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Supporting information for

VCD spectroscopy distinguishes the enamine and iminium ion of a 1,1'-binaphthyl azepine

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1. Experimental and computational details

Materials. Catalyst 1 and its iminium salt were prepared according to literature procedures.^{1, 2}

IR and VCD spectroscopy. The IR and VCD spectra were recorded on a Bruker Vertex FT-IR spectrometer equipped with a PMA 50 module for VCD measurements. Samples were held in a transmission cell with BaF2 windows and 100 μ m path length. Concentration are given in the main text. Spectra were recorded at room temperature with 4 cm⁻¹ spectral resolution by accumulating 32 scans for the IR and ~32000 scans (4 hours accumulation time) for VCD. Baseline correction of the VCD spectra was done by subtraction of the spectra of the solvent recorded under identical conditions.

NMR spectroscopy. ¹H-NMR reaction monitoring was carried out on a 300 MHz Bruker Avance III NMR spectrometer. Concentrations of **1** was 0.5 M with equimolar CH₂Br₂ as internal standard. Reaction monitoring was carried out at room temperature. Spectra analysis and quantification was carried out using MestReNova 14.

Computational details. Details on the conformational analysis can be found in the SI. All geometry optimizations and frequency calculations were carried out at B3LYP/6-31G+(2d,p) level of theory using the Gaussian 09 Rev. E software package.³ Solvent effects were taken into account implicitly by using the integral equation formalism of the polarizable continuum model (IEFPCM)^{4, 5} of chloroform or DMSO. Explicit solvation of **1** with DMSO-d₆ was considered by placing a solvent molecule with its oxygen near the N-H group and re-optimizing the geometry prior to spectra calculations. Relative energy differences and Boltzmann populations generally refer to the zero-point corrected energies of the conformers (ΔE_{ZPC}). Note that we regularly find ΔE_{ZPC} -derived populations to better explain the experimental signatures than Gibbs Free energies (for a detailed discussion see References ⁶⁻⁹, for instance). Vibrational line broadening was simulated by assigning a Lorentzian band shape with half-width at half-height of 6 cm-1 to the calculated dipole and rotational strength. The calculated frequencies were scaled by 0.98 to account for anharmonic effects not captured by the harmonic approximation employed in the frequency calculations. Figures were prepared using CYLview.¹⁰

2. NMR spectra of enamine 2



Figure S1. Reaction monitoring of enamine formation: catalyst 1 + 1 eq of isovaleraldehyde + 1 eq CH₂Br₂ as reference (¹H-NMR, 300 MHz, DMSO-d₆)



Figure S2. Integrals of aldehyde (~9.6 ppm) and enamine (~6.2 ppm) normalized to reference CH₂Br₂.



Figure S3. ¹H-NMR of the mixture after ~ 9hrs of reaction time (top-most spectrum of the reaction monitoring plot in Figure S1)

3. Conformational analysis of 2 and 3



Table S1. Geometries, relative energies (zero-point corrected ΔE_{ZPC} and Gibbs Free energy ΔG_{298K} in kcal/mol) ad corresponding Boltzmann populations χ (in percentage) of the optimized conformations of **2** obtained at B3LYP/6-31G+(2d,p)/IEFPCM(DMSO) level of theory.

	C=C-C=C	C=C-C-N	C-N-C=C	N-C=C-C	С=С-С(СН ₃) ₂ -Н	ΔEzpc	ΔG298K	χ(ΔΕ)	χ(ΔG)
AzE_c1	54.2	-70.5	8.6	Е	3.5	0.00	0.00	78.8	80.7
AzE_c2	54.1	-70.7	8.6	Е	-117.1	1.28	1.46	8.7	6.6
AzE_c3	54.1	-70.6	8.4	Е	123.3	1.29	1.46	8.6	6.5
AzE_c4	54.2	-72.1	-154.2	E	-2.7	1.86	1.57	3.2	5.4
AzE_c5	54.2	-72.1	-153.4	E	-122.8	3.19	3.19	0.3	0.3
AzE_c6	54.1	-72.2	-154.5	Е	117.5	3.20	3.18	0.3	0.3
AzE_c7	53.8	-71.4	7.8	Ζ	-14.8	5.35	5.20	0.0	0.0
AzE_c8	54.0	-73.2	161.9	Ζ	-4.0	5.41	5.28	0.0	0.0
AzE_c9	53.9	-72.1	-163.8	Ζ	37.8	7.13	6.82	0.0	0.0
AzE_c10	54.0	-73.2	155.6	Z	-140.9	9.30	9.42	0.0	0.0
AzE_c11	54.0	-73.8	128.2	Z	178.7	10.11	9.81	0.0	0.0
AzE_c12	53.5	-72.2	24.6	Z	174.6	11.14	10.66	0.0	0.0

