.385141000	1.933501000	0.138663000
C	-3.558771000	-1.244835000	-0.898158000
H	-4.200217000	-1.841003000	-0.230777000
H	-3.282879000	-1.865584000	-1.755296000
H	-4.169567000	-0.401519000	-1.247330000
C	1.509314000	-2.998370000	0.852892000
H	2.293545000	-3.730060000	1.068389000
H	0.881472000	-3.387214000	0.043606000
H	0.875284000	-2.902914000	1.742112000

C2-C3 distance: 2.6

C	-0.827661000	0.081698000	1.429214000
C	-2.251577000	0.251828000	0.912863000
C	-2.330225000	-0.744817000	-0.225441000
C	-0.996231000	-1.224633000	-0.512770000
N	-0.132539000	-0.663452000	0.478709000
H	-2.981180000	0.117730000	1.719186000
O	-0.345391000	0.610206000	2.411128000
O	-0.609295000	-1.933745000	-1.432948000
C	1.280629000	-0.549893000	0.298111000
C	2.102163000	-1.669760000	0.476175000
C	1.779194000	0.705907000	-0.093850000
C	3.475720000	-1.509454000	0.263600000
C	3.158859000	0.823161000	-0.288407000
C	4.001090000	-0.274304000	-0.110887000
H	4.134972000	-2.363520000	0.395745000
H	3.574090000	1.781935000	-0.588917000
H	5.070713000	-0.166328000	-0.269871000
C	0.863179000	1.899682000	-0.311061000
H	1.494026000	2.755303000	-0.571188000
H	0.386914000	2.169316000	0.637100000
C	-0.206411000	1.726246000	-1.435889000
H	-0.101881000	2.567816000	-2.139571000
H	0.050947000	0.842470000	-2.043481000
C	-1.668053000	1.637263000	-1.086515000
H	-2.337398000	1.701371000	-1.941632000
C	-2.327115000	1.674597000	0.284018000
H	-1.882566000	2.412789000	0.965866000
H	-3.380663000	1.947225000	0.158612000
C	-3.551352000	-1.222693000	-0.917980000
H	-4.139832000	-1.887939000	-0.266453000

H	-3.276791000	-1.783656000	-1.815983000
H	-4.212541000	-0.392965000	-1.198908000
C	1.510608000	-2.998489000	0.872786000
H	2.294437000	-3.733414000	1.078602000
H	0.872113000	-3.383768000	0.070123000
H	0.887119000	-2.900954000	1.769187000

C2-C3 distance: 2.5

C	-0.826707000	0.076694000	1.434420000
C	-2.249551000	0.257560000	0.916167000
C	-2.317513000	-0.702152000	-0.264161000
C	-0.988747000	-1.208358000	-0.526107000
N	-0.132134000	-0.669931000	0.485800000
H	-2.981119000	0.095570000	1.715849000
O	-0.344336000	0.602063000	2.418500000
O	-0.593263000	-1.913734000	-1.445218000
C	1.280957000	-0.555595000	0.305644000
C	2.104453000	-1.672448000	0.490079000
C	1.775834000	0.696924000	-0.099766000
C	3.477320000	-1.511392000	0.273762000
C	3.154763000	0.815724000	-0.298766000
C	3.999508000	-0.278434000	-0.112536000
H	4.138480000	-2.363186000	0.411007000
H	3.567621000	1.772445000	-0.609034000
H	5.068585000	-0.169850000	-0.274735000
C	0.856554000	1.887524000	-0.321239000
H	1.485424000	2.741015000	-0.593024000
H	0.387412000	2.164607000	0.628468000
C	-0.222391000	1.712395000	-1.437034000
H	-0.143371000	2.570888000	-2.123790000
H	0.041822000	0.846049000	-2.065562000
C	-1.680164000	1.593993000	-1.077865000
H	-2.355241000	1.689218000	-1.925639000
C	-2.325561000	1.680710000	0.304537000
H	-1.863434000	2.425049000	0.967514000
H	-3.376676000	1.964706000	0.184270000
C	-3.541089000	-1.201661000	-0.940178000
H	-4.080288000	-1.916972000	-0.298568000
H	-3.271897000	-1.718194000	-1.866118000
H	-4.243935000	-0.391296000	-1.169439000
C	1.513662000	-2.999172000	0.894385000
H	2.297436000	-3.736688000	1.091014000
H	0.864833000	-3.381956000	0.098810000
H	0.900823000	-2.899358000	1.797829000

