Supporting Information for

Molecular Balances Based on Aliphatic CH-π and Lone Pair-π Interactions

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Contents

1. The folded/unfolded energetics computed for the molecular balances are presented in terms of ΔE and ΔH in the table S1.

Table S1:. *Difference in total energy (ΔE) and enthalpy (ΔH) in kcal/mol (ΔE = E_{folded} - $E_{unfolded}$) between the folded and unfolded forms of the molecular balances calculated in gas-phase at 298 K.*

	0		**1**		**2**		**3**		**4**	
	ΔE	**ΔH**	**ΔE**	**ΔH**	**ΔE**	**ΔH**	**ΔE**	**ΔH**	**ΔE**	**ΔH**
a	+0.2	+0.3	+0.7	+0.7	+0.3	+0.1	-1.0	-1.2	-0.2	-0.3
b	-0.4	-0.4	+2.9	+2.9	-	-	-0.6	-0.9	-	-
c	-0.3	-0.3	+4.1	+4.1	-	-	+1.3	+1.2	-	-
d	-0.4	-0.5	-0.6	-0.8	-1.5	-1.6	-1.9	-2.0	-2.1	-2.2
e	-		-	-	-	-	-1.1	-1.1	-	-
f	-		-	-	-	-	-2.0	-2.0	-	-

2. Folded/unfolded relative energies for the test calculations carried out in the solvent chloroform for selected molecular balances.

The single point energies were calculated on the gas-phase optimized geometries of 0a, 1a, 2a and 3a using the integral equation formalism polarizable continuum model (IEFPCM) using the M062X/6-31+G(d) level of theory as implemented in Gaussian 09. The ΔE_{sol} (= $E_{folded} - E_{unfolded}$) values computed are shown in the table S2.

System	**ΔE_{solv} (in kcal/mol)**
0a	-0.1
1a	+1.3
2a	-0.2
3a	-0.8

3. Cartesian Coordinates for the optimized structures and their zero point energy corrected total energies in Hartree.

0a – Folded

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-2.96720800	-0.08860600	-1.14819800
C	-2.05914000	-1.21875100	-0.54890400
H	-2.46288000	-2.20695300	-0.78767200
C	-0.60903300	-1.15086900	-0.98773200
C	-0.58596200	-0.65166200	1.30005700
C	-2.04394300	-0.89508400	0.95918600
H	-2.43217200	-1.69945900	1.59069000
C	-2.95224700	0.38051300	1.06076400
C	1.57189800	-0.64314600	0.07940800
C	2.47461300	-1.69174800	0.14779400
C	3.84561600	-1.44312400	0.08264100
H	4.55256400	-2.26420500	0.13638700
C	4.29112900	-0.13303900	-0.04848400
H	5.35582100	0.07621900	-0.09706300
C	3.39017600	0.93115300	-0.12071800
H	3.76404400	1.94329100	-0.22403000
C	2.01934700	0.67987600	-0.06079500
C	1.45888200	2.97175100	-0.26636100
H	2.05656500	3.29010500	0.59572200
H	0.54064900	3.55845600	-0.30944500
N	0.17094100	-0.88601700	0.14473100
O	-0.17276500	-1.28718600	-2.10474800
O	-0.12731500	-0.31194700	2.36307600
O	1.05274100	1.62535400	-0.13204300

H	-3.32928400	-0.30508100	-2.15335600
H	-3.30003500	0.59089600	2.07220100
H	2.08952100	-2.70184700	0.25175100
H	2.03064300	3.12022500	-1.19014000
C	-2.21237300	1.21597300	-0.96005500
H	-1.66344000	1.72772100	-1.74348800
C	-2.20445400	1.49453600	0.34909300
H	-1.64756400	2.27736100	0.85239300
C	-4.00375400	0.02217300	-0.01012300
H	-4.72658400	0.82557700	-0.17557300
H	-4.52701000	-0.91964300	0.19279900

Energy = -898.523031 Hartree.
Low frequencies (cm^{-1}): 14.4527 52.6881 69.3683 87.1750 93.3024 96.9169 161.1429 181.3950 225.6011 236.3246 277.8777 288.6923.

0a – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	3.05058600	0.84684700	-0.97199000
C	1.90232900	1.22362500	0.02726800
H	1.99390900	2.26461800	0.34978500
C	0.50700400	0.98724400	-0.51514800
C	0.77098700	-0.57077400	1.21350100
C	2.07652600	0.19762700	1.16435800
H	2.26420000	0.64590100	2.14409000
C	3.30849900	-0.65378600	0.69617800
C	-1.39536900	-0.51539000	-0.00449300
C	-2.47945200	0.36736100	0.12665400
C	-3.76559900	-0.09190200	-0.16113000
H	-4.61810600	0.57298200	-0.08374800

C	-3.95859300	-1.42136200	-0.53909800
H	-4.96589400	-1.76626900	-0.75380400
C	-2.88584100	-2.30086500	-0.63715100
H	-3.04464100	-3.33527800	-0.92314400
C	-1.59812200	-1.83743200	-0.37312300
N	-0.08499300	-0.02897600	0.24837100
O	-0.01381900	1.53116400	-1.45728800
O	0.50019000	-1.50440900	1.93019700
H	3.27190000	1.62789900	-1.69942100
H	3.76479900	-1.24027800	1.49364500
C	2.71090500	-0.52488800	-1.53111600
H	2.30281300	-0.70277400	-2.52039600
C	2.86501000	-1.41478100	-0.54209700
H	2.61229700	-2.46983200	-0.55987000
C	4.14807600	0.46689500	0.04483500
H	5.05523300	0.08884400	-0.43425400
H	4.39822100	1.27947600	0.73703800
O	-2.18208200	1.61765300	0.55019400
C	-3.21420900	2.58247200	0.53171300
H	-4.00867400	2.32591700	1.24290500
H	-2.75014800	3.52218300	0.83012700
H	-3.63467500	2.68388600	-0.47537300
H	-0.73701000	-2.49506100	-0.44597100

Energy = -898.523394 Hartree.
Low frequencies (cm^{-1}): 35.9423 42.8301 69.6032 80.8786 98.2821 125.0879 155.2223 185.1544 231.1121 242.6476 282.2861 298.3143.

0b - Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	2.89004300	1.14517600	0.49553300

C	2.13125900	-0.01875900	1.22825700
H	2.51435800	-0.14712600	2.24434400
C	0.62632300	0.15192600	1.27999900
C	0.99393300	-1.67701600	-0.13508900
C	2.37287000	-1.22917500	0.30603300
H	2.88828100	-2.06360800	0.78975600
C	3.24811100	-0.63057200	-0.85288300
C	-1.34387600	-0.90516800	0.20045900
C	-2.05102300	-2.06181900	0.50415700
C	-3.41994600	-2.12935800	0.25944100
H	-3.97213300	-3.03221400	0.49772900
C	-4.06981700	-1.02330500	-0.28125700
H	-5.13955200	-1.05750300	-0.46616800
C	-3.36546200	0.13650500	-0.59874600
H	-3.89064600	0.98247600	-1.02843700
C	-1.98747600	0.19904900	-0.37905000
C	-1.77818000	2.53783100	-0.84349500
H	-2.57097700	2.52899100	-1.60245800
H	-0.96642900	3.15974700	-1.22933400
N	0.05138800	-0.82907500	0.46150600
O	0.00581000	0.97470200	1.90905000
O	0.72514100	-2.59165300	-0.87582900
O	-1.19510500	1.24207300	-0.72942200
H	3.07736400	2.01110200	1.13079900
H	3.76128900	-1.38664100	-1.44710000
H	-1.51562000	-2.90331800	0.93310900
C	2.14776400	1.39744000	-0.80449100
H	1.45929400	2.21787800	-0.97360900
C	2.36051800	0.34537200	-1.60483100

H	1.88494100	0.14057900	-2.55798900
C	4.10624600	0.35193500	-0.02798400
H	4.76739500	0.95917100	-0.65191100
H	4.68095400	-0.13651500	0.76772900
C	-2.26985300	3.06533700	0.49440300
H	-2.63606400	4.09035700	0.37633100
H	-3.08404200	2.45298800	0.89254200
H	-1.45350600	3.05378200	1.22099600

Energy = -937.792929 Hartree.
Low frequencies (cm^{-1}): 23.9357 39.0481 49.2184 74.1966 83.9265 100.1029 126.7947 155.2738 169.8023 194.8390 226.7323 241.7768.

0b - Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	3.10331600	0.93522100	-1.02521700
C	1.88808000	1.23791500	-0.08042000
H	1.83754100	2.30446800	0.15662600
C	0.54816900	0.78208000	-0.62389200
C	0.96007300	-0.58396700	1.23300100
C	2.15962200	0.33705900	1.14007500
H	2.26442400	0.88199600	2.08249500
C	3.50099400	-0.38422900	0.76457200
C	-1.17006000	-0.89692200	-0.00714500
C	-2.34985000	-0.13761200	0.05402700
C	-3.57308500	-0.76647600	-0.18464800
H	-4.49689500	-0.20024700	-0.15328600
C	-3.60866800	-2.13641200	-0.44747000
H	-4.56841200	-2.61367400	-0.62298900
C	-2.43984400	-2.89000900	-0.48016500

H	-2.47565100	-3.95594400	-0.67877700
C	-1.21567700	-2.25969100	-0.26309900
N	0.07148400	-0.24099900	0.20746600
O	-0.01406200	1.18415900	-1.61266100
O	0.78750800	-1.47794700	2.02634600
H	3.24544400	1.67954900	-1.80862600
H	4.00429900	-0.84365600	1.61521500
C	2.95679500	-0.50861900	-1.47664600
H	2.60454500	-0.81624000	-2.45548400
C	3.19358600	-1.29063000	-0.41539200
H	3.07747200	-2.36760700	-0.35183400
C	4.21056300	0.77998800	0.04054300
H	5.17160700	0.48566300	-0.38980900
H	4.33488100	1.66982800	0.66882200
O	-2.20137000	1.17008700	0.36503000
C	-3.31825600	2.03247600	0.20068900
H	-4.09606400	1.77178600	0.93157200
H	-3.72900500	1.90303200	-0.80906500
H	-0.28339700	-2.81587400	-0.28829300
C	-2.82354500	3.44802600	0.41040000
H	-2.04945400	3.68631300	-0.32414300
H	-3.64875700	4.15719900	0.29678800
H	-2.40285500	3.56081800	1.41351800

Energy = -937.793551 Hartree.
Low frequencies (cm^{-1}): 22.4897 36.1393 58.9321 69.3155 84.7321 105.8051 121.8061 154.0672 174.2782 209.9412 235.1935 250.7286.

0c - Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-3.40235000	-0.39988600	-0.89788600

C	-2.62124200	-1.12281700	0.25717300
H	-3.23245500	-1.91071900	0.70636000
C	-1.28943300	-1.70184500	-0.17518600
C	-0.75654600	0.02164200	1.31249300
C	-2.26804700	0.02648800	1.21997400
H	-2.69094500	-0.08211200	2.22235600
C	-2.86877300	1.28883900	0.50313900
C	1.10929700	-1.19165900	0.19949900
C	1.67773500	-2.44714000	0.39789600
C	3.01897000	-2.66005900	0.09808700
H	3.46085400	-3.63889300	0.25345900
C	3.78412500	-1.61261600	-0.41294400
H	4.82914500	-1.77325900	-0.66147000
C	3.21412400	-0.36146500	-0.62851500
H	3.79821100	0.44353500	-1.06290900
C	1.87125700	-0.13443100	-0.31834500
C	1.71669400	2.29192100	-0.03594000
H	0.79937000	2.76773700	0.33119500
N	-0.27168800	-0.98496200	0.47226700
O	-1.10530400	-2.60994200	-0.94842000
O	-0.06803200	0.74680500	1.99201800
O	1.23598200	1.03669800	-0.57625700
H	-3.98780400	-1.07667400	-1.52014500
H	-2.96651500	2.15489000	1.15826800
H	1.05510500	-3.25007400	0.77996200
C	-2.39663900	0.48724800	-1.61076200
H	-1.93389700	0.25608600	-2.56423800
C	-2.07768300	1.48614600	-0.77833400
H	-1.29986900	2.22862300	-0.91933700
C	-4.15802600	0.65445800	-0.06136800
H	-4.73253600	1.34858400	-0.68052500
H	-4.80153600	0.21735600	0.71125700
C	2.29319400	3.12353500	-1.17243500
H	2.51233000	4.13860600	-0.82415500
H	3.22289500	2.68421900	-1.54979100
H	1.58181500	3.18486500	-2.00121300
C	2.66774300	2.15198500	1.14347000
H	3.66335300	1.81527200	0.84082500
H	2.77481300	3.13630100	1.61071600
H	2.26190100	1.45983600	1.88469300

Energy = -977.058997 Hartree.
Low frequencies (cm^{-1}): 33.5505 40.1178 60.3843 72.3071 89.7233 95.0581 121.5714 138.9859 166.7517 193.7247 216.9601 234.0069.