Relative energies referenced to $E_{zpc}(c1) = -1098.338939$ hartree and G(c1)=-1098.391084 hartree



Table S2. Geometries, relative energies (zero-point corrected ΔE_{ZPC} and Gibbs Free energy ΔG_{298K} in kcal/mol) ad corresponding Boltzmann populations χ (in percentage) of the optimized conformations of **3** obtained at B3LYP/6-31G+(2d,p)/IEFPCM(DMSO) level of theory.

	C=C-C=C	C=C-C-N	C-N=C-C	N=C-C=C	C-C=C-C _{Ar}	C=C-C _{Ar} -C _{Ar}	ΔEzpc	ΔG298K	χ(ΔΕ)	χ(ΔG)
AzI_c1	54.0	-72.5	177.2	179.6	179.4	-179.0	0.00	0.00	100.0	99.9
AzI_c2	53.9	-72.3	-176.3	-174.0	11.4	-150.1	5.28	4.42	0.0	0.1
AzI_c3	53.7	-72.8	175.2	-24.5	-176.2	174.1	5.99	5.64	0.0	0.0
AzI_c4	53.9	-71.3	-173.7	34.1	175.3	-172.9	8.51	8.33	0.0	0.0
AzI_c5	53.9	-71.9	-177.8	-44.9	-9.9	-23.6	11.03	11.22	0.0	0.0
AzI_c6	53.9	-68.1	2.6	54.0	7.0	-156.0	13.25	13.22	0.0	0.0

Relative energies referenced to $E_{zpc}(c1) = -1249.988727$ hartree and G(c1) = -1250.043312 hartree

4. VCD of catalyst 1



Figure S4. IR and VCD spectra of 1 and different clusters as discussed in the main text.

5. VCD of catalyst 2



Figure S5. Detailed IR and VCD spectra assignment of 2



Figure S6. Comparison of the computed IR and VCD spectra of 2 obtained using the B3LYP and B3PW91 functionals.

