

## Supplementary Information

### Regio- and stereoselective synthesis of novel isoxazolidines heterocycles by 1,3-dipolar cycloaddition between *C*-phenyl-*N*-methylnitron and substituted alkenes. Experimental and DFT investigation of selectivity and mechanism

Djamila Hellel<sup>a</sup>, Fouad Chafaa<sup>a</sup>, Abdelmalek Khorief Nacereddine<sup>a,b</sup>, Abdelhafid Djerourou<sup>a</sup> and Emmanuel Vrancken<sup>c</sup>

<sup>a</sup>Laboratoire de Synthèse et Biocatalyse Organique, Département de Chimie, Faculté des Sciences, Université Badji Mokhtar Annaba, BP 12, 23000 Annaba, Algeria.

<sup>b</sup>Département de Physique et Chimie, Ecole Normale Supérieure d'Enseignement Technologique de Skikda, Cité des frères Boucetta, Azzaba, Skikda, Algeria

<sup>c</sup> Institut Charles Gerhardt, UMR 5253 CNRS-UM2-UM1 ENSCM, Laboratoire Architectures Moléculaires et Matériaux Nanostructurés (AM2N), Ecole Nationale Supérieure de Chimie de Montpellier, 8 Rue de l'Ecole Normale, 34296 Montpellier, France.

### Contents

**S2.** Characterization data and spectroscopic detail for nitron **1**

**S2. Table S1.** B3LYP/6-31G(d) total (E, in a.u.) and relative ( $\Delta E$ , in kcal·mol<sup>-1</sup>) energies, in gas phase, of the stationary points involved in the 13DC reaction of nitron **1** with alkene **2a**.

**S2. Table S2.** B3LYP/6-31G(d) total enthalpies (H, in a.u.), entropies (S, in cal mol<sup>-1</sup>K<sup>-1</sup>) and Gibbs free energies (G, in a.u.), for the stationery points involved in the 13DC between nitron **1** and alkene **2a**.

**S3. Table S3.** B3LYP/6-31G(d) total (E, in a.u.) and relative ( $\Delta E$ , in kcal·mol<sup>-1</sup>) energies, in gas phase, of the stationary points involved in the 13DC reaction of nitron **1** with alkene **2d**.

**S3. Table S4.** B3LYP/6-31G(d) total enthalpies (H, in a.u.), entropies (S, in cal mol<sup>-1</sup>K<sup>-1</sup>) and Gibbs free energies (G, in a.u.), for the stationery points involved in the 13DC between nitron **1** and alkene **2d**.

**S3. Table S5.** B3LYP/6-31G(d) total (E, in a.u.) and relative ( $\Delta E$ , in kcal·mol<sup>-1</sup>) energies, in gas phase, of the stationary points involved in the 13DC reaction of nitron **1** with alkene **2e**.

**S4. Table S6.** B3LYP/6-31G(d) total enthalpies (H, in a.u.), entropies (S, in cal mol<sup>-1</sup>K<sup>-1</sup>) and Gibbs free energies (G, in a.u.), for the stationery points involved in the 13DC between nitron **1** and alkene **2e**.

**S4.** Atomic coordinates (in Å) of the B3LYP/6-31G(d) optimised geometries of stationery points structures.

### Characterization data and spectroscopic detail for nitrone **1**

$R_f = 0.27$  (Et<sub>2</sub>O/ CH<sub>2</sub>Cl<sub>2</sub>) as crystals (recrystallized from diethyl ether).

IR (KBr) : 3055 v C-H, 2993 vC-H, 1589vC=N, 1558v C=C, 1080vN-C, 1296vN-O.

MS: [M]<sup>+</sup>=135 (70), 134 (100), 118(20), 107(25), 89 (30), 77(50), 65(30), 44(73).

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): 3.75 (s, 3H, CH<sub>3</sub>); 7.28-7.38 (m, 5H, C<sub>6</sub>H<sub>5</sub>), 8.15 (q, 1H, J=3.22 Hz, CH=N).

**Table S1.** B3LYP/6-31G(d) total (E, in a.u.) and relative ( $\Delta E$ , in kcal·mol<sup>-1</sup>) energies, in gas phase, of the stationary points involved in the 13DC reaction of nitrone **1** with alkene **2a**.

System	E	$\Delta E$
<b>Alkene 2a</b>	-422.9759669	
<b>Nitronne 1</b>	-440.1687323	
<b>TS-a-mn</b>	-863.1238497	13.08
<b>TS-a-mx</b>	-863.1206696	15.08
<b>TS-a-on</b>	-863.1166294	17.61
<b>TS-a-ox</b>	-863.1173735	17.15
<b>CA-a-mn</b>	-863.164208	-12.24
<b>CA-a-mx</b>	-863.1624402	-11.13
<b>CA-a-on</b>	-863.1599374	-9.56
<b>CA-a-ox</b>	-863.1633643	-11.71

**Table S2.** B3LYP/6-31G(d) total enthalpies (H, in a.u.), entropies (S, in cal mol<sup>-1</sup>K<sup>-1</sup>) and Gibbs free energies (G, in a.u.), for the stationery points involved in the 13DC between nitrone **1** and alkene **2a**.

System	H	S	G
<b>Alkene 2a</b>	-422.839105	103.872	-422.902528
<b>Nitronne 1</b>	-440.021877	103.085	-440.084819
<b>TS-a-mn</b>	-862.836946	160.036	-862.934662
<b>TS-a-mx</b>	-862.833627	160.7	-862.931749
<b>TS-a-on</b>	-862.830376	159.343	-862.927668
<b>TS-a-ox</b>	-862.830417	159.531	-862.927825
<b>CA-a-mn</b>	-862.872782	160.141	-862.970562
<b>CA-a-mx</b>	-862.870968	160.419	-862.968918
<b>CA-a-on</b>	-862.868324	158.058	-862.964832
<b>CA-a-ox</b>	-862.871644	160.01	-862.969344

**Table S3.** B3LYP/6-31G(d) total (E, in a.u.) and relative ( $\Delta E$ , in kcal·mol<sup>-1</sup>) energies, in gas phase, of the stationary points involved in the 13DC reaction of nitrone **1** with alkene **2d**.

System	E	$\Delta E$
<b>Nitron 1</b>	-440.168732	
<b>Alkene 2d</b>	-269.349344	
<b>TS-d-on</b>	-709.488685	18.44
<b>TS-d-ox</b>	-709.493491	15.43
<b>TS-d-mn</b>	-709.496283	13.68
<b>TS-d-mx</b>	-709.500402	11.09
<b>CA-d-on</b>	-709.543075	-15.69
<b>CA-d-ox</b>	-709.545595	-17.27
<b>CA-d-mn</b>	-709.549365	-19.63
<b>CA-d-mx</b>	-709.552707	-21.73

**Table S4.** B3LYP/6-31G(d) total enthalpies (H, in a.u), entropies (S, in cal mol<sup>-1</sup>K<sup>-1</sup>) and Gibbs free energies (G, in a.u.) for the stationary points involved in the 13DC between nitrone **1** and alkene **2d**.

System	H	S	G
<b>Nitron 1</b>	-440.021877	103.085	-440.084819
<b>Alkene 2d</b>	-269.257861	79.702	-269.306507
<b>TS-d-on</b>	-709.247238	135.817	-709.330134
<b>TS-d-ox</b>	-709.252715	137.177	-709.336441
<b>TS-d-mn</b>	-709.254373	137.225	-709.338128
<b>TS-d-mx</b>	-709.25891	137.921	-709.34309
<b>CA-d-on</b>	-709.297281	134.141	-709.379154
<b>CA-d-ox</b>	-709.299436	135.044	-709.38186
<b>CA-d-mn</b>	-709.303247	134.318	-709.385227
<b>CA-d-mx</b>	-709.306405	135.508	-709.389112

**Table S5.** B3LYP/6-31G(d) total (E, in a.u.) and relative ( $\Delta E$ , in kcal·mol<sup>-1</sup>) energies, in gas phase, of the stationary points involved in the 13DC reaction of nitrone **1** with alkene **2e**.