C2-C3 distance: 2.4

C	-0.826803000	0.070157000	1.439025000
C	-2.247688000	0.263151000	0.918215000
C	-2.303563000	-0.655323000	-0.306141000
C	-0.979966000	-1.192883000	-0.539690000
N	-0.132214000	-0.678258000	0.491876000
H	-2.981772000	0.072928000	1.709608000
O	-0.344024000	0.590227000	2.426035000
O	-0.577108000	-1.894829000	-1.457254000
C	1.281039000	-0.562586000	0.312811000
C	2.107049000	-1.675807000	0.504354000
C	1.771372000	0.686739000	-0.106522000
C	3.479129000	-1.513371000	0.284129000
C	3.149506000	0.807488000	-0.310241000
C	3.997369000	-0.282711000	-0.114864000
H	4.142678000	-2.362381000	0.426993000
H	3.559460000	1.762087000	-0.630784000
H	5.065804000	-0.173020000	-0.280501000
C	0.848680000	1.874091000	-0.331764000
H	1.475549000	2.725561000	-0.614408000
H	0.386712000	2.158104000	0.619540000
C	-0.239783000	1.698800000	-1.438507000
H	-0.184340000	2.573368000	-2.107149000
H	0.028565000	0.849573000	-2.087298000
C	-1.694498000	1.556772000	-1.069470000
H	-2.373964000	1.690551000	-1.908688000
C	-2.323805000	1.689274000	0.325619000
H	-1.844504000	2.437325000	0.971709000
H	-3.372676000	1.984037000	0.212295000
C	-3.528748000	-1.181876000	-0.962823000
H	-4.018546000	-1.937714000	-0.327898000
H	-3.267751000	-1.661511000	-1.910758000
H	-4.268483000	-0.394153000	-1.147908000
C	1.518030000	-3.000615000	0.917353000
H	2.302225000	-3.739828000	1.105824000
H	0.859617000	-3.382353000	0.129148000
H	0.915526000	-2.898257000	1.827409000

C2-C3 distance: 2.3

C	-0.828102000	0.061783000	1.443789000
C	-2.245965000	0.267778000	0.920158000
C	-2.288735000	-0.606589000	-0.348456000
C	-0.969994000	-1.180341000	-0.551603000
N	-0.132860000	-0.688864000	0.497437000
H	-2.983358000	0.050631000	1.701667000
O	-0.344219000	0.573974000	2.434355000
O	-0.562433000	-1.880548000	-1.466409000

C	1.280735000	-0.571188000	0.319692000
C	2.110072000	-1.679994000	0.519019000
C	1.765392000	0.675076000	-0.114337000
C	3.481117000	-1.515529000	0.293820000
C	3.142526000	0.798090000	-0.323876000
C	3.994301000	-0.287391000	-0.119390000
H	4.147689000	-2.361124000	0.442690000
H	3.548775000	1.750506000	-0.655450000
H	5.061871000	-0.176109000	-0.289410000
C	0.839477000	1.859537000	-0.342080000
H	1.465102000	2.709046000	-0.633420000
H	0.384384000	2.149212000	0.610921000
C	-0.258193000	1.688186000	-1.440708000
H	-0.226318000	2.582141000	-2.084725000
H	0.014871000	0.860400000	-2.113437000
C	-1.710443000	1.521534000	-1.062640000
H	-2.392353000	1.696243000	-1.892667000
C	-2.321821000	1.698364000	0.345436000
H	-1.826808000	2.449156000	0.975998000
H	-3.368853000	2.002388000	0.240280000
C	-3.514657000	-1.161075000	-0.986003000
H	-3.958323000	-1.948196000	-0.355551000
H	-3.263554000	-1.610638000	-1.951176000
H	-4.284365000	-0.395288000	-1.133871000
C	1.524333000	-3.002843000	0.942804000
H	2.309801000	-3.742066000	1.125877000
H	0.858068000	-3.386631000	0.162174000
H	0.930908000	-2.896869000	1.858368000

C2-C3 distance: 2.2

C	-0.829271000	0.049918000	1.453497000
C	-2.244583000	0.265124000	0.926465000
C	-2.272669000	-0.565581000	-0.371675000
C	-0.960941000	-1.176569000	-0.551641000
N	-0.131612000	-0.701786000	0.506426000
H	-2.988476000	0.026993000	1.695154000
O	-0.345940000	0.550742000	2.449302000
O	-0.559008000	-1.883405000	-1.461559000
C	1.282009000	-0.580197000	0.326793000
C	2.116378000	-1.683458000	0.533074000
C	1.757649000	0.663733000	-0.123154000
C	3.485503000	-1.515495000	0.299134000
C	3.133224000	0.789993000	-0.341799000
C	3.990772000	-0.289608000	-0.130388000
H	4.156657000	-2.356504000	0.453161000
H	3.533731000	1.740572000	-0.685414000