6. Cartesian coordinates

Structure of	1		
С	-1.22314800	1.59737800	-0.88355200
С	-0.72574800	0.50301400	-0.18047500
С	-1.62418800	-0.53877000	0.23300300
C	-2.99713300	-0.48271300	-0.17778800
C	-3,44617800	0.61910300	-0.95000300
C	-2.58508800	1.64064000	-1.27023600
н	-0 20528700	-1 65443300	1 43621000
C	-1 22731600	-1 61219200	1 07983200
C	-3 88932100	-1 51583700	0 22004200
ч	-4 48526900	0 65381500	-1 26391300
н	-2 94278900	2 49707700	-1 83411400
C	-3 46343800	-2 55059700	1 02007200
C	-2 11967900	-2 58840400	1 46373900
u u	-4 92260900	-1 46384700	_0 11097800
и и	-4 15519600	_3 33011300	1 32279500
н	-1 79142200	-3 39199400	2 11544900
C	2 59242200	1 60846900	1 28820100
C	3 44453000	0 58097700	0 96345200
C	2 98744900	-0 51124900	0 18184900
C	1 61503500	-0 55171800	-0 23238000
C	0 72559000	0.49591600	0.18654000
C	1 23033700	1 58188700	0.20031000
u u	4 90432700	-1 50856200	0.09017900
и П	2 95793200	2 45710600	1 85952500
11 U	4 48278300	0 60253300	1 28162500
C	3 87135000	_1 54919300	_0 22142500
C	1 21053800	-1 61596600	-1 08703200
C	2 09503900	-2 59758500	-1 47574800
C	3 43818800	-2 57478300	-1 02950900
U U	0 1996000	-2.57470300	
n u	1 76074700	-2 2020/200	-2 12227700
11 U	4 12363700	-3 35832600	-1 33614500
C	-0 30980100	2 75866600	-1 20317000
u u	0.61805500	2.73000000	-1 65181900
ч	-0 78013800	3 41607200	-1 94020300
11	0.70013000	5.1100/200	1.91020300
C	0 22012000	2 76227400	1 20069500
C	0.32813000	2.76237400	1.20068500
C H	0.32813000 -0.59589100 0.81194000	2.76237400 2.41028400 3.43831700	1.20068500 1.67104800
C H H	0.32813000 -0.59589100 0.81194000 -0.03721400	2.76237400 2.41028400 3.43831700 3.56325800	1.20068500 1.67104800 1.91045500
C H H N	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700	1.20068500 1.67104800 1.91045500 0.00946700
C H H N H	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200
C H H H H	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200
C H H H H Lowest energy C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 conformer of 2 0.10556100	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200
C H H N H Lowest energy C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 conformer of 2 0.10556100 1.06691600	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.51457800 -0.03942000
C H H N H Lowest energy C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 conformer of 2 0.10556100 1.06691600 2.42330000	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.51457800 -0.03942000 0.12028000
C H H N H Lowest energy C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200	1.20068500 1.67104800 1.91045500 -0.20505200 -0.51457800 -0.03942000 0.12028000 -0.31520200
C H H N H Lowest energy C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.51457800 -0.03942000 0.12028000 -0.31520200 -0.85506700
C H H N H Lowest energy C C C C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900	1.20068500 1.67104800 1.91045500 -0.20505200 -0.51457800 -0.03942000 0.12028000 -0.31520200 -0.85506700 -0.92691900
C H H H C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.31457800 -0.31520200 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000
C H H Eowest energy C C C C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.31457800 -0.31520200 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000
C H H N H C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.31520200 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000
C H H N H C C C C C C C C C C C H H C C H	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.31520200 -0.31520200 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.18780200
C H H N H C C C C C C C C C H C C H H C C H H	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.33942000 0.12028000 -0.31520200 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.8780200 -1.31104600
C H H N H C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.18780200 -1.31104600 0.41311400
C H H N H C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.18780200 -1.31104600 0.41311400 0.88558800
C H H N H C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.38160900	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.18780200 -1.31104600 0.41311400 0.88558800 -0.51804700
C H H H C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.31520200 -0.31520200 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400
C H H N H C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600
Lowest energy C C C C C C C C C C C C C H C C H H C C H H H C C C H H C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600 1.77501200
Lowest energy C C C C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800 -3.14099400	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600 1.77501200 1.29264100
Lowest energy C C C C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800 -3.08369300	$\begin{array}{c} 1.20068500\\ 1.67104800\\ 1.91045500\\ 0.00946700\\ -0.20505200\\ \hline\\ \\ -0.31520200\\ -0.31520200\\ -0.31520200\\ -0.31520200\\ -0.85506700\\ -0.92691900\\ 1.11726000\\ 0.74158000\\ -0.17002000\\ -1.18780200\\ -1.31104600\\ 0.41311400\\ 0.88558800\\ -0.51804700\\ 0.52472400\\ 1.36914600\\ 1.77501200\\ 1.29264100\\ 0.28272900\\ \end{array}$