System	E	$\Delta E$
<b>Alkene 2e</b>	-403.128930	
<b>Nitron 1</b>	-440.168732	
<b>TS-e-mn</b>	-843.257674	25.09
<b>TS-e-mx</b>	-843.260581	23.27
<b>TS-e-on</b>	-843.266636	19.47
<b>TS-e-ox</b>	-843.267973	18.63
<b>CA-e-mn</b>	-843.309746	-7.58
<b>CA-e-mx</b>	-843.311227	-8.51
<b>CA-e-on</b>	-843.317355	-12.36
<b>CA-e-ox</b>	-843.317470	-12.43

**Table S6.** B3LYP/6-31G(d) total enthalpies (H. in a.u), entropies (S. in cal mol<sup>-1</sup>K<sup>-1</sup>) and Gibbs free energies (G. in a.u.), for the stationery points involved in the 13DC between nitrone **1** and alkene **2e**.

System	H	S	G
<b>Alkene 2e</b>	-402.979204	98.053	-403.039074
<b>Nitron 1</b>	-440.021877	103.085	-440.084819
<b>TS-e-mn</b>	-842.957197	155.657	-843.052239
<b>TS-e-mx</b>	-842.961207	156.009	-843.056465
<b>TS-e-on</b>	-842.965525	154.595	-843.059918
<b>TS-e-ox</b>	-842.967557	156.577	-843.063161
<b>CA-e-mn</b>	-843.005534	153.881	-843.099491
<b>CA-e-mx</b>	-843.007021	153.64	-843.100831
<b>CA-e-on</b>	-843.012798	153.016	-843.106228
<b>CA-e-ox</b>	-843.012718	153.259	-843.106296

**Atomic coordinates (in Å) of the B3LYP/6-31G(d) optimised geometries of stationery points structures.**

**Nitron 1: E= -440.168732 a.u**

C	-1.09805300	-0.78525100	-0.27378900
H	-1.29314200	-1.79613000	-0.61628800
C	0.28521000	-0.33824900	-0.14454500
C	1.25209200	-1.31513900	0.17502700
C	0.73393400	0.97634800	-0.38580800
C	2.59849000	-0.98503500	0.29130500
H	0.92996700	-2.33954700	0.34385300
C	2.08324300	1.30408500	-0.26399500
H	0.03364100	1.73851400	-0.71138700
C	3.02126200	0.33011400	0.08161700
H	3.32025800	-1.75565800	0.54831600
H	2.40400900	2.32404000	-0.45868100
H	4.07235300	0.58925800	0.17185900
N	-2.21218900	-0.12574900	-0.01759700
O	-3.36851700	-0.60976400	-0.24764200
C	-2.24232400	1.21525700	0.61169100
H	-1.29269100	1.46098400	1.08513000
H	-2.49672600	1.95370200	-0.15261800
H	-3.04734000	1.17040300	1.34511600

**Alkene 2a: E= -422.9759669 a.u**

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.34960528
C	1.26027448	0.00000000	2.09671031

O	1.34259340	0.00001106	3.31232646
C	-1.14709753	-0.00000589	-0.90624652
C	-0.91464631	-0.00000469	-2.29404949
C	-1.97277781	-0.00001012	-3.20014948
C	-3.28825597	-0.00001687	-2.73433229
C	-3.53716241	-0.00001815	-1.35769915
C	-2.48103928	-0.00001273	-0.45330476
H	0.97342865	0.00000000	-0.49436800
H	-0.91020017	-0.00000467	1.94387120
H	2.17641474	0.00001489	1.46188151
H	0.10989508	0.00000056	-2.65891608
H	-1.77091719	-0.00000909	-4.26767928
H	-4.11649287	-0.00002112	-3.43753628
H	-4.55977846	-0.00002340	-0.99055371
H	-2.69022106	-0.00001380	0.61215412

**TS-a-mn: E= -863.1238497 a.u**

1 imaginary frequency = -422.9294 cm<sup>-1</sup>

N	0.94961500	-1.43635100	-1.51056700
C	1.69481700	-0.90522100	-0.51418900
C	0.18193400	-1.30251400	1.02473100
C	-0.98821100	-1.32051600	0.21926300
O	-0.29386700	-1.00477300	-1.59170600
C	1.12771900	-2.83656200	-1.89444700
C	0.69671500	-2.55847400	1.57370900
O	1.54249300	-2.65246800	2.44964900
C	1.89430200	0.54744900	-0.33247800
C	2.89331700	0.95620900	0.56911300
C	3.17325400	2.30730400	0.75673500
C	2.46916200	3.27374900	0.03480100
C	1.47934000	2.87589200	-0.86685500
C	1.18124700	1.52581200	-1.04640000
C	-2.03919900	-0.28410300	0.24775600
C	-3.31905100	-0.60646900	-0.23355200
C	-4.34914800	0.33178900	-0.22453200
C	-4.11756800	1.61795900	0.26573700
C	-2.84832900	1.95473200	0.74274500
C	-1.81972100	1.01541200	0.73466700
H	2.55918600	-1.50948500	-0.24696700
H	0.40364400	-0.43088600	1.63170700
H	-1.36895500	-2.31138600	-0.02385200
H	0.61799600	-3.49770100	-1.18134500
H	0.68262900	-2.96684900	-2.88198200
H	2.19113200	-3.08328500	-1.93315000

H	0.25523300	-3.48010500	1.12034900
H	3.44660300	0.20590800	1.12925800
H	3.94654800	2.60434500	1.45983700
H	2.69009900	4.32847400	0.17435900
H	0.92778600	3.62217400	-1.43246000
H	0.39914000	1.21923700	-1.72997000
H	-3.50349700	-1.60615000	-0.61989200
H	-5.33197400	0.05840400	-0.59924600
H	-4.91850700	2.35231100	0.27653000
H	-2.65818700	2.95431600	1.12469700
H	-0.83867800	1.29836400	1.10171700

**TS-a-mx: E= -863.1206696 a.u**

1 imaginary frequency = -424.3045 cm<sup>-1</sup>

N	0.17821400	-0.94246200	1.42484200
C	1.16773700	-0.03527900	1.26440500
C	-0.13553600	1.23934900	0.00265200
C	-0.89555100	0.21429300	-0.62170600
O	-0.35818900	-1.40133700	0.30928500
C	-0.75840200	-0.81822300	2.54477200
C	-2.37312600	0.08690300	-0.51643000
C	-3.00872900	-1.01999900	-1.10629900
C	-4.39167400	-1.16828000	-1.05049500
C	-5.17589400	-0.20815700	-0.40540700
C	-4.56104500	0.90246000	0.17365100
C	-3.17507100	1.05206600	0.11351800
C	0.87601300	1.96285600	-0.77122500
O	1.33901300	3.04974300	-0.46376100
C	2.36916400	-0.28942800	0.44326200
C	3.47301400	0.56122300	0.63145000
C	4.65505400	0.36283000	-0.07829100
C	4.75896600	-0.69734700	-0.97978200
C	3.66957500	-1.55200800	-1.16872900
C	2.47912600	-1.34998800	-0.47416700
H	1.35118900	0.57153300	2.14875200
H	-0.58046800	1.82838800	0.80186200
H	-0.49502200	-0.14121100	-1.56971500
H	-1.49108700	-0.02676500	2.35131100
H	-1.28231400	-1.77030500	2.63920200
H	-0.20802600	-0.60677800	3.46456000
H	-2.40208900	-1.77655200	-1.59670300
H	-4.85969300	-2.03446900	-1.51094200
H	-6.25588600	-0.32056300	-0.36367400
H	-5.16152000	1.66473200	0.66333200