0c - Unfolded

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-3.18334900	-1.30666200	-0.86485900
C	-2.02427800	-1.33449800	0.19225900
H	-1.92377400	-2.33047900	0.63246200

C	-0.68276200	-0.88883600	-0.35184700
C	-1.30973900	0.76781300	1.17404300
C	-2.43835700	-0.24308100	1.19662400
H	-2.57463600	-0.60575700	2.21918000
C	-3.79245500	0.29127000	0.61056200
C	0.86420100	1.02180900	-0.00159600
C	2.09859800	0.39502500	0.22514900
C	3.26995800	1.10944700	-0.04012800
H	4.23234600	0.64955000	0.15376300
C	3.20292900	2.41246900	-0.52544600
H	4.12420700	2.95203800	-0.72511700
C	1.97209500	3.03083800	-0.73849500
H	1.92389000	4.05060000	-1.10603100
C	0.80075900	2.32992500	-0.47098500
N	-0.33346700	0.30844600	0.27912400
O	-0.03198800	-1.43392400	-1.21216200
O	-1.24940500	1.80624200	1.78649600
H	-3.21960900	-2.19331600	-1.49768800
H	-4.38420300	0.86265200	1.32568000
C	-3.09494900	0.03352000	-1.57609900
H	-2.69211300	0.17684000	-2.57305500
C	-3.45682300	0.98071600	-0.70094500
H	-3.41512400	2.05598500	-0.83984100
C	-4.37295700	-1.03834100	0.08186100
H	-5.31604300	-0.90188700	-0.45414700
H	-4.48967200	-1.80153900	0.86023200
O	2.06519300	-0.84702100	0.76717800
C	2.89410300	-1.91854000	0.26284600
H	-0.17362100	2.78615300	-0.61721200

H	2.25188900	-2.79322000	0.41319600
C	3.20269700	-1.81355700	-1.22433500
H	3.95198200	-1.04750300	-1.44346800
H	3.60130200	-2.77615800	-1.56108500
H	2.29181300	-1.59590400	-1.78755700
C	4.13688600	-2.07584300	1.12984800
H	4.64610300	-3.01317800	0.88094900
H	4.84733100	-1.25771200	0.97488800
H	3.86245400	-2.09950400	2.18814300

Energy = -977.058601 Hartree.
Low frequencies (cm^{-1}): 16.3465 38.4819 55.3068 74.6434 85.1027 98.4325 120.3589 149.8572 157.7392 200.5051 225.4272 238.6782.

0d - Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	3.81273800	0.03461600	-0.00441600
C	2.76509300	0.66852900	0.94413600
C	1.85667600	-0.59264500	1.09801900
H	2.22006600	-1.23051500	1.90851500
C	0.39179000	-0.26881100	1.33773700
C	0.45458000	-1.28180900	-0.76989900
C	1.89818300	-1.26446200	-0.29602800
H	2.28444400	-2.28746700	-0.28283100
C	2.82930700	-0.33820500	-1.14139900
C	2.16625700	1.01282300	-1.27428300
C	2.12972900	1.59781200	-0.06338700
C	-1.76718100	-0.62502600	0.14098300
C	-2.50562200	-1.79823000	0.24841500
C	-3.89395500	-1.75128400	0.16457100
H	-4.47489700	-2.66461100	0.24564000

C	-4.52312800	-0.52425400	-0.02165800
H	-5.60619600	-0.47151000	-0.08422800
C	-3.76957200	0.64311700	-0.13560600
H	-4.28073400	1.58792200	-0.29009300
C	-2.37476100	0.62095100	-0.06508700
C	-2.28934700	3.13592200	-0.57989100
H	-2.83861300	3.01939700	-1.52004100
H	-1.58999900	3.96820400	-0.70206400
H	-3.00282700	3.41729600	0.20126500
N	-0.33983400	-0.71749000	0.23497700
O	4.98892300	-0.13371400	0.11325600
O	-0.07789700	0.28747600	2.29982100
O	0.04293900	-1.69733600	-1.82414200
H	3.12755900	1.09537200	1.87673300
H	3.24645500	-0.79251200	-2.03741800
H	-1.98561800	-2.74072800	0.39377700
C	-1.52745500	1.86523000	-0.21425000
H	-0.76343900	1.66691100	-0.97718300
H	-0.98266400	2.02624800	0.72491700
H	1.77312900	1.40852200	-2.20429600
H	1.70045800	2.56284700	0.18324900

Energy = -936.620811 Hartree.
Low frequencies (cm^{-1}): 20.2139 54.4276 63.6227 74.2220 79.6775 115.4668 126.7730 159.8668 169.4846 193.7204 212.9619 275.0524.

0d – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-3.91751600	0.29613400	0.00537200
C	-3.04013500	-0.64338400	0.86871900

C	-1.86137200	0.35347600	1.10777100
H	-2.05403500	0.97564500	1.98594300
C	-0.51737500	-0.33735200	1.26017000
C	-0.35834200	0.87073900	-0.73545800
C	-1.75804100	1.14732100	-0.21706600
H	-1.90052200	2.22536600	-0.10263600
C	-2.87914500	0.53623100	-1.11748900
C	-2.54160300	-0.91255200	-1.38489100
C	-2.63795500	-1.59849500	-0.23186300
C	1.60574200	-0.48631000	-0.02911100
C	2.71543800	0.36853900	0.01477800
C	3.96825700	-0.20959700	-0.20777800
H	4.85558500	0.41482700	-0.18487900
C	4.10836500	-1.57510000	-0.44942100
H	5.09762700	-1.99195400	-0.61471400
C	2.99002700	-2.40380600	-0.47231400
H	3.09482300	-3.46901300	-0.65280700
C	1.73064600	-1.85214700	-0.26201600
N	0.29148500	0.04088500	0.18177300
O	-5.02353900	0.71722600	0.16470300
O	-0.19113500	-1.09727800	2.13718700
O	0.12291300	1.27410900	-1.76602700
H	-3.48527800	-1.05999800	1.76953600
H	-3.18374800	1.15265700	-1.96036300
H	0.83765000	-2.47049300	-0.26964300
C	2.53607700	1.84359200	0.30195500
H	2.02492800	2.30288000	-0.55311100
H	1.85296900	1.94597700	1.15580100
C	3.82301400	2.61010300	0.59611700

H	3.58887200	3.64553800	0.85878800
H	4.37226200	2.16499700	1.43246300
H	4.48602900	2.63473800	-0.27445100
H	-2.24796400	-1.30006200	-2.35402200
H	-2.44199800	-2.65412900	-0.08007400

Energy = -936.620122 Hartree.
Low frequencies (cm^{-1}): 26.4289 39.6690 53.2245 70.0244 77.1961 115.9507 126.4118 152.3054 160.4219 196.5724 227.1484 273.3993.

1a - Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.77659700	-1.17891800	-0.69653200
C	-1.61164300	-2.00178400	-0.05607300
H	-1.85123800	-3.06722300	-0.06259800
C	-0.24972500	-1.77049400	-0.67503800
C	-0.11967300	-0.85182800	1.47672700
C	-1.53657800	-1.38144500	1.34902900
H	-1.73652000	-2.08690400	2.15823300
C	-2.68229300	-0.31240100	1.27527700
C	-2.24310100	0.80480400	0.35177300
C	-2.28806800	0.23704400	-0.92648200
C	-1.88709800	0.94664100	-2.04393500
H	-1.88737400	0.49700000	-3.03296700
C	-1.48998300	2.27779000	-1.85927800
H	-1.19765900	2.87247000	-2.71971800
C	-1.47331500	2.85204800	-0.58958000
H	-1.17442400	3.89117000	-0.47921400
C	-1.83057000	2.11038400	0.54405200
H	-1.78703700	2.55008100	1.53733000
C	1.89545400	-0.73394700	0.01727400

C	2.82011400	-1.70000800	-0.35694600
C	4.14918900	-1.34890700	-0.58347600
H	4.86872900	-2.10577400	-0.87751600
C	4.54025400	-0.02423700	-0.42012600
H	5.57519000	0.26168600	-0.58401800
C	3.61756700	0.95442600	-0.05215600
H	3.94200700	1.98272600	0.05856600
C	2.27973200	0.60934500	0.15253700
C	1.68319100	2.78956500	0.84042000
H	2.41858400	2.75634200	1.65267900
H	0.77566000	3.27983000	1.19176100
N	0.54297100	-1.09803200	0.26241000
O	-3.62124800	-1.01279600	0.44926800
O	0.10860700	-2.10093600	-1.77938800
O	0.37990900	-0.33625100	2.44443800
O	1.29880300	1.48512900	0.46014000
H	-3.30747600	-1.67278200	-1.50773200
H	-3.12769400	-0.04131300	2.23052000
H	2.48650700	-2.72674600	-0.47059400
H	2.09223500	3.34602300	-0.01207800

Energy = -1087.994689 Hartree.
Low frequencies (cm^{-1}): 38.5586 54.2328 58.0854 77.7710 92.9434 98.6346 129.6474 142.6508 183.3576 205.4677 232.1291 250.4072.

1a - Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.66003700	-1.19340000	-1.07493400
C	-1.25828300	-1.82219900	-0.75982700
H	-1.17436300	-2.81520000	-1.20522600

C	-0.07830800	-0.95869800	-1.16288100
C	-0.08439200	-0.94550600	1.17853100
C	-1.26214400	-1.81364000	0.77914000
H	-1.18013700	-2.80164700	1.23589200
C	-2.66538700	-1.18182100	1.08046100
C	-2.60250800	0.28285600	0.69472200
C	-2.59875700	0.27515600	-0.70460800
C	-2.45049600	1.44397300	-1.43090000
H	-2.40930600	1.43619800	-2.51639400
C	-2.34928500	2.64472200	-0.71556500
H	-2.25916800	3.58308600	-1.25527500
C	-2.35332500	2.65257300	0.67986700
H	-2.26630700	3.59701100	1.20942800
C	-2.45852800	1.46002900	1.40838300
H	-2.42349300	1.46488300	2.49411500
C	1.63308200	0.40380600	0.00464600
C	2.91696900	-0.16101300	-0.00138600
C	4.02716100	0.68444000	-0.00336700
H	5.03246000	0.27943700	-0.00834900
C	3.84059200	2.06816500	0.00121300
H	4.71357500	2.71436600	-0.00025100
C	2.56559700	2.62295500	0.00773500
H	2.43219500	3.69960600	0.01146000
C	1.45599800	1.77774300	0.00928600
C	4.24765100	-2.11950600	-0.00938200
H	4.81077400	-1.84026100	-0.90750900
H	4.81645100	-1.84316000	0.88606200
N	0.50764600	-0.46624300	0.00663800
O	-3.43038100	-1.73444300	0.00378700

O	0.28828200	-0.70096200	-2.28285400
O	0.27681000	-0.67588000	2.29748700
O	2.96995000	-1.51414800	-0.00431200
H	-3.08845600	-1.46293300	-2.03822900
H	-3.09867000	-1.44086100	2.04446100
H	0.44094000	2.16716600	0.01427200
H	4.06909900	-3.19433700	-0.01059800

Energy = -1087.995824 Hartree.
Low frequencies (cm^{-1}): 8.8077 45.3274 61.1224 73.9932 82.6054 107.9115 115.6985 140.6224 177.7995 190.0182 246.6214 252.6497.

1b - Folded

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.78843100	-0.82077000	1.19480400
C	1.63657700	-1.84111000	0.92841300
H	1.83316300	-2.77411600	1.46178500
C	0.22846600	-1.37051600	1.23570800
C	0.31775300	-1.57720100	-1.09618400
C	1.69670300	-1.97620400	-0.60395400
H	1.92516900	-2.98739700	-0.94868900
C	2.87788100	-1.01401800	-0.95223400
C	2.43241000	0.41478300	-0.71864500
C	2.37067800	0.53981400	0.67350600
C	1.99176900	1.72789200	1.27293800
H	1.92074900	1.82224000	2.35308900
C	1.72872500	2.82014300	0.43624700
H	1.47159200	3.78092200	0.87514100
C	1.80127200	2.69698700	-0.95108200
H	1.60285100	3.56366900	-1.57630500
C	2.12811300	1.47556600	-1.55235800

H	2.16048000	1.37611600	-2.63357900
C	-1.86379700	-1.00310000	-0.04149700
C	-2.79471500	-2.02342400	0.09372300
C	-4.15845500	-1.74383900	0.05531200
H	-4.88568000	-2.54131900	0.16341800
C	-4.56836500	-0.42603200	-0.11561400
H	-5.62728400	-0.18538400	-0.14126600
C	-3.64105800	0.60609600	-0.25212600
H	-3.99756500	1.62173500	-0.37453500
C	-2.27090200	0.32671200	-0.22311900
C	-1.63468000	2.61492300	-0.44958300
H	-2.46486600	2.74939500	-1.15311700
H	-0.75546500	3.09158900	-0.88385000
N	-0.47508500	-1.31501200	0.02746700
O	3.72145400	-1.23607900	0.18694400
O	-0.23262800	-1.10339700	2.31805400
O	-0.06143300	-1.51476700	-2.23910200
O	-1.28259800	1.23779300	-0.36850400
H	3.23665200	-0.86898500	2.18523400
H	3.40529900	-1.23613800	-1.87771200
C	-1.93570300	3.19525400	0.92205000
H	-2.14377300	4.26718200	0.84038600
H	-2.79712900	2.71031400	1.39024000
H	-1.07070400	3.05326000	1.57696200
H	-2.43287000	-3.03814300	0.23357400

Energy = -1127.261649 Hartree.
Low frequencies (cm^{-1}): 9.2305 49.1328 57.6198 63.9648 75.1450 86.6530 106.1720 123.1361 139.7847 165.3052 187.8823 196.7142.