Lowest energy C C C C C C C C C C C C C C H H C C C H H H C C C H H C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200 1.18270700	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25376400 -0.2539200 1.98758800 3.14099400 3.08369300 1.80621400	$\begin{array}{c} 1.20068500\\ 1.67104800\\ 1.91045500\\ 0.00946700\\ -0.20505200\\ \hline\\ \\ -0.31520200\\ -0.31520200\\ -0.31520200\\ -0.31520200\\ -0.92691900\\ 1.11726000\\ 0.74158000\\ -0.17002000\\ -1.18780200\\ -1.31104600\\ 0.41311400\\ 0.88558800\\ -0.51804700\\ 0.52472400\\ 1.36914600\\ 1.77501200\\ 1.29264100\\ 0.28272900\\ -0.19969200\\ \end{array}$
Lowest energy C C C C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200 1.18270700 0.62967800	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800 3.14099400 3.08369300 1.80621400 0.61284400	$\begin{array}{c} 1.20068500\\ 1.67104800\\ 1.91045500\\ 0.00946700\\ -0.20505200\\ \hline\\ 0.31520200\\ -0.31520200\\ -0.31520200\\ -0.31520200\\ -0.92691900\\ 1.11726000\\ 0.74158000\\ -0.17002000\\ -1.18780200\\ -1.31104600\\ 0.41311400\\ 0.88558800\\ -0.51804700\\ 0.52472400\\ 1.36914600\\ 1.77501200\\ 1.29264100\\ 0.28272900\\ -0.19969200\\ 0.37781700\\ \end{array}$
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С Н Н Н С С С С С С С С С С С С С С С С	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200 1.18270700 0.62967800 -0.39304600 0.95938200 -1.60407600	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -3.61301500 -2.51376400 -0.25399200 1.98758800 3.14099400 3.08369300 1.80621400 0.61284400 0.71662100 5.22793000 2.04048300	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.1726000 0.74158000 -0.17002000 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600 1.77501200 1.29264100 0.28272900 -0.19969200 0.37781700 1.31703000 0.10728400 2.52422000
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Lowest energy C C C C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200 1.18270700 0.62967800 -0.39304600 0.95938200 -1.60407600 -0.57147800 1.29324800	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800 3.14099400 3.08369300 1.80621400 0.61284400 0.71662100 5.22793000 2.04048300 4.1080900 4.26906700	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600 1.77501200 1.29264100 0.28272900 -0.19969200 0.37781700 1.31703000 0.10728400 2.52422000 1.66104300 -0.27869100
Lowest energy C C C C C C C C C C C C C C C C C C C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200 1.18270700 0.62967800 -0.39304600 0.95938200 -1.60407600 -0.57147800	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800 3.14099400 3.08369300 1.80621400 0.61284400 0.71662100 5.22793000 2.04048300 4.1080900 4.26906700 1.78558200	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600 1.77501200 1.29264100 0.28272900 -0.19969200 0.37781700 1.31703000 0.10728400 2.52422000 1.66104300 -0.27869100 -1.27202800
Lowest energy C C C C C C C C C C C C C C H H C C C H H H C C C H H H H C C C C H H H C	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200 1.18270700 0.62967800 -0.39304600 0.95938200 -1.60407600 -0.57147800 1.29324800 2.11857900 2.61778600	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800 3.14099400 3.08369300 1.80621400 0.61284400 0.71662100 5.22793000 2.04048300 4.1080900 4.26906700 1.78558200 2.95180300	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.18780200 -1.18780200 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600 1.77501200 1.29264100 0.28272900 -0.19969200 0.37781700 1.31703000 0.10728400 2.52422000 1.66104300 -0.27869100 -1.27202800 -1.80812400
С Н Н Н С С С С С С С С С С С С С С С С	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200 1.18270700 0.62967800 -0.39304600 0.95938200 -1.60407600 -0.57147800 1.29324800 2.11857900 2.61778600 2.21309900	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800 3.14099400 3.08369300 1.80621400 0.61284400 0.71662100 5.22793000 2.04048300 4.26906700 1.78558200 2.95180300 4.20938100	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.20505200 -0.31520200 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.18780200 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600 1.77501200 1.36914600 1.77501200 1.31703000 0.28272900 -0.19969200 0.37781700 1.31703000 0.10728400 2.52422000 1.66104300 -0.27869100 -1.27202800 -1.80812400 -1.29975600
С Н Н Н N H Lowest energy С С С С С С С С С С С С С С С С С С С	0.32813000 -0.59589100 0.81194000 -0.03721400 0.72539900 7 conformer of 2 0.10556100 1.06691600 2.42330000 2.78226400 1.78227700 0.47727900 3.17516100 3.43072800 4.12507800 2.05860500 -0.28879500 5.07745800 4.71882000 4.38160900 6.09789700 5.46510200 -0.81954000 -0.25020000 0.74465200 1.18270700 0.62967800 -0.39304600 0.95938200 -1.60407600 2.057147800 1.29324800 2.11857900 2.61778600 2.21309900 2.43473800	2.76237400 2.41028400 3.43831700 3.56325800 4.20084700 -1.64276000 -0.75509200 -1.20212700 -2.52041200 -3.36871700 -2.94625900 0.57212700 -0.41097900 -2.96456800 -4.36482000 -3.61301500 -2.16164200 -0.87639800 -3.96100100 -2.51376400 -0.25399200 1.98758800 3.14099400 3.08369300 1.80621400 0.61284400 0.71662100 5.22793000 2.04048300 4.1080900 4.26906700 1.78558200 2.95180300 4.20938100 0.83310900	1.20068500 1.67104800 1.91045500 0.00946700 -0.20505200 -0.30942000 0.12028000 -0.31520200 -0.85506700 -0.92691900 1.11726000 0.74158000 -0.17002000 -1.18780200 -1.31104600 0.41311400 0.88558800 -0.51804700 0.52472400 1.36914600 1.77501200 1.36914600 1.77501200 1.31703000 0.28272900 -0.19969200 0.37781700 1.31703000 0.10728400 2.52422000 1.66104300 -0.27869100 -1.27202800 -1.80812400 -1.29975600 -1.67990400