H	-2.71848100	1.94047000	0.53961800
H	1.21924600	1.44006300	-1.69202900
H	3.39762600	1.38913300	1.33143800
H	5.49434800	1.03502200	0.07637200
H	5.68077100	-0.85610900	-1.53275400
H	3.74494500	-2.38112400	-1.86737900
H	1.63063600	-2.00509000	-0.62840500

**TS-a-on: E= -863.1166293 a.u**

1 imaginary frequency = -426.7556 cm<sup>-1</sup>

N	2.04284600	1.21230900	0.87262100
C	0.74689300	0.87596900	1.13300300
C	0.92574500	-1.08853500	0.29819700
C	1.79765200	-0.81087300	-0.78295300
O	2.42403500	1.08186000	-0.36903600
C	3.08198700	0.95385800	1.87121400
C	3.16852100	-1.34634200	-0.79102600
O	3.84668700	-1.49861100	-1.78983800
C	-0.47043200	-1.55956500	0.12977300
C	-1.07018000	-2.28286500	1.17568600
C	-2.37380800	-2.76472600	1.06864000
C	-3.11262200	-2.53234900	-0.09235500
C	-2.53192100	-1.81301600	-1.13913900
C	-1.22875200	-1.33195200	-1.03136800
C	-0.38416700	1.51399200	0.42592300
C	-1.64204200	1.47949300	1.05196400
C	-2.75048400	2.08671800	0.46649700
C	-2.61903500	2.75090200	-0.75361700
C	-1.37260000	2.79519000	-1.38289600
C	-0.26377000	2.17546700	-0.80955000
H	0.55916200	0.70449100	2.19155200
H	1.41557500	-1.54574400	1.16117500
H	1.39778800	-0.60675300	-1.77103400
H	3.34421600	-0.11223700	1.88814300
H	2.73588900	1.26982400	2.85780800
H	3.96308000	1.52954500	1.58559100
H	3.55288300	-1.65181800	0.21066900
H	-0.49878500	-2.47786500	2.08124100
H	-2.80906600	-3.32716900	1.89072900
H	-4.12769000	-2.90937000	-0.18228300
H	-3.09619600	-1.62559400	-2.04891300
H	-0.80212300	-0.77187000	-1.85723000
H	-1.75081300	0.96887200	2.00547300
H	-3.71407200	2.04501000	0.96678600

H	-3.48039600	3.22997000	-1.21124400
H	-1.26133100	3.31340100	-2.33175000
H	0.70026100	2.20697000	-1.30202800

**TS-a-ox: E=** -863.1173735 a.u

1 imaginary frequency = -453.1574 cm<sup>-1</sup>

N	-0.39423700	0.99180200	1.69886700
C	-0.49211300	-0.20585500	1.04653600
C	0.58006700	0.35817100	-0.64945100
C	0.36841000	1.76180200	-0.66670700
O	-0.75557700	2.03730200	1.00520600
C	-0.64046100	2.33426100	-1.57543100
O	-0.65293900	3.49368500	-1.94313100
C	1.92318600	-0.26786300	-0.49147700
C	2.06732700	-1.63819600	-0.77660300
C	3.29588700	-2.28240200	-0.64471000
C	4.42099000	-1.57001600	-0.22549200
C	4.29992100	-0.20679100	0.04970600
C	3.06954500	0.43606300	-0.08392600
C	-1.78354400	-0.69572000	0.50184600
C	-1.89798000	-2.07383700	0.24769500
C	-3.07953700	-2.61414300	-0.25562900
C	-4.17634100	-1.78634800	-0.50188600
C	-4.07715700	-0.41805400	-0.24093600
C	-2.89194100	0.13025700	0.24806900
C	0.71508200	1.23172100	2.62695000
H	0.10233900	-0.98768600	1.51490900
H	-0.06166600	-0.19666400	-1.33262600
H	1.15661600	2.45257300	-0.38566300
H	-1.41692700	1.61421900	-1.91672400
H	1.19981900	-2.20141600	-1.11429800
H	3.37541600	-3.34147500	-0.87620100
H	5.38122400	-2.06793100	-0.12411800
H	5.17016400	0.36499800	0.36152300
H	3.01221600	1.50293700	0.11215900
H	-1.05385900	-2.72798700	0.45551500
H	-3.14609200	-3.68217700	-0.44475700
H	-5.10084900	-2.20423200	-0.89070600
H	-4.92816700	0.23272000	-0.42323600
H	-2.81880100	1.19278300	0.44482100
H	0.43719700	2.07642100	3.25917200
H	1.62942500	1.47742300	2.07562300
H	0.88169700	0.34668700	3.24461500



**CA-a-mn:** E= -863.164208 a.u

N	-0.73902200	-1.33025200	1.60285400
C	-1.24888900	-1.18743900	0.21290900
C	0.08709400	-1.10784100	-0.59868700
C	1.16455800	-0.90885900	0.52230300
O	0.40786000	-0.42961300	1.63628800
C	-1.61841600	-0.95362500	2.69666700
C	0.33537100	-2.37718700	-1.38268500
O	0.56587900	-2.42474100	-2.56958000
C	-2.20413700	-0.04247100	-0.08656400
C	-3.42038500	-0.31425800	-0.72522800
C	-4.31810500	0.71068200	-1.02964600
C	-4.01724400	2.02778700	-0.68284000
C	-2.81414900	2.31084000	-0.03196600
C	-1.91265700	1.28737900	0.25995100
C	2.29206700	0.04274100	0.20465600
C	3.61459500	-0.40785800	0.27452900
C	4.67779700	0.44912700	-0.01545100
C	4.42758000	1.77420400	-0.37048300
C	3.11042100	2.23567400	-0.43777100
C	2.05078000	1.37569000	-0.15574500
H	-1.77469400	-2.12661200	-0.00510900
H	0.07712000	-0.26958500	-1.29705700
H	1.57989800	-1.89178900	0.78822500
H	-1.09053300	-1.13807400	3.63587400
H	-1.95179100	0.09245600	2.66593100
H	-2.49596600	-1.60682700	2.65341700
H	0.28893800	-3.30802500	-0.76976100
H	-3.66519100	-1.33952400	-0.99529800
H	-5.25224000	0.47779500	-1.53391200
H	-4.71485400	2.82786200	-0.91514800
H	-2.57497300	3.33318900	0.24911900
H	-0.98484500	1.51116500	0.77590700
H	3.81446800	-1.43820000	0.55906900
H	5.69866200	0.08102500	0.03983000
H	5.25254500	2.44496900	-0.59494300
H	2.90834400	3.26705700	-0.71416800
H	1.03065600	1.74221000	-0.21930100

**CA-a-mx:** E= -863.1624402 a.u

N	-0.20505600	-1.61661100	-0.55822300
C	-0.94787000	-0.39383200	-0.94013300
C	0.16357900	0.66346800	-0.66507100
C	0.93042100	0.05232000	0.55489300
O	0.37197500	-1.25462400	0.74223200