1b - Unfolded

Atomic Coordinates (Angstroms)

Number	X	Y	Z
C	-2.41225100	-1.73939800	-0.85672500
C	-1.05898700	-2.00607100	-0.11249900
H	-0.78644100	-3.06114000	-0.17823700
C	0.08398900	-1.12684600	-0.57721800
C	-0.44088600	-0.37843600	1.57882300
C	-1.39783500	-1.52352500	1.30786000
H	-1.30245600	-2.28947800	2.07974100
C	-2.89660000	-1.08783000	1.13953600
C	-2.90761300	0.18369100	0.31659700
C	-2.58286700	-0.23713500	-0.97747900
C	-2.38224800	0.67447100	-2.00003100
H	-2.08857700	0.35474300	-2.99576500
C	-2.56335200	2.03208700	-1.70560500
H	-2.43469500	2.77140500	-2.49053900
C	-2.89840300	2.45024100	-0.41723100
H	-3.03145800	3.50959900	-0.21661700
C	-3.05426900	1.52547800	0.62374900
H	-3.27538300	1.85467100	1.63528100
C	1.34247300	0.80946900	0.31713600
C	2.68499700	0.44504600	0.13698500
C	3.63968800	1.44867200	-0.03853600
H	4.68237100	1.19346300	-0.19023600
C	3.25094300	2.78799200	-0.00252800
H	4.00523700	3.55832500	-0.13383200
C	1.92101500	3.14372500	0.20061400
H	1.62799900	4.18797600	0.23021700
C	0.96278400	2.14344500	0.35466000
C	4.19856500	-1.32321900	-0.36370700

H	4.35541000	-0.86327400	-1.34798000
H	5.01427900	-1.01274600	0.30321000
N	0.36818100	-0.21712700	0.44816900
O	-3.34068400	-2.05809300	0.18526400
O	0.63159200	-1.15692200	-1.65167100
O	-0.39167500	0.30588800	2.57159000
O	2.95437400	-0.88012100	0.16320800
H	-2.58924500	-2.34775300	-1.74139000
H	-3.49918500	-1.12102000	2.04475000
H	-0.08793600	2.38037400	0.49920100
C	4.12485100	-2.83160100	-0.47170600
H	3.30237600	-3.11845200	-1.13258700
H	5.06032500	-3.22697800	-0.87845500
H	3.95730400	-3.27738300	0.51276700

Energy = -1127.266307 Hartree.
Low frequencies (cm^{-1}): 20.2200 36.8787 48.0382 65.6496 74.2598 81.7068 112.1348 121.8541 137.6062 167.6842 185.8305 222.6640.

1c – Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-3.23092700	-0.87666000	-0.49899800
C	-2.23137400	-1.83001900	0.23051200
H	-2.69521900	-2.80447700	0.39737300
C	-0.89060400	-2.00251700	-0.44798200
C	-0.44597300	-0.78123900	1.49812200
C	-1.94333100	-1.03852600	1.51730600
H	-2.20814300	-1.57028700	2.43388700
C	-2.87204200	0.21170600	1.32776400
C	-2.27532800	1.08649200	0.24762500

C	-2.48230000	0.36865700	-0.93544500
C	-1.99869000	0.82916300	-2.14728200
H	-2.12734800	0.26068200	-3.06416700
C	-1.34275000	2.06768600	-2.15679600
H	-0.97193900	2.46819900	-3.09579600
C	-1.16607500	2.79635700	-0.98207500
H	-0.66665800	3.76113800	-1.02059000
C	-1.61685900	2.30149300	0.24807700
H	-1.45893800	2.85803100	1.16831600
C	1.46068700	-1.36618400	-0.00559800
C	2.12489800	-2.57392500	-0.19909400
C	3.46731600	-2.58398800	-0.56037400
H	3.98316700	-3.52660600	-0.71016800
C	4.13577000	-1.37331800	-0.73166700
H	5.18291600	-1.36559500	-1.02011100
C	3.47163900	-0.16333500	-0.55406900
H	3.99448700	0.77032800	-0.72243000
C	2.12183900	-0.14282200	-0.18815700
C	1.87841900	2.15701700	0.58958300
H	0.95630400	2.61185900	0.96539000
N	0.08075600	-1.37805300	0.34591800
O	-3.96974800	-0.39169300	0.63011200
O	-0.67325600	-2.57311200	-1.48876600
O	0.19818200	-0.19497100	2.33400400
O	1.37264500	0.97678100	-0.06601600
H	-3.88895800	-1.35373400	-1.22255700
H	-3.20738300	0.68703000	2.24742000
C	2.50409900	3.11655500	-0.41689700
H	2.60923900	4.10827400	0.03651900

H	3.49836600	2.79297900	-0.73901400
H	1.86530100	3.20152900	-1.30105800
H	1.57528400	-3.50116300	-0.06889500
C	2.76792900	1.85346900	1.78759700
H	3.75909300	1.49496100	1.49616800
H	2.90177100	2.77547400	2.36310600
H	2.29271100	1.10533400	2.42760700

Energy = -1166.530333 Hartree.
Low frequencies (cm^{-1}): 34.6298 48.6856 55.0521 68.4881 83.5268 95.2195 97.6312 118.9827 141.8945 161.1650 183.0897 194.5214.

1c – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	2.45244700	-1.84916700	0.84751300
C	1.12398000	-2.01194000	0.03012200
H	0.78875500	-3.05075100	0.04523000
C	0.00982900	-1.08236200	0.46799200
C	0.68264700	-0.29862700	-1.63215100
C	1.56036100	-1.50372800	-1.35472800
H	1.46328100	-2.23813900	-2.15651900
C	3.06869100	-1.15697000	-1.09794600
C	3.10486900	0.08319900	-0.22835900
C	2.69720500	-0.36458600	1.03283500
C	2.49461000	0.51914200	2.07898500
H	2.13901500	0.17925800	3.04745400
C	2.75685400	1.87529100	1.84462400
H	2.62883000	2.59232900	2.65004400
C	3.17239300	2.32029300	0.58913300
H	3.36713100	3.37774200	0.43420000

C	3.33232400	1.42598100	-0.47739400
H	3.61901300	1.77929800	-1.46398000
C	-1.09939700	0.94439700	-0.42339100
C	-2.46464800	0.63905100	-0.32507200
C	-3.37711100	1.68673100	-0.17806200
H	-4.43759300	1.48049400	-0.08475500
C	-2.92477000	3.00481500	-0.16000800
H	-3.64817200	3.80749400	-0.04956400
C	-1.56937100	3.30099300	-0.28308500
H	-1.22649700	4.33027500	-0.27118900
C	-0.65390200	2.25962700	-0.41030900
C	-4.02376000	-1.13776700	0.14265900
H	-4.85540800	-0.57834600	-0.30808700
N	-0.16846400	-0.12470900	-0.53465400
O	3.41304100	-2.18222800	-0.16037300
O	-0.59664900	-1.11753100	1.51122100
O	0.71769200	0.41663000	-2.60334300
O	-2.79266300	-0.67090600	-0.42536400
H	2.55034000	-2.49855500	1.71513000
H	3.71324500	-1.19098800	-1.97374600
H	0.41316000	2.44760500	-0.49461600
C	-4.01554500	-0.96978800	1.65599700
H	-3.91812700	0.07914300	1.95010100
H	-4.94713800	-1.36035900	2.07845600
H	-3.16861200	-1.51818800	2.07936600
C	-4.12552000	-2.59445900	-0.27232700
H	-5.06310300	-3.02542800	0.09137300
H	-4.09239000	-2.68871800	-1.36117600
H	-3.29094700	-3.15970000	0.15555900

Energy = -1166.536854 Hartree.
Low frequencies (cm^{-1}): 24.6125 33.5177 56.6227 62.0092 68.5200 77.9249
88.8274 114.5362 136.0810 163.3689 185.2330 206.4684.

1d - Folded

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	3.48020900	-1.05458400	0.14939600
C	2.51288600	-0.52288200	1.23873000
C	1.38022200	-1.56920000	1.01821500
H	1.56229500	-2.46049600	1.62557800
C	-0.02258800	-1.05961800	1.30790000
C	-0.00163200	-1.50478600	-0.98958300
C	1.39731000	-1.84799100	-0.50856400
H	1.61239200	-2.89039600	-0.76042600
C	2.51800600	-0.91950700	-1.05985400
C	2.12222100	0.52098000	-0.83882300
C	2.12973800	0.76312000	0.54826100
C	1.85895400	2.02764700	1.05321500
C	1.58253500	3.05466400	0.14719100
C	1.56076400	2.81232000	-1.22849200
C	1.82757900	1.53799100	-1.73746900
C	-2.15072400	-0.78366300	0.03281900
C	-3.04633700	-1.82539000	-0.18298000
C	-4.40851100	-1.55613000	-0.27491900
H	-5.11339400	-2.36402600	-0.44394400
C	-4.85233100	-0.24337200	-0.14591400
H	-5.91308200	-0.01905200	-0.21194800
C	-3.94148300	0.79134200	0.06116500
H	-4.30940100	1.80886500	0.14668700

C	-2.56854700	0.54785600	0.14908900
C	-2.08557500	3.06544600	0.20283100
H	-2.55531100	3.22069600	-0.77449800
H	-1.26567400	3.78320200	0.29944900
H	-2.82248000	3.30001500	0.97809500
N	-0.75575700	-1.10363400	0.11899600
O	4.59852200	-1.46885100	0.22342500
O	-0.44770300	-0.68229000	2.37191600
O	-0.41074900	-1.56188100	-2.12194700
H	2.89824200	-0.45493900	2.25420100
H	2.90957200	-1.19004400	-2.03870100
H	-2.66713000	-2.83857500	-0.28139300
C	-1.54812400	1.64500400	0.34364100
H	-0.73969500	1.49130300	-0.38320000
H	-1.08775600	1.52294200	1.33240700
H	1.81223000	1.34956600	-2.80726500
H	1.86602700	2.21367500	2.12372500
H	1.33521500	3.62580300	-1.91209300
H	1.38026800	4.05558500	0.51806400

Energy = -1090.180216 Hartree.
Low frequencies (cm^{-1}): 30.2563 55.9037 66.7329 78.9581 85.0506 101.0659
114.8040 126.7869 147.6843 173.2539 199.9647 217.8754.

1d – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	3.43592600	-1.36355800	0.04411100
C	2.62935800	-0.70512300	1.18884700
C	1.31114800	-1.52160800	1.00063200
H	1.33549300	-2.44272500	1.58835700

C	0.07225900	-0.71563200	1.35582600
C	-0.08769900	-1.08882500	-0.94880100
C	1.21210900	-1.75234500	-0.53136700
H	1.20522600	-2.80525800	-0.82460700
C	2.46539500	-1.02554900	-1.11303300
C	2.31426800	0.45217800	-0.84007200
C	2.42191100	0.64641800	0.54970200
C	2.29740700	1.91171800	1.10700100
C	2.06991900	2.99050500	0.24777200
C	1.95492800	2.79753900	-1.13109500
C	2.07065100	1.52186600	-1.69113200
C	-1.82973300	0.31862000	0.12982200
C	-3.09165400	-0.26817600	-0.02447700
C	-4.18871100	0.59468300	-0.07640400
H	-5.18665600	0.18492700	-0.19651300
C	-4.03038300	1.97634000	0.02879400
H	-4.90447200	2.61986100	-0.01193800
C	-2.76355500	2.53122100	0.18718700
H	-2.63770900	3.60636000	0.27005500
C	-1.65328200	1.69296600	0.23573500
N	-0.66403800	-0.51169400	0.18369900
O	4.46257600	-1.97577900	0.05554200
O	-0.22844700	-0.29659300	2.44512300
O	-0.54683900	-1.03774200	-2.06342900
H	3.06058500	-0.73638600	2.18749700
H	2.75708400	-1.33048200	-2.11613800
H	-0.64714500	2.08875500	0.35361500
C	-3.21668500	-1.77281700	-0.12461700
H	-2.67509600	-2.10292900	-1.02039600

H	-2.69320200	-2.21850300	0.73191200
C	-4.64525500	-2.30636500	-0.17446200
H	-4.63531400	-3.39909200	-0.21630800
H	-5.21630100	-2.00967800	0.71148900
H	-5.17707600	-1.94649700	-1.06113800
H	1.96630900	1.37097900	-2.76191100
H	2.36662100	2.05764600	2.18132700
H	1.76762400	3.65005100	-1.77743200
H	1.97404700	3.99141900	0.65853600

Energy = -1090.179287 Hartree.
Low frequencies (cm^{-1}): 18.5823 36.1148 51.7314 57.4150 72.2709 79.5492 112.2337 119.8440 136.6562 163.5967 172.9488 215.0692.

2a – Folded

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.95479700	-3.20505500	-0.00019900
C	-1.31235600	-2.41468600	-1.16765700
C	0.17172200	-2.66827300	-0.77702800
H	0.52600900	-3.60736900	-1.21173700
C	1.12873100	-1.55489900	-1.17191400
C	1.12845500	-1.55484100	1.17233000
C	0.17150200	-2.66822600	0.77726000
H	0.52572000	-3.60727600	1.21212000
C	-1.31270500	-2.41472000	1.16746800
C	-1.69647200	-1.02737200	0.71540500
C	-1.69620000	-1.02733000	-0.71565800
C	-2.03237000	0.09104800	-1.42343400
C	-2.79017700	2.45190300	-1.39950200
C	-2.40867900	1.26752400	-0.71424400
C	-2.40906800	1.26743300	0.71388200

C	-2.79101000	2.45170400	1.39908600
C	-2.03303500	0.09091300	1.42313400
C	2.67132800	-0.00494000	0.00021400
C	4.00893100	-0.37130700	0.00002800
C	5.00667900	0.60105400	-0.00017600
H	6.05234900	0.31248100	-0.00024200
C	4.63889400	1.94167900	-0.00028200
H	5.40191600	2.71488000	-0.00050700
C	3.29631200	2.32030200	-0.00008200
H	3.04298800	3.37341900	-0.00027400
C	2.29377200	1.34625800	0.00020600
C	0.58447100	2.97099400	0.00053500
H	0.95867200	3.47818700	0.89767400
H	-0.50313000	2.98626000	0.00133700
H	0.95752200	3.47797100	-0.89719500
N	1.66874400	-1.01785800	0.00025400
O	-2.68279500	-4.15376200	-0.00032100
O	1.40094500	-1.19645000	-2.28963800
O	1.40010800	-1.19606200	2.29007900
H	-1.58918900	-2.70958000	-2.17785000
H	-1.58983000	-2.70966500	2.17756500
H	4.25698600	-1.42900500	0.00004900
C	-3.15554300	3.58200100	-0.70852000
C	-3.15597800	3.58189700	0.70804400
H	-2.02602600	0.09720700	-2.51090400
H	-2.02718900	0.09697300	2.51060600
H	-2.78556200	2.44777100	-2.48689100
H	-2.78704400	2.44741900	2.48647600
H	-3.44607400	4.47923000	1.24665200

H	-3.44530000	4.47941500	-1.24717300
O	0.96693500	1.60606600	0.00052300

Energy = -1279.631571 Hartree.
Low frequencies (cm^{-1}): 27.4342 55.7589 62.0341 65.2614 73.2641 88.8729
100.0697 112.6838 119.5772 137.1305 171.5417 200.9820.