н		3 32511500	2 90697100	-2 63024000
		0.61006000	E 10110100	1 70500000
н		2.01980200	5.12112100	-1./2520000
С		-1.34793300	-1.23113100	-0.59381700
н		-1.44084600	-0.28189800	-1.14870600
 TT		1 00002000	1 09224200	1 1 5 4 0 2 1 0 0
п		-1.90993900	-1.98324300	-1.15493100
С		-1.10131100	-0.53867500	1.78559500
Н		-0.37337900	-1.29641500	2.08949700
н		-1 72993900	-0 32332200	2 65153400
11		1.06600500	-0.32332200	2.03133400
N		-1.96600700	-1.10490300	0.73141700
C		-3.31196400	-0.74948100	0.75877100
н		-3.68250300	-0.57378600	1.76725100
		4 1 6 0 5 2 2 0 0 0	0 65744200	0.07500000
C		-4.10952200	-0.85744200	-0.2/590000
Н		-3.83007200	-0.81755200	-1.29713700
С		-5.64269300	-0.36902900	-0.10727500
н		-5 83538800	-0 19709800	0 96080800
		5.05550000	1 56564000	0.50000000
C		-6.50581100	-1.56564800	-0.55405000
Н		-6.33408500	-1.79439200	-1.61357100
Н		-6.26646300	-2.46352100	0.02558000
ц		-7 57381300	-1 35066600	-0 42767000
		-7.57501500	-1.35000000	-0.42707000
C		-6.05393100	0.90265900	-0.87375200
Н		-7.12338600	1.11000900	-0.74866600
Н		-5.49260800	1.77503800	-0.52268300
ц		-5 85953100	0 78868500	_1 94786000
11		-3.03933100	0.78888500	-1.94/00000
Lowest	energy	conformer of 3 (ch	narge +1)	
С		1.02450000	-1.21715000	-1.24793600
c		1 01046000	_0 72052400	_0 20596000
		1.91940900	-0./2053400	-0.30308200
C		2.80233100	-1.62965100	0.36907300
С		2.81312100	-3.00939000	-0.02161300
Ċ		1 92805900	-3 45385800	-1 03703000
c		1.02724700	5.15505000	1 (1501100
C		1.03/34/00	-2.58418300	-1.01291100
н		3.62185000	-0.20459000	1.78552100
С		3.64070800	-1.23343900	1.44792800
С		3 69098300	-3 91382300	0 63472200
		1.04706000	1 10702000	1 22270400
н		1.94/96000	-4.49/83000	-1.333/9400
Н		0.34081200	-2.93854800	-2.36961300
С		4.50424300	-3.48982800	1.65905100
C		4 46633300	-2 13817000	2 07599100
		2.60700100	2.15017000	2.07555100
н		3.69/80100	-4.95266700	0.318/5500
H		5.16663300	-4.18989900	2.15737200
н		5.09252500	-1.81291400	2,90035000
C		0 56024200	2 67129200	0 71004200
c		0.50034300	2.07120300	0.71004300
C		1.65994300	3.48918700	0.63776800
C		2.90319600	2.98154700	0.18293300
С		3.01514900	1.59298400	-0.15691900
Ċ		1 97241000		0 01116000
C		1.0/341000	n ./j./uc.jnn	
C		1.07511000	0.73796200	0.01110000
		0.65886800	0.73796200 1.29492300	0.39920300
Н		0.65886800 3.93440900	0.73796200 1.29492300 4.87772000	0.39920300
H H		0.65886800 3.93440900 -0.39508300	0.73796200 1.29492300 4.87772000 3.07546600	0.39920300 0.30531600 1.03784200
H H H		0.65886800 3.93440900 -0.39508300 1.58302700	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200	0.39920300 0.30531600 1.03784200 0.89902100
H H H		0.65886800 3.93440900 -0.39508300 1.58302700	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 2.03101700	0.39920300 0.30531600 1.03784200 0.89902100
H H C		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700
Н Н С С		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400
Н Н С С С		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600
H H C C C		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.47012100
н н С С С		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.24751700	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.47012100
н н С С С С н		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.47012100 -0.99681800
Н Н С С С С Н Н		$\begin{array}{c} 0.65886800\\ 3.93440900\\ -0.39508300\\ 1.58302700\\ 4.03158700\\ 4.25027200\\ 5.31931500\\ 5.21709500\\ 4.34751700\\ 6.24878400 \end{array}$	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.47012100 -0.99681800 -1.26645700
н н С С С С С н н н		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.47012100 -0.99681800 -1.26645700 -0.58856900