H	5.056872000	-0.175521000	-0.307636000
C	0.827348000	1.845083000	-0.351564000
H	1.451874000	2.693210000	-0.649377000
H	0.379752000	2.138911000	0.603871000
C	-0.279841000	1.678848000	-1.442170000
H	-0.273765000	2.594493000	-2.054917000
H	0.002667000	0.877361000	-2.140252000
C	-1.729517000	1.474551000	-1.051840000
H	-2.415518000	1.655889000	-1.877898000
C	-2.320691000	1.699290000	0.359378000
H	-1.806775000	2.449086000	0.974182000
H	-3.366045000	2.012770000	0.267674000
C	-3.498574000	-1.118979000	-1.016157000
H	-3.933551000	-1.920237000	-0.398877000
H	-3.247771000	-1.548314000	-1.990574000
H	-4.271936000	-0.354243000	-1.148118000
C	1.537252000	-3.004407000	0.971695000
H	2.325877000	-3.740823000	1.152447000
H	0.864722000	-3.395433000	0.200008000
H	0.952267000	-2.893250000	1.892025000

C2-C3 distance: 2.1

C	-0.830533000	0.038689000	1.462236000
C	-2.243116000	0.263006000	0.931612000
C	-2.255527000	-0.522060000	-0.395256000
C	-0.951886000	-1.170111000	-0.553660000
N	-0.130363000	-0.712880000	0.513617000
H	-2.993505000	0.004157000	1.686623000
O	-0.348251000	0.526798000	2.464020000
O	-0.555668000	-1.882538000	-1.459495000
C	1.283434000	-0.588487000	0.333144000
C	2.122137000	-1.686669000	0.546212000
C	1.750695000	0.653012000	-0.131570000
C	3.489559000	-1.515525000	0.304764000
C	3.124820000	0.782182000	-0.358147000
C	3.987565000	-0.291926000	-0.139746000
H	4.164894000	-2.352228000	0.463785000
H	3.520161000	1.730801000	-0.712934000
H	5.052332000	-0.175360000	-0.323257000
C	0.815556000	1.830819000	-0.361025000
H	1.438132000	2.677887000	-0.666009000
H	0.375360000	2.128850000	0.596712000
C	-0.301449000	1.667743000	-1.443009000
H	-0.317706000	2.599832000	-2.028928000
H	-0.011976000	0.888469000	-2.161566000
C	-1.748956000	1.430569000	-1.040848000

H	-2.437381000	1.624405000	-1.863031000
C	-2.320152000	1.701171000	0.372416000
H	-1.788394000	2.449798000	0.971777000
H	-3.363756000	2.023356000	0.293918000
C	-3.481435000	-1.079637000	-1.043164000
H	-3.902352000	-1.896603000	-0.438283000
H	-3.232243000	-1.487356000	-2.027254000
H	-4.262139000	-0.319703000	-1.156971000
C	1.548659000	-3.005579000	0.998210000
H	2.339832000	-3.739723000	1.177023000
H	0.870489000	-3.402987000	0.234686000
H	0.971235000	-2.889419000	1.922674000

C2-C3 distance: 2.0

C	-0.831810000	0.026505000	1.469996000
C	-2.241229000	0.260347000	0.936081000
C	-2.237710000	-0.476312000	-0.419082000
C	-0.942716000	-1.159296000	-0.559430000
N	-0.129145000	-0.722193000	0.517815000
H	-2.998316000	-0.019190000	1.676242000
O	-0.350756000	0.499311000	2.478900000
O	-0.552147000	-1.874802000	-1.463287000
C	1.284991000	-0.596042000	0.337910000
C	2.127261000	-1.689407000	0.558959000
C	1.744694000	0.642698000	-0.140887000
C	3.493229000	-1.515659000	0.311415000
C	3.117575000	0.774211000	-0.374123000
C	3.984765000	-0.294755000	-0.147802000
H	4.172349000	-2.348121000	0.476381000
H	3.508501000	1.720557000	-0.739662000
H	5.048408000	-0.176341000	-0.336530000
C	0.804574000	1.816902000	-0.371446000
H	1.424764000	2.662776000	-0.684709000
H	0.372583000	2.119554000	0.588786000
C	-0.323389000	1.655816000	-1.443376000
H	-0.359451000	2.600412000	-2.006308000
H	-0.029630000	0.895233000	-2.179054000
C	-1.768673000	1.389416000	-1.028685000
H	-2.458337000	1.599404000	-1.846932000
C	-2.319811000	1.702884000	0.385572000
H	-1.771173000	2.449870000	0.970180000
H	-3.361631000	2.033009000	0.320310000
C	-3.463414000	-1.042686000	-1.067593000
H	-3.864076000	-1.878272000	-0.476104000
H	-3.217576000	-1.425319000	-2.062596000
H	-4.255669000	-0.291903000	-1.159127000