2a - Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-2.11192300	-3.17005700	-0.04999500
C	-1.38186700	-2.37872100	-1.15845400
C	0.06611500	-2.54714000	-0.59822700
H	0.51817400	-3.47341900	-0.96125100
C	0.95197200	-1.36192200	-0.94006600
C	0.66792000	-1.25951600	1.38420300
C	-0.11063100	-2.48962700	0.94509100
H	0.26334000	-3.37315200	1.46831600
C	-1.64974300	-2.32361600	1.15720100
C	-2.02029200	-0.95891200	0.63044800
C	-1.84657500	-0.98930800	-0.78978900
C	-2.01905100	0.13573800	-1.54630800
C	-2.56439100	2.55357700	-1.63915100
C	-2.39023800	1.35187900	-0.90258300
C	-2.57172500	1.37945300	0.51372700
C	-2.91886400	2.60766700	1.13741900
C	-2.37319800	0.19238000	1.27656500
C	1.94407400	0.55322900	0.26770800
C	3.31901700	0.52040600	-0.00693100
C	4.03522300	1.71816100	-0.00907600
H	5.09735000	1.72639400	-0.22493000

C	3.37778200	2.91666800	0.27508700
H	3.94857700	3.84070400	0.27304300
C	2.01583200	2.94147300	0.55643500
H	1.51214800	3.87743000	0.77371500
C	1.29659000	1.74722300	0.54626100
N	1.21279100	-0.66649500	0.24358900
O	-2.78472300	-4.15789000	-0.10370000
O	1.33095200	-1.03235500	-2.03520000
O	0.77402500	-0.83626400	2.50807300
H	-1.52667500	-2.70774400	-2.18561500
H	-2.02114200	-2.60908900	2.13924600
C	-2.89849700	3.72605700	-1.00741400
C	-3.07782000	3.75350000	0.39748300
H	-1.85696000	0.12531500	-2.62171600
H	-2.47915500	0.22464900	2.35858600
H	-2.42146600	2.52837000	-2.71670000
H	-3.05297600	2.62355000	2.21643200
H	-3.34137100	4.68593800	0.88808900
H	-3.02504500	4.63826200	-1.58304000
H	0.22842200	1.72844400	0.75003700
O	3.84638500	-0.70312800	-0.24433900
C	5.20651600	-0.77030300	-0.62411400
H	5.41336000	-1.82377600	-0.80986700
H	5.38483900	-0.19413400	-1.53947200
H	5.85856200	-0.40492000	0.17821700

Energy = -1279.631981 Hartree.
Low frequencies (cm^{-1}): 21.9970 26.1406 42.6462 47.2955 77.2931 89.4745
94.7360 107.2317 113.8173 139.5003 174.0127 198.1275.

2d - Folded

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
C	1.81161000	3.28070500	-0.02100500
C	1.21596000	2.44868300	-1.18480200
C	-0.28188900	2.63357500	-0.80860800
H	-0.68228600	3.54256000	-1.26685600
C	-1.18014200	1.46357900	-1.18057400
C	-1.22357900	1.54123200	1.15868900
C	-0.29457300	2.67037500	0.74487900
H	-0.67755000	3.60908100	1.15537000
C	1.19490600	2.47477900	1.15080200
C	1.64616100	1.10069800	0.71752100
C	1.66387200	1.08718300	-0.71431900
C	2.07718000	-0.01518300	-1.40696300
C	2.96069600	-2.33197700	-1.35554400
C	2.50220600	-1.16756400	-0.68424600
C	2.47863100	-1.15781100	0.74359700
C	2.90625300	-2.31747100	1.44304100
C	2.03819400	0.00740900	1.43790700
C	-2.71570900	-0.09231000	0.02093100
C	-4.05037400	0.27242800	0.15034100
C	-5.03387900	-0.71212700	0.18494700
H	-6.07854200	-0.43536100	0.28652300
C	-4.66045400	-2.04922200	0.08970200
H	-5.41710900	-2.82828100	0.11707800
C	-3.31649200	-2.39943800	-0.03593500
H	-3.04683900	-3.44892400	-0.10157300
C	-2.31256300	-1.42948600	-0.07246600
C	-0.49680100	-3.24294900	-0.11252600
H	-0.84385700	-3.67746200	0.83141000

H	0.58802200	-3.37386800	-0.16453600
H	-0.94054900	-3.81265400	-0.93611000
N	-1.73136000	0.95132000	-0.00308500
O	2.49609300	4.26094200	-0.02532000
O	-1.39476000	1.03999800	-2.28894700
O	-1.49120000	1.19960600	2.28334000
H	1.48747300	2.74536800	-2.19588100
H	1.45098400	2.79285500	2.15950500
H	-4.30791700	1.32524000	0.22561500
C	-0.84426900	-1.76097900	-0.20135200
H	-0.30095700	-1.21724100	0.58237900
H	-0.47965200	-1.35452800	-1.15458200
C	3.34957200	-3.42726600	0.76532300
H	3.67600200	-4.30539400	1.31456900
C	3.37974200	-3.43383300	-0.65026000
H	3.73053300	-4.31633200	-1.17715500
H	2.87970200	-2.30916900	2.53004000
H	2.97578400	-2.33403000	-2.44285900
H	2.02488300	0.01136600	2.52553300
H	2.09113000	-0.02705300	-2.49461100

Energy = -1509.370027 Hartree.
Low frequencies (cm^{-1}): 14.5347 40.9828 41.7781 62.4599 68.4975 68.9337 90.5634 102.1966 108.3654 113.5296 152.7937 160.0339.

2d – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	2.06847700	-3.20254100	-0.03601300
C	1.58105900	-2.35703700	1.16297200
C	0.04758200	-2.51298900	0.91037800

H	-0.34310300	-3.39804600	1.41886700
C	-0.73936400	-1.28256300	1.33325200
C	-0.96125700	-1.37194400	-0.99494700
C	-0.08943000	-2.56218100	-0.63682400
H	-0.53697300	-3.48428900	-1.01625800
C	1.37220600	-2.40050900	-1.15963900
C	1.84230800	-1.01776900	-0.77329100
C	1.98219300	-0.99535600	0.65094100
C	2.35670600	0.14299600	1.30778600
C	2.98355100	2.53961600	1.18704600
C	2.60969300	1.32489100	0.55261900
C	2.45569600	1.30695000	-0.86714100
C	2.68257100	2.50424500	-1.59642700
C	2.06272100	0.10380700	-1.52247700
C	-1.94342000	0.57519900	0.19931000
C	-3.32213000	0.63362100	-0.03782600
C	-3.91396000	1.89871000	-0.01769900
H	-4.98042100	1.99363800	-0.19656900
C	-3.16461100	3.04753700	0.23509200
H	-3.65688700	4.01584700	0.24601200
C	-1.79645000	2.95826500	0.47503900
H	-1.20878300	3.84892000	0.67487900
C	-1.18196000	1.71005100	0.45491000
N	-1.27025200	-0.68949400	0.18265400
O	2.73644600	-4.19386700	-0.07701700
O	-0.87109500	-0.86104200	2.45463900
O	-1.31108400	-1.04066100	-2.10111700
H	1.92499400	-2.64977900	2.15279900
H	1.54051600	-2.72634300	-2.18422000

C	3.04162300	3.66361800	-0.95431300
H	3.20986200	4.57256600	-1.52431100
C	3.19397100	3.68150200	0.45391200
H	3.47784900	4.60363900	0.95254900
H	-0.11504200	1.60464800	0.63642100
C	-4.09963300	-0.63865200	-0.29776500
H	-3.73290500	-1.08066800	-1.23296000
H	-3.85708900	-1.35722900	0.49654700
C	-5.61445600	-0.47255200	-0.37799900
H	-6.08961800	-1.44674700	-0.52351800
H	-6.01951400	-0.03516900	0.54058600
H	-5.90574600	0.16523700	-1.21866600
H	1.92836000	0.09930900	-2.60172400
H	2.56040100	2.48632400	-2.67664100
H	3.09622800	2.54873100	2.26854500
H	2.44337600	0.16894100	2.39167700

Energy = -1509.369720 Hartree.
Low frequencies (cm^{-1}): 19.5474 23.9981 31.0799 48.0374 66.6373 76.4412
83.0888 90.8757 108.9313 121.1519 151.9711 164.6402.

3a - Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.92686600	3.03060100	-0.51841100
C	-1.07784000	2.61272500	0.70664200
C	0.32010100	2.88605200	0.07879200
H	0.60583900	3.93320800	0.21190400
C	1.40156500	1.98669000	0.64333000
C	1.16363500	1.32893600	-1.59293200
C	0.16252800	2.45826000	-1.40254700
H	0.38444600	3.25593300	-2.11674800
C	-1.32995400	2.01554900	-1.52359900
C	-1.54057500	0.78347800	-0.67657500
C	-1.36513500	1.13023300	0.63578700
C	-1.46679000	0.16858200	1.69383700
C	-1.16718700	0.50007500	3.03217400
H	-0.82452200	1.50448800	3.26446600
C	-1.27161300	-0.44576200	4.02959000

H	-1.02957200	-0.18630100	5.05566700
C	-1.67735500	-1.75218400	3.70832600
H	-1.75601200	-2.50263200	4.48945400
C	-1.96503800	-2.09476100	2.40185100
H	-2.25577700	-3.11730200	2.18756900
C	-1.86919400	-1.15112600	1.35609900
C	-2.15206000	-1.49588600	-0.03646200
C	-2.64332400	-2.76461600	-0.41560700
H	-2.85318600	-3.51304700	0.34058200
C	-2.87419600	-3.08251600	-1.74021000
H	-3.25855100	-4.06493000	-1.99869300
C	-2.60604500	-2.14479800	-2.75289700
H	-2.77016500	-2.40363400	-3.79457100
C	-2.13804100	-0.89162900	-2.41495000
H	-1.92345800	-0.16211000	-3.19057700
C	-1.92971700	-0.54026400	-1.06436100
C	2.80452400	0.11634400	-0.16655800
C	4.08772800	0.45469900	0.23934200
C	5.04087300	-0.53993100	0.44667300
H	6.04397200	-0.27521600	0.76360500
C	4.69157700	-1.87000300	0.23592700
H	5.42682500	-2.65485000	0.38731400
C	3.40219700	-2.21907300	-0.16450100
H	3.14823400	-3.26270800	-0.30973400
C	2.43883700	-1.22543300	-0.35570300
C	0.82784800	-2.74759300	-1.17814100
H	1.53432800	-3.06009100	-1.95569900
H	-0.17136800	-2.67039700	-1.60315800
H	0.82426900	-3.47725500	-0.35871500
N	1.82869300	1.13035500	-0.37425700
O	-2.75983800	3.87696300	-0.65128400
O	1.82175600	1.99190500	1.77422500
O	1.37480300	0.71616100	-2.60781500
O	1.15363400	-1.45472300	-0.70104400
H	-1.27943800	3.13014600	1.64262500
H	-1.74102900	2.02970400	-2.53080000
H	4.32858600	1.50216000	0.39316500

Energy = -1433.174103 Hartree.
Low frequencies (cm^{-1}): 24.8086 44.5212 61.2155 65.0625 70.6025 82.4432
88.6782 106.5264 116.6930 134.5190 136.0356 152.9122.

3a – Unfolded

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.91577200	3.14322400	-0.30237600
C	-1.12138300	2.51646900	0.86392200
C	0.30403900	2.62044700	0.22828800
H	0.77562700	3.57664600	0.46927200
C	1.20246200	1.47144600	0.65718600
C	0.86544900	1.15597600	-1.63912300
C	0.06646400	2.39830800	-1.28798700
H	0.37792900	3.23475600	-1.91866700
C	-1.47285100	2.15256700	-1.40098700

C	-1.78617200	0.87471000	-0.65721700
C	-1.59125000	1.09208000	0.67986800
C	-1.74784000	0.04842200	1.64975800
C	-1.50866300	0.26700700	3.02324900
H	-1.16124500	1.24220000	3.35107100
C	-1.69035200	-0.74707700	3.93784200
H	-1.50030200	-0.57178600	4.99228700
C	-2.11613300	-2.01222900	3.49724500
H	-2.26538900	-2.81307600	4.21534900
C	-2.33452200	-2.24870600	2.15493100
H	-2.65233900	-3.23923600	1.84979500
C	-2.14967100	-1.23434200	1.18934800
C	-2.32667900	-1.47522500	-0.24257300
C	-2.65731800	-2.74759900	-0.76016500
H	-2.82340300	-3.58168800	-0.08774600
C	-2.76496500	-2.96652300	-2.11929000
H	-3.01620600	-3.95794900	-2.48475700
C	-2.53858700	-1.92006800	-3.03038100
H	-2.60289500	-2.10236500	-4.09867300
C	-2.22273600	-0.66421900	-2.55911500
H	-2.01873000	0.14474500	-3.25448200
C	-2.12463800	-0.41932500	-1.17239200
C	2.21806300	-0.52026000	-0.40850600
C	3.56998100	-0.45944900	-0.03880700
C	4.29541100	-1.64746500	0.06339500
H	5.33804500	-1.63328700	0.35940900
C	3.67604500	-2.86332500	-0.22972600
H	4.25424900	-3.77956200	-0.15224000
C	2.34219100	-2.91452400	-0.62069000
H	1.86948600	-3.86339300	-0.85117100
C	1.60958500	-1.73162700	-0.70365700
N	1.47010500	0.68763300	-0.47104700
O	-2.62201500	4.10679300	-0.34708600
O	1.58448400	1.23388600	1.77449900
O	0.93853600	0.63110900	-2.72282900
H	-1.23476800	2.98164000	1.84078200
H	-1.89780100	2.29515000	-2.39248700
O	4.07317400	0.77782900	0.17854700
C	5.38163300	0.87187900	0.70563800
H	5.56103100	1.93352300	0.87269900
H	5.45736800	0.33204600	1.65656200
H	6.12208900	0.48315700	-0.00339800
H	0.56233400	-1.73532500	-0.99739400

Energy = -1433.172526 Hartree.
Low frequencies (cm^{-1}): 11.3757 23.7737 27.3962 51.4295 63.2922 75.9704
88.2755 96.0938 106.6506 118.3408 125.4985 151.5678.