Н Н С С С С С Н Н Н С		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.47012100 -0.99681800 -1.26645700 -0.58856900 -1.85615100
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н н н С С С С н н н С н .		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.47012100 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200
н н С С С С н н н С С н н н н С		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.47012100 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200 -2.71317200
н н С С С С н н н С н н С		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.58641900	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.47012100 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200 -2.71317200 0.48761500
н н С С С С н н н С н н С н		$\begin{array}{c} 0.65886800\\ 3.93440900\\ -0.39508300\\ 1.58302700\\ 4.03158700\\ 4.25027200\\ 5.31931500\\ 5.21709500\\ 4.34751700\\ 6.24878400\\ 6.07091600\\ -0.01070500\\ 0.42862900\\ -0.49600600\\ -0.58641900\\ -0.40770300\\ \end{array}$	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900	0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.47012100 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200 -2.71317200 0.48761500 1.06567100
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нннсссснннснноннмснснс		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.58641900 -0.40770300 -1.38373600 -1.06873900 -2.33123400 -2.52780000 -3.45279800 -3.31253700 -4.70227300	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400	0.39920300 0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200 -2.71317200 0.48761500 1.06567100 0.97028600 -0.85726000 -1.5131300 -2.16624200 -0.30459100 0.72399900 -0.81194000
нннССССнннСннСннонснон		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.58641900 -0.49600600 -0.58641900 -0.40770300 -1.38373600 -1.06873900 -2.33123400 -2.5278000 -3.45279800 -3.31253700 -4.70227300 -4.76853400	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400 -0.47951700	0.39920300 0.39920300 0.30531600 1.03784200 0.03028700 -0.69468400 -0.84834600 -0.47012100 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200 0.48761500 0.48761500 0.97028600 -0.85726000 -1.15131300 -2.16624200 0.72399900 -0.81194000 -1.85230900
нннсссснннсннсныснснснснс		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.58641900 -0.40770300 -1.38373600 -1.06873900 -2.33123400 -2.52780000 -3.45279800 -3.31253700 -4.76853400 -5.97166500	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400 -0.47951700 -0.3489200	0.39920300 0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.47012100 -0.99681800 -1.26645700 -1.26645700 -2.77317200 0.48761500 1.06567100 0.97028600 -1.15131300 -2.16624200 -0.30459100 0.72399900 -0.81194000 -1.85230900 -0.13287300
нннсссснннсннкиснснснсс		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.58641900 -0.49600600 -0.58641900 -0.49600600 -1.38373600 -1.38373600 -1.38373600 -2.33123400 -2.5278000 -3.45279800 -3.31253700 -4.76253400 -5.97166500	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400 -0.47951700 -0.03489200	0.39920300 0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200 -2.71317200 0.48761500 1.06567100 0.97028600 -0.85726000 -1.15131300 -2.16624200 -0.30459100 0.72399900 -0.81194000 -1.85230900 -0.13287300 -0.13287300