C	-0.97897400	-2.82853800	-0.33344400
C	2.43544400	0.03171100	0.37365700
C	3.23023700	0.98801600	1.01273200
C	4.61526700	0.99654600	0.83315700
C	5.21811100	0.03782100	0.01924600
C	4.42969600	-0.92656500	-0.61496200
C	3.04668900	-0.92981600	-0.44225700
C	-0.34436700	2.06871600	-0.40684500
O	-0.15513900	2.99982000	-1.15721700
C	-2.29734400	-0.13929200	-0.27692600
C	-3.39818600	0.15675500	-1.09243800
C	-4.65565600	0.41339200	-0.54377100
C	-4.83597100	0.36585000	0.83838200
C	-3.75109800	0.06112300	1.66327500
C	-2.49218600	-0.18524300	1.11463100
H	-1.10986000	-0.45687500	-2.02139300
H	0.82312000	0.70899900	-1.53415700
H	0.69046600	0.60827100	1.47132700
H	-1.44652400	-3.10069400	-1.28511500
H	-0.28794800	-3.62411900	-0.04331000
H	-1.75670600	-2.72518300	0.43490000
H	2.76620900	1.73084800	1.65883600
H	5.22048500	1.74650900	1.33551900
H	6.29612100	0.03834400	-0.11832900
H	4.89519700	-1.67894500	-1.24647300
H	2.42878800	-1.67479500	-0.93448900
H	-0.90888400	2.20470000	0.54050700
H	-3.26840000	0.19289900	-2.17212500
H	-5.49199100	0.64689100	-1.19722800
H	-5.81341700	0.56281400	1.27027200
H	-3.88323500	0.01603200	2.74116400
H	-1.65947300	-0.43558600	1.76277300

**CA-a-on:** E= -863.1599374 a.u

N	0.84469600	2.24828700	-0.74408500
C	0.67848300	0.79051600	-0.97464700
C	-0.84521500	0.67685600	-0.65989600
C	-1.00919400	1.72608100	0.48981600
O	0.22622100	2.42644300	0.57712900
C	2.20322900	2.75231400	-0.60950900
C	-2.13514100	2.70944700	0.20748900
O	-3.27785700	2.55822900	0.58083700
C	-1.45741500	-0.69067200	-0.40350000
C	-0.95750200	-1.83815400	-1.03598900
C	-1.56476100	-3.08031100	-0.85220500
C	-2.69188500	-3.19931700	-0.03827300

C	-3.21035400	-2.06231700	0.58076500
C	-2.60173600	-0.81933200	0.39817000
C	1.63481500	-0.12315100	-0.22370200
C	2.60823000	-0.81839900	-0.95592200
C	3.53829800	-1.64565600	-0.32527700
C	3.51468500	-1.78677900	1.06207400
C	2.55732900	-1.09477200	1.80635800
C	1.62583000	-0.27232200	1.17246400
H	0.83726600	0.64171700	-2.04845200
H	-1.34100100	1.09453900	-1.54758800
H	-1.18558200	1.24651000	1.45762600
H	2.71239300	2.59313800	-1.56526100
H	2.77414200	2.26658900	0.19289600
H	2.14861500	3.82706600	-0.41725100
H	-1.81732900	3.59831400	-0.37914300
H	-0.07963600	-1.77013900	-1.67042000
H	-1.15203800	-3.95647700	-1.34551000
H	-3.16385000	-4.16736700	0.10689200
H	-4.09572700	-2.13637900	1.20675400
H	-3.04210700	0.05871700	0.86215500
H	2.63610300	-0.71293100	-2.03909500
H	4.27857200	-2.17686900	-0.91775900
H	4.23479800	-2.43041800	1.56004600
H	2.53157600	-1.19692800	2.88805200
H	0.89783600	0.26133600	1.77163600

**CA-a-ox:** E= -863.1633643 a.u

N	-0.59067300	1.03705200	1.67135500
C	-0.54360500	-0.14768200	0.77187400
C	0.55833200	0.27858800	-0.25944400
C	0.67135600	1.82746200	0.00470100
O	-0.49074100	2.16354600	0.74108000
C	0.67067200	2.61597400	-1.28911700
O	1.67706900	2.92197600	-1.88584100
C	1.88023500	-0.44731800	-0.12692900
C	2.46147200	-1.07122900	-1.23629800
C	3.68127700	-1.74143300	-1.12265200
C	4.33630900	-1.79784400	0.10719800
C	3.76553100	-1.17807500	1.22202800
C	2.54938900	-0.50723700	1.10576400
C	-1.84865000	-0.59139000	0.12971700
C	-2.31395000	-1.89301300	0.35756400
C	-3.50155900	-2.34591100	-0.21991600
C	-4.25247000	-1.49416300	-1.02992100
C	-3.80629500	-0.19013000	-1.25754800
C	-2.61467600	0.25697200	-0.68740200

C	-1.79895400	1.24900900	2.45219100
H	-0.16804400	-0.97322100	1.38427300
H	0.16840800	0.10746800	-1.26782000
H	1.58216900	2.04549900	0.57416900
H	-0.34198800	2.86422700	-1.67826300
H	1.95665900	-1.03092300	-2.19877400
H	4.11719800	-2.21866900	-1.99631600
H	5.28556500	-2.31892500	0.19794500
H	4.27010400	-1.21550400	2.18398700
H	2.11034400	-0.02247500	1.97484100
H	-1.73521000	-2.56324300	0.98986300
H	-3.83858600	-3.36245500	-0.03469600
H	-5.17838200	-1.84171300	-1.48016000
H	-4.38754000	0.48230900	-1.88318400
H	-2.28193600	1.27510700	-0.86141000
H	-1.66345900	2.15409500	3.04987000
H	-1.90829600	0.39492800	3.12797300
H	-2.70940700	1.34447000	1.84544200

**Alkene 2d: E=-269.349344 a.u**

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.53938792
C	1.41933872	0.00000000	1.97335530
C	2.23262661	-0.00040235	0.90760210
C	1.48938750	-0.00083924	-0.40881785
H	-0.54180328	0.87858473	-0.36446269
H	1.70309542	0.00029111	3.01999146
H	3.31858680	-0.00047379	0.94798635
H	1.76055984	-0.87769413	-1.01098758
H	1.76138098	0.87486454	-1.01227242
H	-0.54306626	-0.87771916	-0.36462301
O	-0.98291475	0.00017409	2.25676869

**TS-d-mn: E= -709.496283 a.u**

1 imaginary frequency = -404.7805 cm<sup>-1</sup>

O	1.88133100	-1.92041300	-0.11493200
C	-0.15543900	-1.07168100	-0.50265400
H	-0.04634300	-1.51042700	-1.48722600
N	0.68329700	-1.63113800	0.38486500
C	-1.46737600	-0.47863400	-0.20179500
C	-2.55420600	-0.85867000	-1.01146500
C	-1.68281600	0.48051200	0.80401800
C	-3.82432100	-0.33096300	-0.79763500

H	-2.39659600	-1.58224300	-1.80752800
C	-2.95482200	1.00909400	1.01410600
H	-0.85207700	0.85016500	1.39273900
C	-4.02923700	0.60168400	0.22167200
H	-4.65243200	-0.64419400	-1.42731300
H	-3.10142700	1.75693200	1.78814700
H	-5.01821000	1.01999700	0.38743400
C	1.42158900	0.41059800	-1.24367300
C	2.53251700	-0.41823400	-0.93040000
C	0.63961000	-1.43466800	1.83113700
H	-0.39410300	-1.48614200	2.17711900
H	1.22243600	-2.24277400	2.27566700
H	1.07750900	-0.47429500	2.12194400
C	3.41967400	0.27735800	0.10286400
C	1.40221800	1.58779500	-0.37425100
C	2.59210500	1.47539500	0.60752400
H	2.22518500	1.35163800	1.63323900
H	3.14925300	2.41780600	0.59654200
H	0.93000200	0.44118400	-2.20896300
H	3.02526500	-1.01157800	-1.69440300
H	3.73786000	-0.40933200	0.89271500
H	4.33235300	0.62538700	-0.39812500
O	0.61132800	2.52270500	-0.39166000