3b – Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.99905300	3.10418600	-0.58451700
C	-1.22657700	2.67829300	0.68854600
C	0.20519600	2.99652200	0.16561200

H	0.45390800	4.04677100	0.34207900
C	1.27938100	2.11491500	0.77545000
C	1.19959200	1.50751500	-1.48538300
C	0.15866500	2.60513000	-1.33369600
H	0.40764600	3.42778400	-2.00988100
C	-1.30698500	2.12722900	-1.56714900
C	-1.54264900	0.87133200	-0.76297800
C	-1.47811600	1.19334800	0.56543900
C	-1.67115600	0.21410900	1.59365400
C	-1.50699300	0.52819000	2.95915700
H	-1.18482900	1.52785500	3.23622300
C	-1.72162400	-0.42654000	3.92983600
H	-1.58464200	-0.18034600	4.97831800
C	-2.10729900	-1.72452000	3.55362500
H	-2.27710000	-2.48088300	4.31417700
C	-2.25915300	-2.05121000	2.22054000
H	-2.54238900	-3.06732600	1.96756400
C	-2.04029400	-1.09969100	1.19983200
C	-2.15992000	-1.43151500	-0.21956400
C	-2.55789300	-2.71170900	-0.66537200
H	-2.81527600	-3.48222800	0.05345800
C	-2.63014900	-3.01688800	-2.01062200
H	-2.94274000	-4.00974800	-2.32067200
C	-2.29200000	-2.05366200	-2.97742900
H	-2.32938400	-2.30321100	-4.03351700
C	-1.91008100	-0.79034600	-2.57611200
H	-1.63291200	-0.04284800	-3.31403000
C	-1.85860200	-0.45445900	-1.20632200
C	2.83533700	0.35292000	-0.01941300
C	4.09817100	0.76956800	0.37782400
C	5.11684300	-0.16215200	0.56058200
H	6.10329300	0.16173200	0.87452500
C	4.85243600	-1.50774800	0.32409300
H	5.63888400	-2.24625600	0.44943100
C	3.58365000	-1.93510600	-0.06453300
H	3.40440100	-2.99067700	-0.22977800
C	2.54992700	-1.00683000	-0.22146900
C	0.95818500	-2.62333000	-0.98171600
H	1.75496500	-2.99130500	-1.63997100
H	0.05600900	-2.50391500	-1.58492800
N	1.80508700	1.31049100	-0.23759100
O	-2.84278600	3.93256300	-0.75626500
O	1.62751200	2.10043400	1.93058200
O	1.47850300	0.91366000	-2.49556400
O	1.27424000	-1.30186800	-0.54925900
H	-1.50582600	3.17070500	1.61799700
H	-1.64877900	2.15156400	-2.59979100
H	4.27180500	1.82935400	0.53951200
C	0.69532900	-3.56030600	0.18647800
H	0.32634700	-4.52108400	-0.18855700
H	1.59174000	-3.74313800	0.78565300
H	-0.06549100	-3.12803500	0.84301700

Energy = -1472.443982 Hartree.
Low frequencies (cm^{-1}): 25.6956 45.6839 50.8953 61.3804 67.9399 80.8356 86.4194 94.9507 103.9059 119.8628 126.0176 147.8220.

3b – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.65174700	3.30297900	-0.50937400
C	-0.87450600	2.66059800	0.66007800
C	0.50281700	2.50146700	-0.06516300
H	1.11953000	3.39525000	0.06025000
C	1.25992200	1.27274100	0.41223600
C	0.71004800	0.82133900	-1.81871500
C	0.12782600	2.19458400	-1.53798700
H	0.51160400	2.91963800	-2.25993000
C	-1.43430500	2.17260000	-1.53836500
C	-1.87395900	1.01920800	-0.66608300
C	-1.55716400	1.31229000	0.63265400
C	-1.80206600	0.38823400	1.70116300
C	-1.45212400	0.68407700	3.03594000
H	-0.94739300	1.62028600	3.25496400
C	-1.72850700	-0.20837400	4.04860500
H	-1.45471500	0.02550900	5.07288000
C	-2.36253200	-1.42611000	3.74739300
H	-2.58772100	-2.13042300	4.54283100
C	-2.69185000	-1.74031300	2.44433900
H	-3.17296800	-2.69195800	2.24856900
C	-2.41489300	-0.85267300	1.38108000
C	-2.71162900	-1.18439000	-0.01180000
C	-3.24138900	-2.43728500	-0.39315800
H	-3.46698700	-3.18382900	0.36004200
C	-3.46684900	-2.75047000	-1.71894600
H	-3.86873800	-3.72532800	-1.97943400
C	-3.16644500	-1.82268000	-2.73151200
H	-3.32754400	-2.08018000	-3.77379900
C	-2.65395800	-0.58881600	-2.39386300
H	-2.39255000	0.12452900	-3.16989700
C	-2.42857200	-0.24790600	-1.04276000
C	1.87614600	-0.94020900	-0.52164000
C	3.23782000	-1.06689300	-0.21073000
C	3.77438600	-2.34445300	-0.03940200
H	4.82107400	-2.47064300	0.21307800
C	2.96150900	-3.46511800	-0.21107400
H	3.39413000	-4.45292400	-0.08143300
C	1.61777800	-3.33271800	-0.54815500
H	0.99335400	-4.20933300	-0.68548300
C	1.07349800	-2.05873800	-0.69780400
N	1.32009700	0.36261200	-0.64901300
O	-2.21459600	4.35376800	-0.59969200
O	1.69406000	1.08210600	1.52017400
O	0.62798800	0.20436700	-2.85202100
H	-0.84939100	3.21484600	1.59577300
H	-1.90373700	2.29744600	-2.51208500
O	3.93854300	0.08620200	-0.11858100
C	5.21866400	0.04875500	0.49832000
H	5.13652600	-0.46550000	1.46486600
H	5.91938000	-0.50857300	-0.13802200
H	0.02464200	-1.91932600	-0.95046800

C	5.66855400	1.48304200	0.67909600
H	4.95549900	2.02269700	1.30829400
H	6.65281300	1.51221500	1.15592100
H	5.73572700	1.98716900	-0.28910300

Energy = -1472.443045 Hartree.

Low frequencies (cm^{-1}): 19.2978 23.0241 26.2916 46.4136 55.8032 68.5568 75.9356 92.7538 103.4779 105.5235 114.4307 125.9514.

3c – Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	2.78664400	-2.46823800	-1.02869000
C	1.93330000	-2.49310400	0.26257400
C	0.62187200	-3.02157800	-0.38987900
H	0.64358600	-4.11267900	-0.46092800
C	-0.62951100	-2.58688400	0.34467000
C	-0.69208800	-1.44223000	-1.69567600
C	0.56500800	-2.30122400	-1.76079300
H	0.48199300	-2.98507600	-2.61032900
C	1.89632500	-1.48930000	-1.83174700
C	1.83924400	-0.40347600	-0.78531300
C	1.82559300	-0.99624900	0.44840800
C	1.71577500	-0.22883800	1.65417800
C	1.59336700	-0.84252100	2.91875600
H	1.56190800	-1.92662200	2.98049400
C	1.48033500	-0.07975600	4.06136700
H	1.37520500	-0.55913800	5.02978300
C	1.48568600	1.32200900	3.96444100
H	1.39250600	1.92713800	4.86152600
C	1.59724400	1.93791000	2.73357200
H	1.58265800	3.02170500	2.69489500
C	1.71378800	1.18759900	1.54340300
C	1.81445400	1.81967300	0.22907500
C	1.88176700	3.22096400	0.06598600
H	1.88833700	3.86926500	0.93540600
C	1.94026800	3.79994100	-1.18706200
H	1.99275000	4.88114100	-1.27759500
C	1.92853000	2.99858600	-2.34258500
H	1.96210200	3.45751200	-3.32616300
C	1.87620100	1.62590600	-2.21796000
H	1.85560600	0.99794700	-3.10374100
C	1.83450800	1.01924700	-0.94448800
C	-2.54397700	-1.07881000	-0.06636600
C	-3.65031600	-1.87403500	0.21185000
C	-4.84168400	-1.29082900	0.62841900
H	-5.70626900	-1.90913900	0.84563500
C	-4.90604500	0.09385200	0.76727600
H	-5.82814800	0.56457400	1.09606900
C	-3.79551100	0.89143400	0.50613300
H	-3.85832000	1.96265300	0.64896900
C	-2.59218900	0.31491300	0.08554700
C	-1.43276000	2.29873900	-0.73635500
H	-0.42376900	2.34363400	-1.14934600

N	-1.32638300	-1.69468900	-0.47507400
O	3.79585100	-3.03819600	-1.31905300
O	-0.97436900	-2.93695500	1.44618200
O	-1.09518200	-0.69043600	-2.54817200
O	-1.43889900	0.98665200	-0.13141800
H	2.31383500	-3.08815000	1.09066600
H	2.23617000	-1.23032300	-2.83225800
H	-3.56215500	-2.95076000	0.10127100
C	-1.55369000	3.40059600	0.31103800
H	-1.19447700	4.34321500	-0.11663800
H	-2.58199700	3.55854200	0.64987800
H	-0.93277400	3.15884900	1.17981200
C	-2.40795800	2.42642200	-1.89837000
H	-3.45056800	2.50005300	-1.57657500
H	-2.16319000	3.33725300	-2.45516400
H	-2.30457400	1.56837500	-2.56891600

Energy = -1511.711028 Hartree.
Low frequencies (cm^{-1}): 26.8102 31.9019 54.3045 60.2801 71.6844 75.1503
85.0036 93.2027 102.7100 105.8266 123.5786 135.6625.

3c – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.82161400	3.33444100	-0.23952600
C	-0.95206300	2.61884300	0.81681900
C	0.35409800	2.49757700	-0.03498000
H	0.98451000	3.38311300	0.08073300
C	1.14142100	1.24532500	0.31232900
C	0.38314200	0.90174200	-1.87491500
C	-0.15258600	2.26647400	-1.48172700
H	0.18107100	3.02008100	-2.19951100
C	-1.71013800	2.26474400	-1.34767900
C	-2.08958600	1.06695800	-0.50794700
C	-1.64716800	1.27721400	0.77009400
C	-1.79169800	0.28609800	1.79589600
C	-1.29189300	0.48624900	3.10033200
H	-0.74979200	1.40026500	3.32378100
C	-1.46474900	-0.47330000	4.07385100
H	-1.07198900	-0.31433200	5.07344800
C	-2.14511900	-1.66336700	3.76299900
H	-2.28904700	-2.42058700	4.52797800
C	-2.62127500	-1.88416500	2.48649800
H	-3.13150900	-2.81820200	2.28018100
C	-2.45218100	-0.92641500	1.46195700
C	-2.90160200	-1.16156400	0.09012100
C	-3.50277900	-2.37586900	-0.30996200
H	-3.67388900	-3.16253700	0.41604200
C	-3.87233900	-2.59857200	-1.62143700
H	-4.32799600	-3.54505100	-1.89758500
C	-3.65065600	-1.61515100	-2.60151500
H	-3.92446300	-1.80298000	-3.63517300
C	-3.07263600	-0.41638800	-2.24421600
H	-2.87445000	0.33987200	-2.99806200

C	-2.70217100	-0.16661400	-0.90504700
C	1.66301400	-0.91843500	-0.77659000
C	3.04391100	-1.05247100	-0.57484100
C	3.58973600	-2.33698500	-0.51220200
H	4.65175300	-2.47321100	-0.34003600
C	2.76852300	-3.44982800	-0.682810
H	3.20958600	-4.44137600	-0.63554200
C	1.40272600	-3.30630200	-0.91539900
H	0.77107500	-4.17758300	-1.05359800
C	0.84889000	-2.02981700	-0.95690300
N	1.09735100	0.38690800	-0.78975000
O	-2.37773000	4.39232300	-0.21801200
O	1.67146600	1.00166400	1.36784400
O	0.19674800	0.33123800	-2.92098800
H	-0.83944200	3.11419400	1.77894300
H	-2.25898300	2.45127400	-2.26841400
O	3.75151700	0.09980100	-0.50219400
C	5.01715200	0.11454100	0.17138400
H	5.67692200	-0.62801900	-0.29876600
H	-0.21504700	-1.88089500	-1.12680700
C	5.57894000	1.50333900	-0.07451700
H	4.91295100	2.25325900	0.36506700
H	6.56680100	1.59996400	0.38569900
H	5.66873300	1.69889100	-1.14659500
C	4.83959000	-0.18107600	1.65402200
H	4.39916900	-1.16790100	1.82225000
H	5.81027200	-0.14477900	2.15941000
H	4.17296800	0.56461900	2.09707500

Energy = -1511.713087 Hartree.
Low frequencies (cm^{-1}): 20.2870 23.5555 29.7630 48.2665 64.8738 69.7882
75.8149 86.1399 94.1867 106.2842 114.7020 123.2567.