нннсссснннсннсниснснсс		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.58641900 -0.40770300 -1.38373600 -1.06873900 -2.52780000 -3.31253700 -4.70227300 -4.76853400 -5.97166500 -7.14438100	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400 -0.47951700 -0.33642400	0.39920300 0.39920300 0.30531600 1.03784200 0.03028700 -0.69468400 -0.84834600 -0.47012100 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200 0.48761500 1.06567100 0.97028600 -0.85726000 -1.15131300 -2.16624200 0.72399900 -0.81194000 -1.85230900 -0.13287300 -0.85670900
нннсссснннсннснонснснссс		$\begin{array}{c} 0.65886800\\ 3.93440900\\ -0.39508300\\ 1.58302700\\ 4.03158700\\ 4.25027200\\ 5.31931500\\ 5.21709500\\ 4.34751700\\ 6.24878400\\ 6.07091600\\ -0.01070500\\ 0.42862900\\ -0.49600600\\ -0.58641900\\ -0.58641900\\ -0.58641900\\ -0.58641900\\ -0.58641900\\ -0.38373600\\ -1.06873900\\ -2.33123400\\ -2.52780000\\ -3.31253700\\ -4.76853400\\ -5.97166500\\ -7.14438100\\ -6.09184100\\ \end{array}$	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400 -0.3642400 0.37486400	0.39920300 0.39920300 0.30531600 1.03784200 0.03028700 -0.69468400 -0.47012100 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.71317200 0.48761500 1.06567100 0.97028600 -1.15131300 -2.16624200 -0.30459100 0.72399900 -0.81194000 -1.85230900 -0.13287300 -0.13287300 -0.85670900 1.21286200
нннсссснннсннсннонснонсссс		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.49600600 -0.58641900 -0.40770300 -1.38373600 -1.06873900 -2.33123400 -2.52780000 -3.45279800 -3.31253700 -4.70227300 -4.76853400 -5.97166500 -7.14438100 -6.09184100 -8.39558300	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400 -0.3642400 -0.37486400 -0.23402000	0.39920300 0.39920300 0.30531600 1.03784200 0.03028700 -0.69468400 -0.84834600 -0.99681800 -1.26645700 -1.26645700 -2.71317200 0.48761500 1.06567100 0.97028600 -1.15131300 -2.16624200 -0.85726000 -1.15131300 -2.16624200 -0.30459100 0.72399900 -0.81194000 -1.85230900 -0.13287300 -0.85670900 1.21286200 -0.25903400
нннсссснннсннсниснснснссссн		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.58641900 -0.49600600 -0.58641900 -0.40770300 -1.38373600 -1.06873900 -2.33123400 -2.52780000 -3.45279800 -3.45279800 -3.45279800 -3.45279800 -3.76253400 -5.97166500 -7.14438100 -6.09184100 -8.39558300 -7.06256100	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400 -0.3642400 -0.33642400 0.37486400 -0.23402000 -0.65331700	0.39920300 0.39920300 0.30531600 1.03784200 0.89902100 0.03028700 -0.69468400 -0.84834600 -0.99681800 -1.26645700 -1.26645700 -2.17858200 -2.71317200 0.48761500 1.06567100 0.97028600 -1.5131300 -2.16624200 -0.85726000 -1.5131300 -2.16624200 0.72399900 -0.81194000 -1.85230900 -0.13287300 -0.85670900 1.21286200 0.25903400 -1.89181500
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нннсссснннсннсныснснснсссснс		0.65886800 3.93440900 -0.39508300 1.58302700 4.03158700 4.25027200 5.31931500 5.21709500 4.34751700 6.24878400 6.07091600 -0.01070500 0.42862900 -0.49600600 -0.58641900 -0.40770300 -1.38373600 -1.06873900 -2.33123400 -2.52780000 -3.45279800 -3.31253700 -4.70227300 -4.76853400 -5.97166500 -7.14438100 -6.09184100 -8.39558300 -7.06256100 -7.34203000	0.73796200 1.29492300 4.87772000 3.07546600 4.53998200 3.83181700 1.13494100 1.98821100 3.34791100 0.09970700 1.61568300 4.00684300 -0.30007800 0.64726800 -0.76593300 0.44218100 -0.46981900 1.00292100 0.01744700 -0.14587000 -0.48194700 0.05451400 0.35830800 -0.16497400 -0.3642400 0.37486400 -0.23402000 -0.65331700 0.47639600	0.39920300 0.39920300 0.30531600 1.03784200 0.03028700 -0.69468400 -0.84834600 -0.99681800 -1.26645700 -0.58856900 -1.85615100 -2.17858200 -2.71317200 0.48761500 1.06567100 0.97028600 -0.85726000 -1.15131300 -2.16624200 -0.30459100 0.72399900 -0.81194000 -1.85230900 -0.81287300 -0.85670900 1.21286200 -0.25903400 -1.89181500 1.80563200