C	1.558072000	-3.005497000	1.024321000
H	2.350956000	-3.737789000	1.203103000
H	0.875272000	-3.409424000	0.268285000
H	0.986736000	-2.883136000	1.951753000

C2-C3 distance: 1.9

C	-0.833264000	0.012607000	1.476903000
C	-2.239137000	0.256979000	0.939615000
C	-2.220133000	-0.429214000	-0.442854000
C	-0.934190000	-1.145751000	-0.568308000
N	-0.128187000	-0.730894000	0.519482000
H	-3.003138000	-0.042526000	1.664028000
O	-0.353949000	0.467547000	2.494066000
O	-0.549335000	-1.862580000	-1.471722000
C	1.286428000	-0.603317000	0.341218000
C	2.132129000	-1.691628000	0.571526000
C	1.739177000	0.632576000	-0.150745000
C	3.496835000	-1.515430000	0.318977000
C	3.110958000	0.766328000	-0.389598000
C	3.982318000	-0.297517000	-0.154819000
H	4.179593000	-2.343522000	0.490761000
H	3.497805000	1.710269000	-0.765523000
H	5.044981000	-0.177429000	-0.348011000
C	0.794192000	1.803169000	-0.382854000
H	1.411704000	2.647573000	-0.705427000
H	0.370864000	2.111198000	0.579769000
C	-0.345246000	1.642554000	-1.443653000
H	-0.399340000	2.596498000	-1.987210000
H	-0.049144000	0.897578000	-2.193554000
C	-1.788046000	1.349663000	-1.015426000
H	-2.477632000	1.578454000	-1.829850000
C	-2.318917000	1.704372000	0.398757000
H	-1.754050000	2.449025000	0.969374000
H	-3.358806000	2.042023000	0.346400000
C	-3.445897000	-1.006448000	-1.090219000
H	-3.819957000	-1.865132000	-0.516328000
H	-3.207007000	-1.356531000	-2.098888000
H	-4.252895000	-0.268424000	-1.151482000
C	1.566943000	-3.004374000	1.050891000
H	2.361405000	-3.734534000	1.231389000
H	0.880371000	-3.415696000	0.302205000
H	1.000638000	-2.874710000	1.980387000

C2-C3 distance: 1.8

C	-0.834515000	-0.002322000	1.482969000
C	-2.236863000	0.252918000	0.942730000

C	-2.203152000	-0.381082000	-0.465795000
C	-0.926532000	-1.130731000	-0.579086000
N	-0.127437000	-0.738896000	0.519220000
H	-3.007613000	-0.065448000	1.651064000
O	-0.357195000	0.433261000	2.508884000
O	-0.547932000	-1.848801000	-1.482468000
C	1.287723000	-0.610542000	0.343057000
C	2.136677000	-1.693678000	0.583057000
C	1.734124000	0.622690000	-0.160921000
C	3.500323000	-1.514989000	0.326453000
C	3.104867000	0.758677000	-0.404493000
C	3.980133000	-0.300180000	-0.161218000
H	4.186611000	-2.338629000	0.505407000
H	3.487973000	1.700328000	-0.789866000
H	5.041930000	-0.178477000	-0.358120000
C	0.784321000	1.789711000	-0.394012000
H	1.398682000	2.632914000	-0.725813000
H	0.369437000	2.102571000	0.570972000
C	-0.366529000	1.629125000	-1.443351000
H	-0.437808000	2.591074000	-1.968659000
H	-0.068532000	0.899158000	-2.206772000
C	-1.806693000	1.310211000	-1.002152000
H	-2.494536000	1.559136000	-1.813542000
C	-2.317995000	1.705359000	0.410922000
H	-1.737661000	2.447615000	0.967734000
H	-3.355881000	2.049951000	0.370601000
C	-3.429118000	-0.970994000	-1.110619000
H	-3.775237000	-1.851875000	-0.554802000
H	-3.198807000	-1.288128000	-2.132238000
H	-4.250799000	-0.247353000	-1.140864000
C	1.575459000	-3.002636000	1.076948000
H	2.371524000	-3.730165000	1.260934000
H	0.886061000	-3.422379000	0.335492000
H	1.013064000	-2.864638000	2.007621000