3d – Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.82352700	3.16926000	-0.18591900
C	-1.09919100	2.49921500	1.00785400
C	0.35809200	2.77957200	0.53140300
H	0.68161100	3.77224700	0.85756100
C	1.37642500	1.75133600	0.99332600
C	1.24605400	1.47797900	-1.32582300
C	0.29223700	2.61942600	-1.00977600
H	0.61217800	3.51117800	-1.55656300
C	-1.20281800	2.29771300	-1.30509900
C	-1.53192300	0.95593700	-0.69485300
C	-1.46299400	1.07291900	0.66762500
C	-1.72666200	-0.03555300	1.53726300
C	-1.56713800	0.06260100	2.93571600
H	-1.20938500	0.99525200	3.36231100
C	-1.82911000	-1.01850800	3.74974400
H	-1.69636300	-0.93805000	4.82427900
C	-2.25650600	-2.22973000	3.17911900
H	-2.46385800	-3.08498900	3.81554100

C	-2.40396500	-2.34641600	1.81109000
H	-2.72126000	-3.30087700	1.40560000
C	-2.14088300	-1.26070500	0.94704900
C	-2.23653700	-1.37754600	-0.50768700
C	-2.62857000	-2.57494200	-1.14607000
H	-2.91923200	-3.43665000	-0.55502000
C	-2.64095200	-2.68697200	-2.52215400
H	-2.94145500	-3.62403500	-2.9817240
C	-2.25737000	-1.60133200	-3.32876800
H	-2.24799600	-1.70125200	-4.4097810
C	-1.89027600	-0.41096300	-2.73881200
H	-1.57547600	0.42905000	-3.35123400
C	-1.88860900	-0.27551700	-1.33418200
C	2.91214900	0.10798500	-0.07253100
C	4.21969800	0.55356900	0.08395600
C	5.25979100	-0.36850400	0.15327200
H	6.28273900	-0.02696900	0.27626000
C	4.97028000	-1.72667400	0.06251500
H	5.77161600	-2.45824700	0.11417300
C	3.65312000	-2.15829400	-0.08769100
H	3.44975100	-3.22281600	-0.14651800
C	2.59156100	-1.25270600	-0.15462500
C	0.90427500	-3.18222800	-0.16237200
H	1.39563900	-3.74544900	-0.96284200
H	-0.16780300	-3.38866500	-0.22597800
H	1.26640900	-3.56143300	0.79940700
N	1.87125200	1.09261200	-0.13699800
O	-2.59415100	4.08092000	-0.23057900
O	1.71037800	1.52623300	2.12986400
O	1.43921700	0.97782400	-2.40646600
H	-1.34642800	2.87192700	1.99991800
H	-1.53575800	2.49922800	-2.32117600
H	4.41123000	1.62072100	0.15361500
C	1.14956600	-1.68287100	-0.29650500
H	0.77356300	-1.33377100	-1.26807800
H	0.56065300	-1.15281300	0.46429000

Energy = -1397.262318 Hartree.
Low frequencies (cm^{-1}): 24.6947 36.8862 50.7445 56.6791 73.1485 75.1648 82.4876 101.9794 106.3452 121.3173 126.7309 158.1383.

3d – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.92765600	3.15560800	-0.25241900
C	-1.15987000	2.50511600	0.91958500
C	0.28099600	2.64959100	0.33029900
H	0.72551600	3.60853500	0.60934600
C	1.18679400	1.50811500	0.76056100
C	0.91491500	1.22974500	-1.54466400
C	0.09293500	2.45810000	-1.19638800
H	0.41548800	3.31051700	-1.79956400
C	-1.43992000	2.20075900	-1.36423100
C	-1.76578600	0.90039200	-0.66575800

C	-1.60684200	1.08108000	0.68162400
C	-1.78318900	0.00993800	1.61768200
C	-1.56851900	0.18812000	3.00103500
H	-1.22327000	1.15212500	3.36269800
C	-1.76777000	-0.85220000	3.88193900
H	-1.59571500	-0.70876800	4.94425200
C	-2.18757400	-2.10287300	3.39651400
H	-2.35088500	-2.92422800	4.08794000
C	-2.38174100	-2.29967200	2.04409500
H	-2.69564300	-3.28017000	1.70445100
C	-2.17773100	-1.25798200	1.11224000
C	-2.32630800	-1.45712400	-0.32920200
C	-2.64812600	-2.71368800	-0.88902600
H	-2.83277300	-3.56529300	-0.24385800
C	-2.72326400	-2.89506700	-2.25580100
H	-2.96742100	-3.87548800	-2.65436600
C	-2.47194700	-1.82493700	-3.13216500
H	-2.51048300	-1.97821500	-4.20620200
C	-2.16359700	-0.58361000	-2.61943400
H	-1.93974700	0.24297900	-3.28746500
C	-2.09822200	-0.37701900	-1.22464200
C	2.20084100	-0.50045700	-0.30908300
C	3.56150000	-0.53317200	0.02253100
C	4.16936300	-1.79068500	0.07075800
C	3.45709300	-2.95576600	-0.21002500
H	3.96233300	-3.91633000	-0.16472700
C	2.10898300	-2.89100700	-0.55155000
H	1.55007900	-3.79338200	-0.77915600
C	1.47738500	-1.65312900	-0.59993700
N	1.50406200	0.75029100	-0.36890600
O	-2.64504300	4.11079000	-0.29130500
O	1.55075800	1.26632100	1.88528300
O	1.02240800	0.72266200	-2.63325200
H	-1.30804000	2.94076500	1.90535500
H	-1.83508900	2.36771900	-2.36419300
H	0.42675600	-1.57045600	-0.86873400
H	5.22207500	-1.86466100	0.32491500
C	4.31104200	0.75121200	0.30348600
H	4.05830100	1.47443600	-0.48332800
H	3.92891000	1.17496700	1.24013700
C	5.82883700	0.61503100	0.38970300
H	6.28414600	1.59971200	0.52844100
H	6.13089800	-0.00801300	1.23748400
H	6.24542800	0.17650500	-0.52324700

Energy = -1397.259349 Hartree.
Low frequencies (cm^{-1}): 17.2814 24.6129 35.9201 49.0118 57.4678 67.6747
79.4607 94.1809 106.8189 119.5381 125.2102 150.1086.

3e – Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.55282600	3.49202500	-1.05319700
C	0.19524800	3.02447400	0.21814400

C	1.53022600	2.61579700	-0.47116900
H	2.20168200	3.47479300	-0.55795600
C	2.24432400	1.48614400	0.24564600
C	1.59148600	0.58616400	-1.81638700
C	1.09056900	2.02164400	-1.83342000
H	1.51925100	2.53750900	-2.69710900
C	-0.46411700	2.15778400	-1.83313700
C	-1.03248700	1.27986500	-0.74366900
C	-0.62740600	1.77996800	0.46467500
C	-0.99012000	1.14870600	1.69889800
C	-0.48122900	1.59231100	2.93816500
H	0.22570000	2.41711000	2.95343200
C	-0.84457700	0.96835700	4.11229500
H	-0.44036200	1.31107400	5.05994400
C	-1.72705000	-0.12457200	4.07428800
H	-2.00909000	-0.62647800	4.99520100
C	-2.22674800	-0.57668400	2.86883200
H	-2.88737200	-1.43664900	2.87421900
C	-1.87822100	0.04028700	1.64796500
C	-2.38322000	-0.43620600	0.35974900
C	-3.33159600	-1.47409000	0.26327500
H	-3.73592800	-1.92995800	1.16160400
C	-3.77967000	-1.94484900	-0.96374000
C	-3.25433200	-1.38577100	-2.15086100
H	-3.57460600	-1.77472200	-3.11423800
C	-2.34105200	-0.35950700	-2.08310700
H	-1.93707300	0.06058000	-2.99980800
C	-1.90669500	0.15216300	-0.84195000
C	2.80740900	-0.88176700	-0.21933900
C	4.16074900	-0.97738300	0.07139700
C	4.71415200	-2.20395500	0.43219900
H	5.77208700	-2.27819300	0.66041000
C	3.89564500	-3.32748800	0.48929100
H	4.31473100	-4.29180300	0.76196600
C	2.53285300	-3.23867700	0.20669400
H	1.91256800	-4.12519800	0.26879300
C	1.97149300	-2.00690700	-0.13766200
C	-0.16331700	-2.93936900	-0.54252100
H	0.26902400	-3.63525000	-1.27057900
H	-1.11888100	-2.57182200	-0.91156900
H	-0.31035500	-3.44568800	0.41950000
N	2.24068800	0.36875300	-0.59268000
O	-1.03282700	4.54670000	-1.34633100
O	2.73131300	1.53027800	1.34856700
O	1.47704800	-0.22791800	-2.69678800
O	0.66249300	-1.79951400	-0.39095700
H	0.28723600	3.74863300	1.02532700
H	-0.93418700	2.13547700	-2.81429900
H	4.77233400	-0.08192800	0.01533300
N	-4.67594700	-3.01224300	-1.04248300
H	-5.24958100	-3.14986300	-0.21956400
H	-5.23154200	-3.04035400	-1.88851100

Energy = -1488.494165 Hartree.
Low frequencies (cm^{-1}): 21.1708 38.7159 53.0193 58.2720 67.2045 82.0277 89.6091 96.8462 105.0864 117.0116 128.1532 143.2487.

3e – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.02375900	3.53377000	-0.88877900
C	-0.25993600	3.00139000	0.34076200
C	1.06839700	2.60574900	-0.38829100
H	1.77104800	3.44259600	-0.41504300
C	1.72282600	1.39030300	0.24908800
C	1.04755600	0.67334000	-1.87589600
C	0.60648200	2.12265200	-1.78814600
H	1.02383700	2.69383300	-2.62130900
C	-0.95076200	2.24979600	-1.74253200
C	-1.45343500	1.28104500	-0.69608500
C	-1.05978800	1.73338300	0.53467300
C	-1.31792900	0.98639200	1.72973200
C	-0.88025400	1.43417000	2.99476300
H	-0.30959600	2.35575700	3.05959700
C	-1.15039300	0.70617300	4.13257100
H	-0.80432200	1.05714700	5.09994200
C	-1.86909600	-0.49778200	4.03280700
H	-2.08882800	-1.07442900	4.92645700
C	-2.29020700	-0.95867800	2.80179400
H	-2.83458200	-1.89542200	2.76113500
C	-2.02493000	-0.24139500	1.61449500
C	-2.42162200	-0.73792600	0.29581700
C	-3.06789800	-1.97864200	0.12599100
H	-3.31395900	-2.59025200	0.98797700
C	-3.39187100	-2.46892500	-1.13164900
C	-3.05365900	-1.71194400	-2.27692900
H	-3.27115000	-2.10867600	-3.26538000
C	-2.43400000	-0.49413800	-2.13829700
H	-2.15551500	0.06957900	-3.02386100
C	-2.11677800	0.02475500	-0.86387000
C	2.07856500	-0.98739800	-0.35142000
C	3.43469900	-1.22421100	-0.08138600
C	3.83633800	-2.51329700	0.27290300
H	4.87473500	-2.72497200	0.50055600
C	2.89449900	-3.54201500	0.32410300
H	3.22246900	-4.54083000	0.59715400
C	1.55571700	-3.30605000	0.02905500
H	0.83003600	-4.11179500	0.06554500
C	1.14837700	-2.01596400	-0.30544500
N	1.65924200	0.33438900	-0.66807000
O	-1.49562600	4.60799300	-1.12106100
O	2.17604500	1.31562800	1.36266500
O	0.86692000	-0.07746900	-2.80288800
H	-0.14825100	3.68477800	1.18004500
H	-1.44599100	2.27541800	-2.71140500
O	4.26170000	-0.15991000	-0.20487100
C	5.60570200	-0.32083500	0.20165800
H	6.07161600	0.65742200	0.08713700
H	5.66041600	-0.63359600	1.25076900
H	6.12582700	-1.04957300	-0.43163900
H	0.10811400	-1.79426500	-0.53327200

N	-3.97423200	-3.72587600	-1.28553000
H	-4.47927800	-4.07021900	-0.47880700
H	-4.50105700	-3.85433400	-2.14009300

Energy = -1488.492464 Hartree.
Low frequencies (cm^{-1}): 19.5305 24.8089 37.0491 48.3460 63.0231 78.8587
94.2534 98.3296 104.5161 117.1810 124.2917 145.0273.