**TS-d-mx:** E= -709.500402 a.u

1 imaginary frequency = -390.0699 cm<sup>-1</sup>

O	-1.85078700	1.66313300	-0.73169100
C	0.03549100	0.46230200	-0.62198700
H	-0.44234100	-0.19248100	-1.33974000
N	-0.53620300	1.68023800	-0.60216700
C	1.43765400	0.14583600	-0.30967700
C	2.09035800	-0.78330500	-1.14046600
C	2.14015900	0.65740400	0.79757400
C	3.40961700	-1.15832700	-0.90015700
H	1.55283100	-1.21076400	-1.98242900
C	3.45978900	0.28141400	1.03666700
H	1.64706900	1.32491100	1.49563400
C	4.10196500	-0.62136600	0.18625300
H	3.89442800	-1.87402900	-1.55799700
H	3.98376500	0.68388500	1.89920900
H	5.13001300	-0.91523300	0.37876000
C	-1.39496100	-0.30546400	0.98556800
C	-1.63628700	-1.65033100	0.44622000
C	-2.89485200	-1.56551600	-0.44232300

C	-3.55884800	-0.22682800	-0.07029300
C	-2.47296400	0.54617700	0.66233400
H	-0.70517200	-0.14988700	1.80762800
H	-2.58692500	-1.59106200	-1.49618300
H	-3.52961200	-2.44103100	-0.27767400
H	-2.76100900	1.37677000	1.29940100
C	-0.01721700	2.85120800	0.09776900
H	1.05796100	2.94369100	-0.06253400
H	-0.53312200	3.71799400	-0.31690500
H	-0.23200800	2.78984600	1.17320500
H	-4.40869200	-0.38601700	0.60610400
H	-3.93177100	0.33285500	-0.93381500
O	-0.97188900	-2.65942400	0.62639300

**TS-d-on: E= -709.488685 a.u**

1 imaginary frequency = -429.2008 cm<sup>-1</sup>

O	1.67388700	-1.86508000	-0.05185700
C	-0.28358700	-0.88651600	-0.48566000
H	-0.22998600	-1.42067900	-1.42942500
N	0.52350200	-1.51146600	0.42922400
C	-1.63462800	-0.35004300	-0.19350100
C	-2.64464200	-0.60330700	-1.14064300
C	-1.96373700	0.44551300	0.92016700
C	-3.93405000	-0.10404100	-0.97620700
H	-2.41083500	-1.20692400	-2.01424900
C	-3.25686300	0.94165400	1.08721400
H	-1.21270800	0.69174000	1.66174800
C	-4.24745400	0.66892800	0.14351200
H	-4.69478000	-0.32176400	-1.72082100
H	-3.48628400	1.55087600	1.95722900
H	-5.25257600	1.05907300	0.27658700
C	1.01869700	0.53622500	-1.17492700
C	2.24738300	-0.15321200	-1.11357700
C	3.16403200	0.50640400	-0.15916600
C	1.07746800	1.78209900	-0.28042200
H	1.13206300	2.67403300	-0.91760800
C	2.37476400	1.63188000	0.54027800
O	4.34571400	0.26635200	0.01370700
H	0.18154300	1.91005900	0.33598600
H	2.98323900	2.54136300	0.55698500
H	2.19824200	1.36056300	1.58750800
H	2.63870900	-0.80817200	-1.88021000
H	0.48601500	0.62778300	-2.11825600
C	0.48177900	-1.31895900	1.88036700
H	-0.54660900	-1.39068800	2.23752800

H	1.08242600	-2.12058400	2.31037500
H	0.91524500	-0.35633800	2.17263700

**TS-d-ox:** E= -709.493491 a.u

1 imaginary frequency = -409.6217cm<sup>-1</sup>

O	-1.65066900	1.49562900	-0.92085700
C	0.16146100	0.24600200	-0.54809600
H	-0.26480800	-0.43143300	-1.28235200
N	-0.37955600	1.48993300	-0.69652600
C	1.59418400	-0.00451000	-0.24957900
C	2.31663100	-0.84445000	-1.11462600
C	2.24942700	0.49837900	0.88839500
C	3.65491800	-1.14829600	-0.87031700
H	1.82252600	-1.25275400	-1.99268200
C	3.58871300	0.19756800	1.13161400
H	1.70714500	1.11374000	1.59967900
C	4.29728300	-0.62374200	0.25230700
H	4.19506400	-1.79416000	-1.55704400
H	4.07643900	0.59685400	2.01668700
H	5.33986900	-0.85988900	0.44615400
C	-1.06234100	-0.44778700	0.95502700
C	-1.35535300	-1.89089400	0.52461600
C	-2.64542100	-1.77292300	-0.30987000
C	-3.28974400	-0.45817600	0.15886200
C	-2.22608900	0.32483900	0.81958100
H	-0.36574700	-0.27807000	1.77271200
H	-1.52878300	-2.51057800	1.41378100
H	-0.52283500	-2.35309400	-0.01940800
H	-2.42827500	-1.67883500	-1.38254800
H	-3.33824900	-2.61033100	-0.19152200
H	-2.45855000	1.23070900	1.36495400
O	-4.46031000	-0.15009100	0.02853500
C	0.14151100	2.69626900	-0.05146200
H	1.22808700	2.73796700	-0.13647300
H	-0.31312300	3.54532200	-0.56220900
H	-0.15511000	2.71703700	1.00582400

**CA-d-mn:** E= -709.549365 a.u

O	-2.23561000	1.49866100	-0.08691800
C	-0.15337000	0.73714400	-0.64167900
H	-0.10762200	1.41925900	-1.50926400
N	-0.88239500	1.38295900	0.46474500
C	1.25652800	0.33302100	-0.26543100
C	2.26105900	0.36601000	-1.24042900

C	1.59025700	-0.07736200	1.03222800
C	3.56669700	-0.01717900	-0.93462300
H	2.01746000	0.69349300	-2.24890700
C	2.89819900	-0.44972600	1.34255100
H	0.82283300	-0.09137100	1.79959000
C	3.88938500	-0.42592300	0.36023300
H	4.33182800	0.00985700	-1.70596500
H	3.14149100	-0.76311200	2.35434000
H	4.90687900	-0.72066000	0.60270300
C	-1.14551600	-0.40201200	-1.02446000
C	-2.51977200	0.23508400	-0.69862700
C	-0.47350900	2.75681800	0.72104800
H	0.55305100	2.73992700	1.09615000
H	-0.52650800	3.38307100	-0.18400800
H	-1.12626900	3.18073500	1.48814400
C	-3.25523200	-0.74781800	0.24670000
C	-1.05301000	-1.65416900	-0.13469000
C	-2.16216500	-1.59657100	0.91185800
H	-1.75538900	-1.07993600	1.79212200
H	-2.46912900	-2.60038800	1.21800500
H	-1.00733500	-0.69125200	-2.06941900
H	-3.12164000	0.46857100	-1.58115700
H	-3.87768700	-0.19371900	0.95497500
H	-3.91717100	-1.38823400	-0.34966600
O	-0.25005600	-2.54751800	-0.28294800