C2-C3 distance: 1.7

C	-0.835179000	-0.015514000	1.488645000
C	-2.233843000	0.250566000	0.945856000
C	-2.186683000	-0.332233000	-0.486269000
C	-0.920016000	-1.114509000	-0.589436000
N	-0.126858000	-0.745843000	0.518904000
H	-3.011176000	-0.084666000	1.638343000
O	-0.359898000	0.400915000	2.522905000
O	-0.548491000	-1.834967000	-1.492386000
C	1.288844000	-0.617108000	0.344612000
C	2.140734000	-1.695675000	0.592829000

C	1.729669000	0.613881000	-0.169285000
C	3.503538000	-1.514264000	0.333664000
C	3.099638000	0.752460000	-0.415814000
C	3.978428000	-0.301771000	-0.164858000
H	4.193017000	-2.333882000	0.518715000
H	3.479393000	1.692348000	-0.808732000
H	5.039598000	-0.178220000	-0.363963000
C	0.774983000	1.776992000	-0.404425000
H	1.385800000	2.618858000	-0.746220000
H	0.368029000	2.095591000	0.562298000
C	-0.386601000	1.614012000	-1.442430000
H	-0.474437000	2.582007000	-1.952138000
H	-0.086742000	0.897436000	-2.217525000
C	-1.824382000	1.270155000	-0.989071000
H	-2.508191000	1.538470000	-1.799233000
C	-2.317376000	1.707195000	0.420582000
H	-1.723342000	2.448591000	0.962768000
H	-3.353645000	2.056827000	0.390550000
C	-3.412809000	-0.937646000	-1.126718000
H	-3.732143000	-1.836731000	-0.585916000
H	-3.191151000	-1.226769000	-2.158699000
H	-4.248237000	-0.229119000	-1.130501000
C	1.582799000	-3.001829000	1.097548000
H	2.380202000	-3.727153000	1.284400000
H	0.891595000	-3.428096000	0.361453000
H	1.023005000	-2.857549000	2.028822000

C2-C3 distance: 1.6

C	-0.835773000	-0.028574000	1.493640000
C	-2.230745000	0.248472000	0.948576000
C	-2.170691000	-0.282078000	-0.505621000
C	-0.914268000	-1.096289000	-0.600997000
N	-0.126705000	-0.752446000	0.517788000
H	-3.014484000	-0.102818000	1.625051000
O	-0.362722000	0.368472000	2.536097000
O	-0.550248000	-1.818642000	-1.504194000
C	1.289581000	-0.623577000	0.345459000
C	2.144174000	-1.697754000	0.601661000
C	1.725533000	0.605293000	-0.177345000
C	3.506265000	-1.513834000	0.340376000
C	3.094759000	0.746168000	-0.426643000
C	3.976744000	-0.303736000	-0.168408000
H	4.198669000	-2.329607000	0.531437000
H	3.471493000	1.684369000	-0.826448000
H	5.037362000	-0.178578000	-0.369465000
C	0.766553000	1.765027000	-0.414198000

H	1.373856000	2.605264000	-0.766292000
H	0.367649000	2.089675000	0.554113000
C	-0.405618000	1.599356000	-1.440511000
H	-0.509807000	2.572503000	-1.935465000
H	-0.104677000	0.895617000	-2.226728000
C	-1.840989000	1.230798000	-0.975316000
H	-2.519072000	1.517895000	-1.785536000
C	-2.317506000	1.709051000	0.429115000
H	-1.711706000	2.450311000	0.957280000
H	-3.352544000	2.062029000	0.407501000
C	-3.396441000	-0.905747000	-1.140733000
H	-3.687214000	-1.822283000	-0.614830000
H	-3.184176000	-1.167396000	-2.182193000
H	-4.246375000	-0.214763000	-1.118272000
C	1.589632000	-3.001021000	1.117322000
H	2.388611000	-3.723507000	1.308420000
H	0.897679000	-3.434728000	0.386236000
H	1.031271000	-2.850168000	2.048396000