3f – Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-0.68775600	3.57224300	-0.78329300
C	0.00743800	2.99112300	0.47153200
C	1.38586600	2.69108100	-0.19004300
H	2.02181400	3.58079500	-0.17011500
C	2.13786300	1.52958800	0.43516200
C	1.54333600	0.78767700	-1.70190900
C	1.02289900	2.21406300	-1.62103400
H	1.49115500	2.80737800	-2.41188100
C	-0.52951300	2.32624800	-1.68921300
C	-1.12258000	1.32698600	-0.72433500
C	-0.79668500	1.71416800	0.54890900
C	-1.22137300	0.96365600	1.69356200
C	-0.81482200	1.30696300	3.00086300
H	-0.14381100	2.14973700	3.14101400
C	-1.23421900	0.56735900	4.08570800
H	-0.90904100	0.83423200	5.08661300
C	-2.07215300	-0.54317300	3.88772100
H	-2.39946500	-1.13355000	4.73843900
C	-2.46998200	-0.89956100	2.61430300
H	-3.10173500	-1.77345300	2.49809500
C	-2.06089400	-0.16452300	1.47991300
C	-2.43484700	-0.55585100	0.11982600
C	-3.26805500	-1.66146200	-0.13983300
H	-3.69375500	-2.23151700	0.68026300
C	-3.56007600	-2.06999100	-1.43393200
C	-2.99963000	-1.36487800	-2.52386200
H	-3.19603800	-1.70243900	-3.53839000
C	-2.20631000	-0.26639600	-2.29812000
H	-1.76977200	0.26312300	-3.14016600
C	-1.92106800	0.17104500	-0.98666600
C	2.92616200	-0.72107500	-0.27358900
C	4.31600600	-0.67930200	-0.29268600
C	5.04573900	-1.84134500	-0.06291500
H	6.13080500	-1.81468700	-0.07468600
C	4.36696700	-3.03173700	0.18054500
H	4.92188300	-3.94820500	0.35987700
C	2.97335900	-3.05621400	0.20475600
H	2.46569100	-3.99371200	0.40835400
C	2.21778000	-1.90157400	-0.01547200
C	0.06236800	-3.14824600	0.59651500
H	0.25972900	-4.02217400	-0.03314200
H	-1.02250000	-3.01772000	0.64388500
H	0.42494500	-3.36166300	1.60810600

N	2.21856100	0.50301200	-0.51228500
O	-1.17523100	4.64331300	-0.99216200
O	2.59295900	1.48057400	1.55066300
O	1.40637200	0.02176300	-2.62397100
H	0.04019000	3.63274500	1.35002600
H	-0.95331300	2.39396800	-2.68911500
H	4.81458600	0.26713700	-0.48207000
C	0.70685200	-1.88628500	0.03130500
H	0.32459300	-1.69873100	-0.98132300
H	0.39528000	-1.02351900	0.63502200
N	-4.33473800	-3.20300700	-1.67269100
H	-4.95801900	-3.46862700	-0.92084100
H	-4.79881200	-3.22786300	-2.57168200

Energy = -1452.582765 Hartree.
Low frequencies (cm^{-1}): 24.6997 32.4948 43.5935 58.1463 67.6861 70.8041 81.2238 97.4564 99.7705 106.0088 124.1082 147.9241.

3f – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	-1.06883300	3.51005200	-0.89829800
C	-0.33077700	2.99422100	0.35557400
C	1.03261800	2.64802000	-0.33014500
H	1.70344400	3.51113800	-0.33324600
C	1.71263300	1.45892400	0.32699500
C	1.12315500	0.71353100	-1.80904000
C	0.63407500	2.14903800	-1.74323300
H	1.06387000	2.73067200	-2.56286500
C	-0.92665800	2.23199100	-1.75352100
C	-1.44475200	1.24934500	-0.72804500
C	-1.10129900	1.70420700	0.51694400
C	-1.40090200	0.95540300	1.70133500
C	-1.00801200	1.40100400	2.98171300
H	-0.43981100	2.32244200	3.06870600
C	-1.31926900	0.67130700	4.10805700
H	-1.00689500	1.01994000	5.08765300
C	-2.03544400	-0.53139800	3.98085100
H	-2.28643600	-1.10958800	4.86514400
C	-2.41327800	-0.98997000	2.73496700
H	-2.95586200	-1.92659400	2.67354200
C	-2.10508000	-0.27133800	1.55894400
C	-2.45562200	-0.76604300	0.22620300
C	-3.10254800	-2.00242800	0.03177600
H	-3.38574600	-2.61181700	0.88387200
C	-3.38091100	-2.49128400	-1.23751300
C	-2.99292500	-1.73747400	-2.36924400
H	-3.17447500	-2.13366700	-3.36508300
C	-2.37114200	-0.52384100	-2.20692300
H	-2.05577600	0.03844600	-3.08097000
C	-2.10180700	-0.00589800	-0.92132400
C	2.13081000	-0.93092400	-0.24193000
C	3.47823000	-1.20744200	0.02344100
C	3.79642300	-2.52332100	0.37096700

C	2.82002000	-3.51617400	0.43497600
H	3.10300700	-4.52936700	0.70582600
C	1.49145200	-3.21617500	0.14677100
H	0.72690100	-3.98605600	0.18687200
C	1.14560600	-1.91262600	-0.19332200
N	1.72435100	0.39972900	-0.58486400
O	-1.56824100	4.56892600	-1.14127100
O	2.14776000	1.41184700	1.45145200
O	0.99220300	-0.04771200	-2.73503000
H	-0.26878200	3.67562600	1.20162700
H	-1.38661500	2.24726800	-2.73971900
H	0.11696100	-1.64896000	-0.42800800
H	4.82767300	-2.78324400	0.58796800
C	4.51976400	-0.11450000	-0.08341700
H	4.36104300	0.41588400	-1.03194400
H	4.33517600	0.61931000	0.71041200
C	5.96900100	-0.58791700	-0.00980500
H	6.64647100	0.25764600	-0.15899200
H	6.20064600	-1.02608000	0.96636400
H	6.18701500	-1.33520400	-0.78020500
N	-3.96602000	-3.74334600	-1.41312700
H	-4.50306800	-4.08556700	-0.62649200
H	-4.45799400	-3.87112900	-2.28825200

Energy = -1452.579718 Hartree.
Low frequencies (cm^{-1}): 16.4664 24.7184 32.1636 42.7825 53.4076 64.2012 80.5604 98.0964 103.9545 110.6339 123.5191 146.4864.

4a – Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.40165200	3.73182000	0.00028100
C	0.02784300	2.77830500	-1.16184200
C	-1.46523600	2.56512900	-0.77552400
H	-2.09250900	3.34678800	-1.21394700
C	-2.01966800	1.20664700	-1.17098200
C	-2.01971200	1.20639800	1.17090100
C	-1.46530200	2.56496600	0.77577400
H	-2.09252700	3.34656600	1.21435700
C	0.02777000	2.77808900	1.16221700
C	0.82449300	1.58791100	0.68478200
C	0.82457300	1.58804000	-0.68454100
C	1.52597900	0.59570300	-1.44832100

C	1.48987400	0.53298800	-2.84464200
H	0.87174200	1.23443700	-3.39738600
C	2.22013300	-0.43810500	-3.52504500
H	2.18046700	-0.47909500	-4.60936600
C	2.99134400	-1.35960800	-2.82503500
H	3.55877600	-2.11674300	-3.36089200
C	3.03735500	-1.33989600	-1.42465600
C	2.29404700	-0.35575200	-0.71662200
C	2.29397200	-0.35587100	0.71675600
C	3.03720100	-1.34012700	1.42472300
C	2.99091600	-1.36013500	2.82509100
H	3.55827700	-2.11735500	3.36090500
C	2.21955300	-0.43879200	3.52514200
H	2.17968600	-0.48000600	4.60944900
C	1.48940600	0.53243600	2.84480700
H	0.87115800	1.23374200	3.39760000
C	1.52576900	0.59543200	1.44850400
C	-2.98110400	-0.75880100	-0.00019200
C	-4.36394800	-0.86081100	-0.00019700
C	-4.97836800	-2.11123000	-0.00016200
H	-6.06021300	-2.18999100	-0.00017800
C	-4.18218300	-3.25099300	-0.00008300
H	-4.64204100	-4.23508200	-0.00000900
C	-2.79036800	-3.15850300	-0.00011700
H	-2.19872000	-4.06564000	-0.00006500
C	-2.17179400	-1.90514000	-0.00021600
C	-0.01895000	-2.86633900	-0.00038300
H	-0.20250700	-3.46720500	0.89802400
H	1.01196400	-2.52038200	-0.00072700

H	-0.20296900	-3.46755600	-0.89845500
N	-2.37414900	0.53038600	-0.00010500
O	0.82315400	4.84966200	0.00040200
O	-2.14939000	0.77611300	-2.28927900
O	-2.14942200	0.77561400	2.28911400
H	0.20489700	3.14482400	-2.17111700
H	0.20475800	3.14443400	2.17156500
H	-4.95136500	0.05296300	-0.00019500
C	3.79782300	-2.30990800	-0.67815100
C	3.79777600	-2.30999900	0.67815200
O	-0.83435800	-1.70576600	-0.00039800
H	4.36757400	-3.05283700	1.23124100
H	4.36764100	-3.05268200	-1.23130400

Energy = -1509.370027 Hartree.
Low frequencies (cm^{-1}): 14.5347 40.9828 41.7781 62.4599 68.4975 68.9337 90.5634 102.1966 108.3654 113.5296 152.7937 160.0339.

4a – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.78667500	3.73861800	0.05361100
C	0.58262300	2.80269800	-1.15757800
C	-0.96138200	2.60729200	-1.00705600
H	-1.50985600	3.39406400	-1.53077400
C	-1.40490500	1.24187900	-1.50102500
C	-1.73449800	1.18909400	0.81706400
C	-1.19246100	2.57964800	0.52596300
H	-1.89003800	3.33986200	0.88640300
C	0.23383100	2.78666800	1.13631800
C	1.05663400	1.57285300	0.77346300

C	1.25347800	1.57713200	-0.58198000
C	1.90702100	0.49342900	-1.26142300
C	2.05065200	0.43340500	-2.65200500
H	1.64115300	1.22797600	-3.26887500
C	2.68654300	-0.65249600	-3.24758600
H	2.78663700	-0.69003600	-4.32809600
C	3.18524300	-1.69181200	-2.46901000
H	3.68173900	-2.53663700	-2.94014800
C	3.04455900	-1.67708700	-1.07504200
C	2.39187300	-0.57682000	-0.45305900
C	2.19977700	-0.57271600	0.96708800
C	2.67468800	-1.66183900	1.74815800
C	2.45732000	-1.65926500	3.13176200
H	2.82124300	-2.49500900	3.72448800
C	1.77166200	-0.61513700	3.74384600
H	1.59761200	-0.63741500	4.81533800
C	1.29603000	0.45410600	2.99079500
H	0.74183100	1.25320200	3.47401100
C	1.51060700	0.49714800	1.60934100
C	-2.16712900	-0.88146500	-0.46976600
C	-3.46165000	-1.27242900	-0.09751200
C	-3.79142400	-2.62856600	-0.12786400
C	-2.84356900	-3.56242000	-0.54875400
H	-3.11580100	-4.61369300	-0.57071700
C	-1.56846800	-3.16575300	-0.93859800
H	-0.83774700	-3.89646100	-1.26912500
C	-1.23065200	-1.81463500	-0.89126700
N	-1.81412100	0.49445000	-0.39490400
O	1.20754500	4.85512600	0.12572900

O	-1.37145200	0.84376600	-2.63907100
O	-2.00220900	0.73185200	1.89880400
H	0.91543300	3.16950100	-2.12652100
H	0.25606100	3.14295700	2.16403700
C	3.53011200	-2.75648300	-0.25322300
C	3.35586800	-2.74784100	1.09072100
H	-0.23996800	-1.47122200	-1.18081900
H	-4.77977700	-2.96213800	0.16619800
O	-4.30767700	-0.27649200	0.25467200
C	-5.56406200	-0.64090700	0.79031900
H	-6.05103600	0.29226100	1.07202700
H	-6.17601400	-1.16163700	0.04412100
H	-5.44003700	-1.27325300	1.67716800
H	3.72025900	-3.57024500	1.70154800
H	4.03752500	-3.58504100	-0.74121700

Energy = -1509.369720 Hartree.
Low frequencies (cm^{-1}): 19.5474 23.9981 31.0799 48.0374 66.6373 76.4412 83.0888 90.8757 108.9313 121.1519 151.9711 164.6402.

4d – Folded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.38919000	3.73931800	-0.04194800
C	0.05434400	2.76597800	-1.19969900
C	-1.44563400	2.53874400	-0.84887000
H	-2.07447300	3.29609800	-1.32572300
C	-1.96767900	1.15929300	-1.21957700
C	-2.07053100	1.23781200	1.11537500
C	-1.49153200	2.58026000	0.70101800
H	-2.12327500	3.37866200	1.10074200
C	-0.00812900	2.79864900	1.12360000

C	0.81074500	1.60769500	0.68417500
C	0.85089800	1.59122400	-0.68520000
C	1.58280900	0.59694800	-1.41775600
C	1.58607100	0.51910000	-2.81424700
H	0.98559000	1.21545500	-3.39213400
C	2.33260000	-0.46215100	-3.46195700
H	2.32321600	-0.51621700	-4.54624400
C	3.08438300	-1.37499000	-2.72958400
H	3.66751900	-2.13685300	-3.24094000
C	3.09225900	-1.33956000	-1.32862100
C	2.32587600	-0.35000600	-0.65349200
C	2.28119400	-0.33679200	0.77887000
C	2.99995300	-1.31651600	1.51728300
C	2.90957100	-1.32353700	2.91594700
H	3.45806800	-2.07699100	3.47578000
C	2.12161000	-0.39278400	3.58449200
H	2.04892400	-0.42435500	4.66723900
C	1.41803400	0.57731800	2.87453100
H	0.78818500	1.28752900	3.40229800
C	1.49671200	0.62745900	1.47903600
C	-3.00803900	-0.76634800	-0.02580600
C	-4.39226600	-0.80840700	0.09172000
C	-5.04544400	-2.03749700	0.11598000
H	-6.12606600	-2.07841700	0.20856100
C	-4.29647000	-3.20646600	0.02013400
H	-4.79238500	-4.17264800	0.03631700
C	-2.90758800	-3.14792400	-0.09223000
H	-2.34280500	-4.07240300	-0.15821900
C	-2.22966600	-1.92691300	-0.11486700

C	0.03194200	-3.13768100	-0.12799100
H	-0.18984600	-3.65950700	0.80930400
H	1.10960800	-2.95354700	-0.16063400
H	-0.21511900	-3.80463100	-0.96078100
N	-2.37336200	0.51988900	-0.04531600
O	0.80090800	4.86060100	-0.04639000
O	-2.02661600	0.68285600	-2.32604400
O	-2.24359800	0.84236600	2.24131300
H	0.25373500	3.11906100	-2.20934900
H	0.14037700	3.17925700	2.13214300
H	-4.94666200	0.12284600	0.16589400
C	-0.72580300	-1.81738900	-0.21968100
H	-0.37718300	-1.14869800	0.57859900
H	-0.47721900	-1.31568900	-1.16550100
C	3.79342800	-2.28514100	0.80424600
H	4.35050800	-3.01840400	1.38207400
C	3.83945900	-2.29473800	-0.55056600
H	4.43350300	-3.03610400	-1.07914300

Energy = -1473.460170 Hartree.
Low frequencies (cm^{-1}): 21.0903 35.1443 51.9834 53.5506 69.4733 74.6159
78.6080 87.5731 101.8256 113.2952 157.2198 158.7468.