**CA-b-mx:** E= -709.552707 a.u

O	-1.85829500	1.61434200	-0.08471600
C	-0.04242200	0.24091300	-0.36147000
H	-0.28265000	-0.07893800	-1.39022500
N	-0.40177600	1.66657200	-0.17526600
C	1.42864600	-0.00285900	-0.10600800
C	2.16698900	-0.82581200	-0.96389200
C	2.07121500	0.58067800	0.99466100
C	3.52101000	-1.06924900	-0.72566400
H	1.67754500	-1.28349400	-1.81984400
C	3.42440300	0.34233700	1.23014700
H	1.50489400	1.23656700	1.64943900
C	4.15315200	-0.48529200	0.37186600
H	4.08081600	-1.71210100	-1.39982300
H	3.91118200	0.80434800	2.08496100
H	5.20771400	-0.67101900	0.55767400
C	-1.02670900	-0.46210000	0.62661500
C	-1.80536700	-1.59505700	-0.05872000
C	-3.23153100	-1.10583200	-0.33810100



C	-3.46246300	-0.00376800	0.70962300
C	-2.07788500	0.63176900	0.93014000
H	-0.50335700	-0.84325300	1.50627700
H	-3.23296400	-0.67924600	-1.35244100
H	-3.95104400	-1.92995600	-0.32083000
H	-1.96078400	1.08279400	1.92417200
C	-0.10412600	2.50310100	-1.32979700
H	0.98324300	2.53220100	-1.44657600
H	-0.56286800	2.12387100	-2.25887700
H	-0.46694400	3.51581900	-1.13673400
H	-3.80727900	-0.44304100	1.65535400
H	-4.19934800	0.74617700	0.40709300
O	-1.35110500	-2.68430500	-0.32892800

**CA-d-on:** E= -709.543075 a.u

O	-1.93900200	1.50449900	-0.28562500
C	0.12581800	0.61712400	-0.71109700
H	0.23098100	1.23308200	-1.62235500
N	-0.60805100	1.37542000	0.32038700
C	1.50449300	0.18208900	-0.25888000
C	2.50052100	-0.03575800	-1.22058700
C	1.81789800	-0.02775100	1.09160500
C	3.77266000	-0.46917600	-0.84817500
H	2.27651200	0.13874900	-2.27094100
C	3.09395100	-0.45271700	1.46631300
H	1.05951400	0.15909800	1.84537300
C	4.07367500	-0.67972300	0.49899700
H	4.53072300	-0.63424300	-1.60931200
H	3.32124400	-0.60513100	2.51820500
H	5.06619900	-1.01115500	0.79211100
C	-0.88811000	-0.51455500	-1.03650200
C	-2.23687200	0.20454100	-0.76946900
C	-2.99434300	-0.69165200	0.24172500
C	-0.86797200	-1.76256000	-0.10762900
H	-0.34620300	-2.60559400	-0.56879500
C	-2.34287300	-2.06918200	0.21086100
O	-3.92038100	-0.33214300	0.92904400
H	-0.34198200	-1.53002200	0.82224300
H	-2.80775100	-2.64647400	-0.60322000
H	-2.51259900	-2.61525800	1.14237500
H	-2.86218700	0.34037000	-1.65985300
H	-0.78591700	-0.81681300	-2.08270800
C	-0.15581700	2.74957200	0.48815800
H	0.85598300	2.72640600	0.90133500
H	-0.15268700	3.30609900	-0.46273100

H -0.81859200 3.25259900 1.19629100

**CA-d-ox:** E= -709.545595 a.u

O 0.00000000 0.00000000 0.00000000  
C 0.00000000 0.00000000 2.28179711  
H 1.10392393 0.00000000 2.34206604  
N -0.43920752 0.81821173 1.13713012  
C -0.57062107 0.49112206 3.59360594  
C 0.24054207 0.57604145 4.73083832  
C -1.92362273 0.84691051 3.69944018  
C -0.28740438 0.99341935 5.95466710  
H 1.29452626 0.31690877 4.65752156  
C -2.44972310 1.27202412 4.91832015  
H -2.55074035 0.80390266 2.81393343  
C -1.63425079 1.34269612 6.05124973  
H 0.35619351 1.05171117 6.82845552  
H -3.49823729 1.55036589 4.98472498  
H -2.04603098 1.67315757 7.00109590  
C -0.47027770 -1.41699554 1.85513514  
C 0.51697719 -2.55801987 2.21914831  
C 1.46896833 -2.68159807 1.01506174  
C 0.59877720 -2.30244320 -0.18131007  
C -0.47733366 -1.31111021 0.31094446  
H -1.46855973 -1.60711425 2.25636353  
H -0.03519616 -3.49581758 2.34881337  
H 1.03761465 -2.36235498 3.16225609  
H 2.28438048 -1.94734414 1.07800082  
H 1.92072624 -3.66767753 0.88145809  
H -1.45161095 -1.49643631 -0.15705072  
O 0.69742908 -2.71403622 -1.31338935  
C 0.27862923 2.07572641 0.99166088  
H 0.02020822 2.70829929 1.84528222  
H 1.37122381 1.93495180 0.95440153  
H -0.05118708 2.56638162 0.07272584

**Alkene 2e:** E=-403.1289297 a.u

C 0.15128800 -0.33275200 0.00016700  
C -0.38888000 0.98533700 0.00010100  
C -1.78547600 1.14370400 0.00028000  
C -2.59440900 0.01426000 0.00021100  
C -2.03752600 -1.28123500 -0.00019300  
C -0.66030900 -1.47325400 -0.00034800  
C 1.86076400 1.12086400 -0.00028800  
C 0.72675800 1.88883900 -0.00032300

H	-2.22506700	2.13806800	0.00041500
H	-3.67528300	0.12706900	0.00034200
H	-2.69644400	-2.14538400	-0.00046700
H	-0.23486700	-2.47306700	-0.00098200
H	2.90172300	1.41610200	0.00002800
H	0.69046800	2.96962400	-0.00047600
N	1.52981300	-0.22415600	0.00008400
C	2.46029300	-1.33291000	0.00030600
H	2.32794300	-1.95906000	0.89093000
H	2.32773100	-1.95958000	-0.88991900
H	3.48008800	-0.94179300	0.00006400

**TS-e-mn: E= -843.2576736 a.u**

1 imaginary frequency = -457.9068 cm<sup>-1</sup>

C	-1.93993900	-0.88063300	-0.27505700
C	-1.45473700	1.16477100	-1.23695000
C	-0.32378100	0.29244700	-1.38988900
C	1.12386000	1.29593500	-0.36071200
O	-0.64818800	2.58212600	0.06252700
N	0.35433000	1.92647100	0.58285200
C	0.13824100	1.44854000	1.95102300
H	1.09198500	1.18720100	2.41345800
H	-0.31953500	2.27671100	2.49378500
H	-0.54070000	0.58961100	1.97726200
C	2.29007000	0.44010100	-0.02811200
C	3.50590200	0.68515400	-0.69158100
C	2.23307900	-0.64539600	0.86568200
C	4.62998100	-0.10391400	-0.45547100
H	3.56778800	1.51344300	-1.39346400
C	3.35958400	-1.43226400	1.10557900
H	1.29830900	-0.89168800	1.35593900
C	4.56283200	-1.16429600	0.45034000
H	5.55940800	0.11247800	-0.97549100
H	3.29321400	-2.26398400	1.80219500
H	5.43820800	-1.77957900	0.63957100
H	1.30699900	1.97645600	-1.18933500
H	0.23960000	0.23226600	-2.31674300
H	-1.66028300	2.00530800	-1.88262900
C	-2.46813400	0.41352000	-0.53235400
N	-0.65483700	-0.95939300	-0.78966400
C	-3.76540700	0.72764400	-0.10902800
C	-2.68651300	-1.84985100	0.40277000
H	-4.17578800	1.71617900	-0.29792100
H	-2.28728000	-2.84159200	0.59545800