C		-8 49612100	0 17258700	1 07272800
U U		-0.20060100	-0.46040200	_0 02721700
11		-9.20000100	0.70011000	-0.02/21/00
H		-7.42449100	0.79211800	2.8398/600
н		-9.47066200	0.25405200	1.54251800
Lowest	energy	conformer of 3 with	th perchlorate	
С		-1.33377200	1.12282500	-0.02701200
C		-2.41607600	0.36100300	0.40089000
С		-3.24148200	0.85288700	1,46776500
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c		-1 01705000	2.10103300	1 47211000
C		-1.91705000	2.93037300	1.4/211900
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H		-4.45382900	-0.92958400	1.71451700
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Н		-1.73999900	3.92562000	1.86865100
н		-0.24653200	2.98741300	0.13715700
C		-4 81088200	1 89199900	3 58507800
C		-5 03391000	0 58189000	3 09885600
		3.61450000	2 66119500	2 4207070700
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п		-5.423/1600	2.20032300	4.39204400
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C		-1.74398800	-3.16624000	-0.83106300
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С		-2.63441200	-0.97330900	-0.23380000
С		-1.58553900	-1.88780800	-0.24221100
ч		-5 31835100	-3 93820200	-2 57638000
и и		-0.91422000	-2 96599700	_0 00021000
п		2 05141400	-3.80598700	1 95236400
H G		-3.05141400	-4.514//000	-1.05350400
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п		0.30911000	1 5410000	-1.42499200
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Н		4.06142100	-3.33534500	1.50857300
С		7.43988200	-3.01940200	1.61600300
Н		8.57495800	-1.40748700	0.74240500
Н		6.05211800	-4.48567100	2.37724500
н		8.31391700	-3.53398600	2.00163500
Cl		3,06567400	3,19059100	-1.49111300
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0		2.00/19300	4.00710100	-0.11021900
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0		3.88920700	2.44/9//00	-0.51013400



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