4d – Unfolded

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
C	0.82370100	3.72705900	0.01624600
C	0.56764500	2.78271100	-1.17922900
C	-0.97180400	2.60413300	-0.97332900
H	-1.53004800	3.38884200	-1.49006800
C	-1.44919500	1.23630900	-1.42848200
C	-1.71463500	1.22890400	0.89441500
C	-1.15237200	2.60197100	0.56644100
H	-1.82186100	3.38129100	0.93969900
C	0.29582600	2.79018700	1.12555800
C	1.09264800	1.56450200	0.74538900

C	1.24965600	1.55799800	-0.61536900
C	1.89601000	0.47591800	-1.30421100
C	2.00648100	0.40835000	-2.69744100
H	1.57400500	1.19464100	-3.30934700
C	2.64022300	-0.67427400	-3.30116900
H	2.71523200	-0.71790100	-4.38346800
C	3.16790900	-1.70339800	-2.52823200
H	3.66161000	-2.54615200	-3.00591100
C	3.06019600	-1.68139500	-1.13152300
C	2.41220200	-0.58333600	-0.50079700
C	2.25313100	-0.57278100	0.92348900
C	2.75369300	-1.65405700	1.69921600
C	2.56693800	-1.64601000	3.08728200
H	2.95055200	-2.47587800	3.67584300
C	1.88761600	-0.60376100	3.70962200
H	1.73740900	-0.62225000	4.78475600
C	1.38859600	0.45883500	2.96233900
H	0.84000700	1.25687800	3.45373200
C	1.57159400	0.49576200	1.57609600
C	-2.19542100	-0.87524600	-0.34754400
C	-3.49442100	-1.28731700	-0.02349200
C	-3.75456900	-2.65917300	-0.08025900
H	-4.74712000	-3.02437300	0.16388600
C	-2.76946600	-3.57246900	-0.45278500
H	-3.00684800	-4.63189300	-0.48768000
C	-1.49056200	-3.13268300	-0.78278500
H	-0.71982500	-3.83769700	-1.07876300
C	-1.20270900	-1.77290000	-0.72800500
N	-1.85094200	0.51489200	-0.29812200
O	1.26078200	4.83825100	0.06478400
O	-1.45538400	0.81729100	-2.55866900
O	-1.97466800	0.80388900	1.99332800
H	0.86983800	3.13848200	-2.16220000
H	0.35845200	3.15442200	2.14889500
C	3.42933100	-2.73774400	1.03228000
H	3.81469700	-3.55357800	1.63899200
C	3.57422100	-2.75166700	-0.31507200
H	4.07828900	-3.57823800	-0.80976900
H	-0.21399200	-1.39858000	-0.98340500
C	-4.54640000	-0.26895800	0.35916100
H	-4.25924900	0.17897800	1.31839500
H	-4.51912300	0.54492500	-0.37776400
C	-5.97089100	-0.80818400	0.45809400
H	-6.66366400	0.00752700	0.68368100
H	-6.29160000	-1.27243400	-0.48052500
H	-6.06703400	-1.55042400	1.25689700

Energy = -1473.456837 Hartree.
Low frequencies (cm^{-1}): 17.5991 21.4938 28.3783 34.9734 47.4201 70.2755
76.9854 83.5939 107.8743 121.2767 150.4220 154.8820.

TS1

Atomic Coordinates (Angstroms)

Number X Y Z

C	-1.96675300	2.96282300	-0.75395100
C	-0.87603000	2.74035300	0.32450500
C	0.35786900	2.80403900	-0.62155700
H	0.69359000	3.83752600	-0.74822400
C	1.53469900	1.95637000	-0.16726200
C	0.80061200	0.96443600	-2.15744400
C	-0.13064300	2.14464600	-1.93762600
H	-0.07461100	2.80693000	-2.80649300
C	-1.60723200	1.74920700	-1.64668900
C	-1.62995100	0.70915700	-0.55177900
C	-1.19873400	1.29216400	0.60864900
C	-1.14957900	0.57161600	1.84616200
C	-0.62960000	1.14977100	3.02341300
H	-0.20840300	2.14999700	2.97801400
C	-0.62739100	0.44757400	4.20948600
H	-0.21925100	0.89619600	5.10997200
C	-1.14967600	-0.85685100	4.24448400
H	-1.15657500	-1.41317900	5.17722400
C	-1.64739500	-1.44265400	3.09712200
H	-2.03346400	-2.45435300	3.16040000
C	-1.65499700	-0.75572600	1.86291000
C	-2.12342500	-1.37645300	0.62346400
C	-2.60778800	-2.70257000	0.57781200
H	-2.68153000	-3.28664800	1.48893200
C	-2.99007800	-3.28922000	-0.61247400
H	-3.35585000	-4.31185700	-0.61397200
C	-2.89953400	-2.57479400	-1.81965000
H	-3.18333900	-3.04653300	-2.75548300
C	-2.44376100	-1.27416700	-1.80845500

H	-2.35359100	-0.71891000	-2.73766100
C	-2.06490400	-0.65504900	-0.59869900
C	2.82594000	0.03617800	-1.06789500
C	2.61984200	-1.18695900	-0.41269600
C	3.67240700	-2.10471700	-0.36142300
H	3.54734300	-3.06069500	0.13238200
C	4.89745500	-1.79363500	-0.95190100
H	5.70323600	-2.52024500	-0.90069200
C	5.09692800	-0.57821800	-1.59687400
H	6.05264700	-0.34323600	-2.05301400
C	4.04745500	0.33689400	-1.65074200
N	1.76005000	0.97896600	-1.14021300
O	-2.80319600	3.80809500	-0.86991500
O	2.17886500	2.09532400	0.84195900
O	0.74632800	0.15616000	-3.04979700
H	-0.86513600	3.43844600	1.15904400
H	-2.23136300	1.58714700	-2.52327400
O	1.39640800	-1.38297200	0.12711900
C	1.18334200	-2.61127400	0.80021800
H	0.16233900	-2.57733800	1.17365700
H	1.29442700	-3.45595500	0.11017200
H	1.87900700	-2.71843900	1.64074400
H	4.16415400	1.29665100	-2.14601100

Energy = -1433.171985 Hartree.
Low frequencies (cm^{-1}): -24.8049 33.3257 43.1830 55.1476 60.9910 65.5663 85.8076 94.1855 103.9971 110.3229 117.3598 147.6952.

TS2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

C	-1.93507200	3.01893500	-0.53666800
C	-1.07873900	2.61113300	0.68578700
C	0.31263000	2.87842100	0.03998400
H	0.58381500	3.93362100	0.13355600
C	1.40743500	2.01389900	0.62948600
C	1.11089400	1.22388500	-1.55454200
C	0.14549300	2.39363800	-1.42266900
H	0.39890500	3.15277900	-2.16800900
C	-1.35858600	1.98469900	-1.53237700
C	-1.57355600	0.76620400	-0.66755800
C	-1.36851500	1.12718000	0.63652600
C	-1.43214000	0.17282200	1.70411300
C	-1.11338100	0.52207400	3.03351200
H	-0.79067900	1.53637800	3.25161500
C	-1.17521900	-0.41767500	4.04011200
H	-0.91902400	-0.14425600	5.05910100
C	-1.55751500	-1.73541400	3.73698000
H	-1.60401100	-2.48086400	4.52552900
C	-1.86300600	-2.09512100	2.43919700
H	-2.13628500	-3.12530000	2.23950700
C	-1.80869800	-1.15920000	1.38405700
C	-2.11210800	-1.52256200	0.00041800
C	-2.56559500	-2.80977700	-0.36167200
H	-2.71834800	-3.56567800	0.40072900
C	-2.83215800	-3.13774200	-1.67713100
H	-3.18483400	-4.13563200	-1.92138200
C	-2.64942000	-2.18880000	-2.69794500
H	-2.85185900	-2.45236500	-3.73176800
C	-2.21498900	-0.91980400	-2.37710000
H	-2.06235000	-0.18127200	-3.15896300
C	-1.95534500	-0.56430800	-1.03670700
C	2.76678700	0.07624400	-0.09447100
C	4.05428500	0.41038700	0.31241900
C	4.98774300	-0.59200700	0.55551600
H	5.99263400	-0.33255900	0.87174100
C	4.62109400	-1.92661600	0.38832800
H	5.34259300	-2.71582300	0.57850500
C	3.32929500	-2.26439900	-0.00487400
H	3.03684800	-3.30562000	-0.10025700
C	2.38543000	-1.26257100	-0.24254500
C	0.81997400	-2.48898400	-1.55752600
H	1.73975700	-2.97046200	-1.90030800
H	0.34788100	-1.98011700	-2.40083400
H	0.13803300	-3.23503800	-1.14266100
N	1.80646700	1.09561200	-0.34547600
O	-2.76088500	3.87184800	-0.67358700
O	1.85650100	2.08456700	1.74688500
O	1.27211500	0.52964800	-2.52696700
O	1.09138300	-1.51278700	-0.55312800
H	-1.26971000	3.14114600	1.61703800
H	-1.77474400	1.99234400	-2.53738200
H	4.31173000	1.45776600	0.43625800

Energy = -1433.171674 Hartree.
Low frequencies (cm^{-1}): -215.0476 24.5225 33.0095 55.0219 63.9078 75.7221 90.7573 99.1018 106.2893 120.9456 134.4306 142.8044.

Barrier for C-N bond rotation in 3a

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.98523100	3.14620100	-0.53783400
C	-0.98444500	2.74109600	0.56521500
C	0.32587800	2.85528100	-0.28745700
H	0.76221700	3.85400700	-0.21005800
C	1.36322800	1.82918700	0.13261900
C	0.77382200	1.26123300	-2.04227400
C	-0.09211900	2.44972300	-1.69943000
H	0.03860000	3.22173300	-2.46123400
C	-1.60150600	2.05640100	-1.56236400
C	-1.68267300	0.86603000	-0.63553300
C	-1.33825200	1.27504600	0.62417600
C	-1.22768200	0.35677100	1.71856800
C	-0.84623500	0.78188100	3.00933900
H	-0.62429200	1.83172600	3.17652400
C	-0.72403000	-0.12401000	4.04039700
H	-0.42415700	0.21012100	5.02907000
C	-0.97453600	-1.48652600	3.79985500
H	-0.87261200	-2.20706800	4.60599400
C	-1.34462800	-1.91936500	2.54161400
H	-1.52274300	-2.97816400	2.39176000
C	-1.48473200	-1.01740900	1.46326800
C	-1.85014100	-1.45650400	0.11639200
C	-2.10910400	-2.81018200	-0.19206200
H	-2.05743700	-3.56473200	0.58463200
C	-2.42668700	-3.20794100	-1.47529500
H	-2.61943700	-4.25686700	-1.67993900
C	-2.49283600	-2.26696200	-2.51718600
H	-2.72961700	-2.58657200	-3.52740500
C	-2.25011200	-0.93695200	-2.24997300
H	-2.28264700	-0.20437800	-3.05140700
C	-1.93977100	-0.51099100	-0.94077500
C	2.37243500	-0.33661800	-0.91442800
C	3.18076200	-0.78862000	0.16092000
C	3.95055300	-1.94744800	0.02298000
H	4.55833600	-2.21677800	0.88187000
C	3.95422500	-2.70991200	-1.13283000
H	4.56909100	-3.60169500	-1.20676000
C	3.14666100	-2.29510200	-2.18244100
H	3.10418100	-2.85854000	-3.10939500
C	2.38114500	-1.14040700	-2.07290200
N	1.54630200	0.86819400	-0.91567800
O	-2.77997700	4.03696400	-0.59508900
O	1.89335900	1.87443300	1.20711500
O	0.74496200	0.75672500	-3.13938200
H	-0.99852300	3.32468100	1.48284100
H	-2.16239700	2.03448600	-2.49435200
O	3.30564700	-0.16953600	1.36753200
C	2.35984200	-0.61035800	2.33201900
H	2.43571100	0.07272100	3.17871100
H	1.34030400	-0.57321900	1.93115000
H	2.58709000	-1.63780300	2.64718300

H 1.78536600 -0.85995900 -2.92228600

Energy = -1433.142772 Hartree.
Low frequencies (cm^{-1}): -64.9734 22.3315 33.5679 46.7384 58.4208 78.8437
102.0273 106.1945 120.0171 140.0828 144.7981 158.3612.

4. References

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