C	-4.51659100	-0.23891300	0.55575100
C	-3.97796600	-1.51211400	0.80918800
H	-5.52614000	-0.00868800	0.88456000
H	-4.58118800	-2.25435700	1.32572900
C	-0.02337500	-2.20566500	-1.17424500
H	-0.02306500	-2.91063600	-0.33637700
H	-0.53203500	-2.68239200	-2.02669500
H	1.01692400	-2.01368800	-1.44345500

**TS-e-mx: E= -843.2605812 a.u**

l imaginary frequency = -422.8351 cm<sup>-1</sup>

C	2.24992900	-0.89252200	-0.27132200
C	1.40616400	1.16193800	-0.88491900
C	0.37499800	0.17289600	-1.01945400
C	-0.86658700	0.59363600	0.51178400
O	0.60987100	2.24604200	0.80308100
H	-0.25752000	0.05034100	1.23188500
N	-0.64856500	1.93945800	0.65420600
C	-1.45568700	2.96296300	-0.00733000
H	-2.52020500	2.75325800	0.11117400
H	-1.20720800	3.91374300	0.46608800
H	-1.20675800	3.02768200	-1.07685600
H	1.41176600	2.11100200	-1.39960700
H	-0.34328600	0.18164100	-1.83593100
C	-2.22966300	0.02365800	0.31740100
C	-2.73546800	-0.86587800	1.28103000
C	-3.01748700	0.28818700	-0.81619700
C	-3.99119600	-1.45214500	1.13163300
H	-2.13671400	-1.08829400	2.16100100
C	-4.27553800	-0.29594300	-0.96660400
H	-2.64304200	0.94803900	-1.59357000
C	-4.76804800	-1.16650500	0.00689000
H	-4.36393000	-2.13034300	1.89460700
H	-4.86795900	-0.07592600	-1.85077900
H	-5.74681300	-1.62292300	-0.11264900
C	2.57724700	0.48623200	-0.39904900
N	0.97066900	-1.09225100	-0.74743500
C	0.24275900	-2.33780700	-0.68262200
H	-0.14333300	-2.56124200	0.32297500
H	-0.60644300	-2.29527000	-1.37037900
H	0.89378600	-3.16207300	-0.99296700
C	3.16941500	-1.81674500	0.24078300
C	3.86185100	0.92546900	-0.05262200
H	2.91275500	-2.86492900	0.36420100

H	4.12201600	1.97656500	-0.14650000
C	4.43806700	-1.34970800	0.57849100
C	4.78769300	0.00496900	0.42923700
H	5.17292300	-2.05016600	0.96717600
H	5.78557500	0.33393300	0.70531000

**TS-e-on: E=** -843.2666359 a.u

1 imaginary frequency = -449.8871 cm<sup>-1</sup>

C	2.23213000	0.67130700	-0.20597200
C	0.98959700	0.81622400	-0.87584000
C	0.36908200	2.06716800	-0.89516800
C	0.96207600	3.13557800	-0.21426000
C	2.15804100	2.95621400	0.49281800
C	2.80948600	1.71830600	0.51201300
C	1.73211300	-1.35980900	-1.09414400
C	0.62430100	-0.49669200	-1.41244500
H	-0.56942700	2.20616300	-1.42487400
H	0.48609700	4.11228400	-0.22649700
H	2.59591600	3.79359400	1.02981800
H	3.74370700	1.59213000	1.05164000
N	2.70280900	-0.62003600	-0.42824400
C	3.82837500	-1.22002800	0.25256200
H	3.57258100	-1.52388400	1.27661300
H	4.14498200	-2.10992600	-0.29785700
H	4.66501300	-0.51523800	0.28319800
C	-0.88745000	-1.46809100	-0.29497500
O	0.94055800	-2.64760000	0.20535100
N	-0.11172200	-2.00083300	0.68759400
C	0.06959200	-1.42129200	2.01724500
H	-0.90251200	-1.18837200	2.45691200
H	0.56760400	-2.18263700	2.61978000
H	0.68944500	-0.51639900	1.99563800
C	-2.07579700	-0.61712200	-0.06438000
C	-3.25530100	-0.93744300	-0.76222200
C	-2.08369200	0.52249900	0.76063800
C	-4.40921400	-0.17086600	-0.62020700
H	-3.26409000	-1.80681500	-1.41537000
C	-3.24118500	1.28767400	0.90516000
H	-1.17826700	0.83188700	1.26782000
C	-4.40800800	0.94391400	0.22110900
H	-5.30962600	-0.44514100	-1.16341400
H	-3.22481000	2.16402400	1.54765900
H	-5.30666000	1.54395300	0.33606600
H	-1.01093600	-2.18867500	-1.09826500
H	0.09408000	-0.59374900	-2.35343500

H 2.05996800 -2.21155500 -1.67528700

**TS-e-ox: E= -843.2679725 a.u**

1 imaginary frequency = -435.7547 cm<sup>-1</sup>

C 2.51074900 0.46859800 0.14320300  
C 1.25049000 0.83273400 0.67905400  
C 0.87751700 2.17762400 0.69932500  
C 1.75621400 3.13600300 0.18615900  
C 2.98822900 2.75486500 -0.36328300  
C 3.38112300 1.41448200 -0.40010500  
C 1.51030400 -1.45368900 0.80884500  
C 0.55755300 -0.40672300 1.03824600  
H -0.08551300 2.47480400 1.10666200  
H 1.47905100 4.18645900 0.20643800  
H 3.65277600 3.51316900 -0.76904100  
H 4.33584700 1.12755400 -0.83123800  
N 2.67717500 -0.90488200 0.30558400  
C 3.75664300 -1.68571800 -0.25781700  
H 3.61647000 -1.85476000 -1.33292500  
H 4.71222800 -1.17731900 -0.09386000  
H 3.79171100 -2.65757500 0.24160900  
C -0.76001200 -0.74685700 -0.54950500  
O 0.66662200 -2.45542600 -0.77418800  
H -0.11112200 -0.22484700 -1.24555100  
N -0.60110800 -2.09265800 -0.67292600  
C -1.45360700 -3.08361400 -0.02606300  
H -2.50759500 -2.84934400 -0.18771400  
H -1.21485900 -4.04675900 -0.47962700  
H -1.24895300 -3.14397900 1.05355700  
H 1.57607800 -2.39416900 1.33774600  
H -0.15708400 -0.45829300 1.85267600  
C -2.06075400 -0.07633300 -0.30972100  
C -2.42685800 0.98292000 -1.15884100  
C -2.91399700 -0.38670400 0.76494300  
C -3.61658800 1.68327900 -0.96555700  
H -1.76962400 1.25177100 -1.98146300  
C -4.10522900 0.31119500 0.95714800  
H -2.63804900 -1.16424000 1.47005500  
C -4.46431400 1.34574700 0.09064700  
H -3.88040300 2.49316200 -1.64041100  
H -4.74919800 0.05337000 1.79382200  
H -5.39198400 1.89033000 0.24408800

**CA-e-mn: E= -843.3097458 a.u**

C	1.77804800	-0.90991300	0.29547300
C	1.43549500	1.34467500	0.96611000
C	0.20130500	0.46017100	1.35638600
C	-0.95224900	1.16591400	0.56741500
O	0.91807800	2.40891400	0.16888400
N	-0.21991800	1.81509300	-0.53303200
C	-0.92067100	2.94368900	-1.12499800
H	-1.80997100	2.56097300	-1.63318300
H	-1.22028300	3.69334600	-0.37388800
H	-0.26642100	3.41636900	-1.86177200
C	-2.05727100	0.26745500	0.06589900
C	-3.26802000	0.18902200	0.76523100
C	-1.88783700	-0.51661300	-1.08497800
C	-4.28594400	-0.66511200	0.33778000
H	-3.41569700	0.80409400	1.65056600
C	-2.90819400	-1.36423100	-1.51711300
H	-0.95662700	-0.44459000	-1.63660700
C	-4.10785500	-1.44546000	-0.80542100
H	-5.21898600	-0.71394600	0.89312800
H	-2.76632400	-1.96260200	-2.41349600
H	-4.90071800	-2.10722100	-1.14406800
H	-1.37865600	1.93007300	1.24333000
H	-0.02951500	0.47246600	2.42839700
H	1.91324700	1.83975600	1.81779200
C	2.35347300	0.37216800	0.26313300
N	0.54573500	-0.88840200	0.92894300
C	3.59061700	0.57952600	-0.32375400
C	2.44819900	-2.00541400	-0.25916900
H	4.02520900	1.57607800	-0.34678300
H	2.00983000	-2.99877900	-0.25074900
C	4.27277700	-0.50895000	-0.88737400
C	3.69970700	-1.78205500	-0.84611100
H	5.24220800	-0.36252500	-1.35446400
H	4.23227700	-2.62349000	-1.28284200
C	-0.10077500	-2.07204800	1.45247900
H	-0.76804400	-1.78762200	2.27186300
H	-0.70630500	-2.59068200	0.69777700
H	0.64460600	-2.77678800	1.84662800

**CA-e-mx: E= -843.3097458 a.u**

C	2.34094000	-0.83735100	0.04562400
C	1.12325300	1.02836400	-0.74896200
C	0.17063100	-0.18036200	-0.50937500
C	-0.92396900	0.42234200	0.42392000
O	0.72077100	2.00295300	0.21950000

H	-0.65435500	0.14425600	1.45574900
N	-0.73638400	1.87427100	0.20997000
C	-1.20253400	2.69666900	1.31576100
H	-2.28974600	2.59445100	1.37727200
H	-0.75040600	2.40258700	2.27682200
H	-0.95545000	3.74068900	1.10740000
H	1.01480700	1.45151300	-1.75587200
H	-0.26851300	-0.55612000	-1.44284900
C	-2.34384000	-0.00827200	0.12859900
C	-3.00458500	-0.89729100	0.98543000
C	-3.01277100	0.44726200	-1.01713900
C	-4.29932900	-1.33586000	0.70026900
H	-2.50193300	-1.24440200	1.88567700
C	-4.30817700	0.01519700	-1.29969700
H	-2.51425800	1.15689800	-1.67054400
C	-4.95453100	-0.88102700	-0.44449000
H	-4.79676200	-2.02617800	1.37655600
H	-4.81557800	0.38006600	-2.18907100
H	-5.96371400	-1.21745100	-0.66675900
C	2.48464100	0.47503600	-0.44335700
N	0.99927400	-1.20891200	0.12500300
C	0.58610900	-2.59550700	0.03981800
H	1.11173500	-3.19342100	0.79079200
H	-0.48469300	-2.66630100	0.24972900
H	0.77624000	-3.04029600	-0.95246500
C	3.46938100	-1.58975900	0.38824700
C	3.73876600	1.05237700	-0.57665400
H	3.38066700	-2.60825700	0.75356200
H	3.83685700	2.06657300	-0.95569000
C	4.72786200	-0.99597300	0.24888100
C	4.87376000	0.31085300	-0.22458600
H	5.61175400	-1.57243800	0.51075000
H	5.86331000	0.74649800	-0.32560100

**CA-e-on: E= -843.3173551 a.u**

C	2.12271100	0.78465600	-0.06836200
C	0.87466000	0.86595300	-0.71494600
C	0.20216200	2.07638300	-0.78580000
C	0.75810100	3.21131900	-0.17477200
C	1.97518000	3.11082600	0.49967700
C	2.67623900	1.90022100	0.56447200
C	1.74503100	-1.38248500	-0.86909100
C	0.51874200	-0.49704600	-1.26651100
H	-0.75421200	2.14486900	-1.29686600
H	0.23584900	4.16239200	-0.22087600



H	2.39669100	3.98922300	0.98241500
H	3.62545000	1.83933000	1.08784800
N	2.67710200	-0.47721000	-0.23206100
C	3.80092600	-0.97704200	0.52471600
H	4.62552400	-0.25571200	0.49610700
H	3.55090400	-1.18349600	1.57588000
H	4.15107100	-1.90898700	0.07051300
C	-0.65098900	-1.26943800	-0.57323300
O	1.23843500	-2.41736100	-0.02945400
N	0.02889100	-1.86353100	0.59094200
C	-0.65605200	-3.02080300	1.14769200
H	-1.59329900	-2.67735400	1.59359700
H	-0.87008500	-3.78893300	0.38648100
H	-0.03004400	-3.45715200	1.93016700
C	-1.87323100	-0.46926100	-0.18393800
C	-2.99059400	-0.46339000	-1.02887700
C	-1.92170100	0.27357600	1.00446400
C	-4.12720500	0.27959800	-0.70704800
H	-2.97041600	-1.04763000	-1.94665900
C	-3.06288000	1.00537400	1.33388400
H	-1.06208000	0.26824400	1.66590100
C	-4.16653900	1.01637200	0.47849400
H	-4.98368100	0.27345500	-1.37620300
H	-3.08671400	1.57319700	2.26035500
H	-5.05293300	1.58997100	0.73642600
H	-0.96042000	-2.06904300	-1.27050400
H	0.34875600	-0.47559100	-2.34736900
H	2.23285400	-1.92157800	-1.68867800

**CA-e-ox: E= -843.3174696 a.u**

C	-2.59184800	0.27493300	-0.27231900
C	-1.33500600	0.90819000	-0.31290100
C	-1.22279900	2.25967000	-0.02626400
C	-2.37068100	2.98506200	0.32986400
C	-3.60725400	2.34212600	0.39559400
C	-3.73805400	0.97916500	0.09923300
C	-1.10299400	-1.43847200	-0.74864000
C	-0.28643800	-0.11333700	-0.69285100
H	-0.25378000	2.75180500	-0.06748700
H	-2.29394000	4.04379600	0.55960200
H	-4.49146300	2.90542200	0.68319200
H	-4.70636700	0.49193000	0.15961800
N	-2.48377100	-1.05338600	-0.68344400
C	-3.53243800	-2.03466000	-0.50705700

H	-3.70457500	-2.29217700	0.54851400
H	-4.47007000	-1.66112500	-0.93363200
H	-3.25696500	-2.94783100	-1.04267800
C	0.78281200	-0.41361900	0.40461500
O	-0.70443100	-2.15358100	0.43215100
H	0.43691800	0.02902800	1.35212000
N	0.73291000	-1.89176400	0.48404700
C	1.17826500	-2.42842100	1.76040100
H	2.24319000	-2.20251100	1.86607700
H	0.62581800	-1.99991400	2.61241900
H	1.04473700	-3.51319400	1.75472400
H	-0.89640500	-2.06494200	-1.62538000
H	0.19662300	0.11289400	-1.64862500
C	2.17838700	0.08364100	0.09693200
C	2.70431000	1.18181200	0.78759400
C	2.95867800	-0.52675400	-0.89606400
C	3.97665400	1.67225800	0.48619100
H	2.11243800	1.65582300	1.56749400
C	4.23234900	-0.04323500	-1.19247500
H	2.56367600	-1.39337800	-1.41767600
C	4.74419300	1.06055600	-0.50529300
H	4.36856300	2.52726400	1.03085700
H	4.82790700	-0.52926800	-1.96103600
H	5.73635400	1.43758700	-0.73889500