Electronic Supplementary Material (ESI) for RSC Advances.

A comprehensive spectroscopic investigation of α- (2-naphthyl) - *N*-methylnitrone: A computational study on its photochemical nitrone-oxaziridine conversion and thermal *E-Z* isomerization processes

Praveen Saini[a], Anjan Chattopadhyay[a]*

Department of Chemistry, Birla Institute of Technology and Science (BITS), Pilani –K.K. Birla Goa Campus, Goa, 403 726, India

SUPPLEMENTARY DATA

Orbitals involved in the (4, 4) active space in CASSCF/6-31G* calculations

In the CASSCF (4,4) calculation the chosen HOMO is of π symmetry (MO#49) on the CNO moiety while the LUMO is of corresponding π* symmetry (MO#50). Figure S1 shows all the four orbitals involved in the (4, 4) active space of CASSCF calculations.

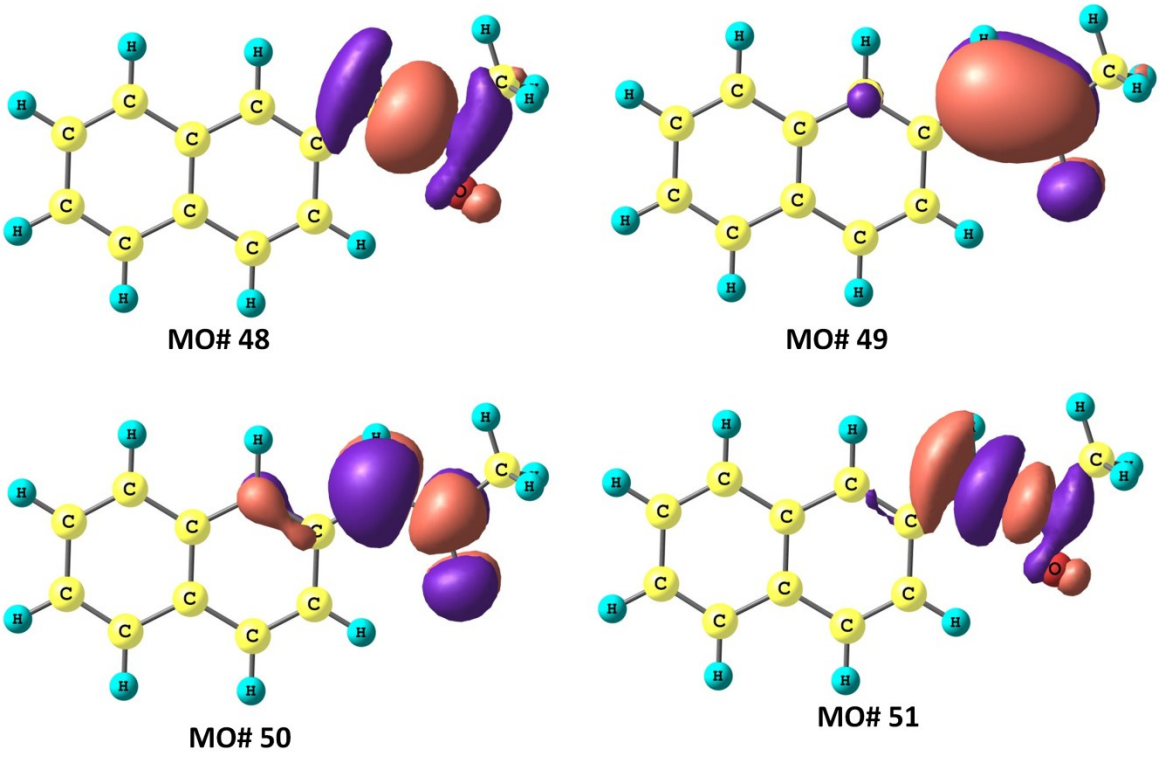


Fig. S1. Orbitals involved in the (4, 4) active space in CASSCF/6-31G* calculations for the α-(2-naphthyl)-*N*-methylnitrone

Semi-empirical CI (PM3/CI) level of studies

Rough estimations of the ground and excited state geometries have been carried out at (4x4) PM3/CI level of calculations using MOPAC. These have predicted non-planar geometries (Figure S2) for the second CI roots for both the isomers. In case of the Z-isomer, the <C-C-N-O dihedral angle value in the excited state is roughly 43^0 which is predicted to be around 57^0 at the

CASSCF level. An interesting situation arises as we give an optimization run on this excited state geometry using a biradical option as the keyword in the input file; the energy drops with a further twist in the CNO part of the molecule.

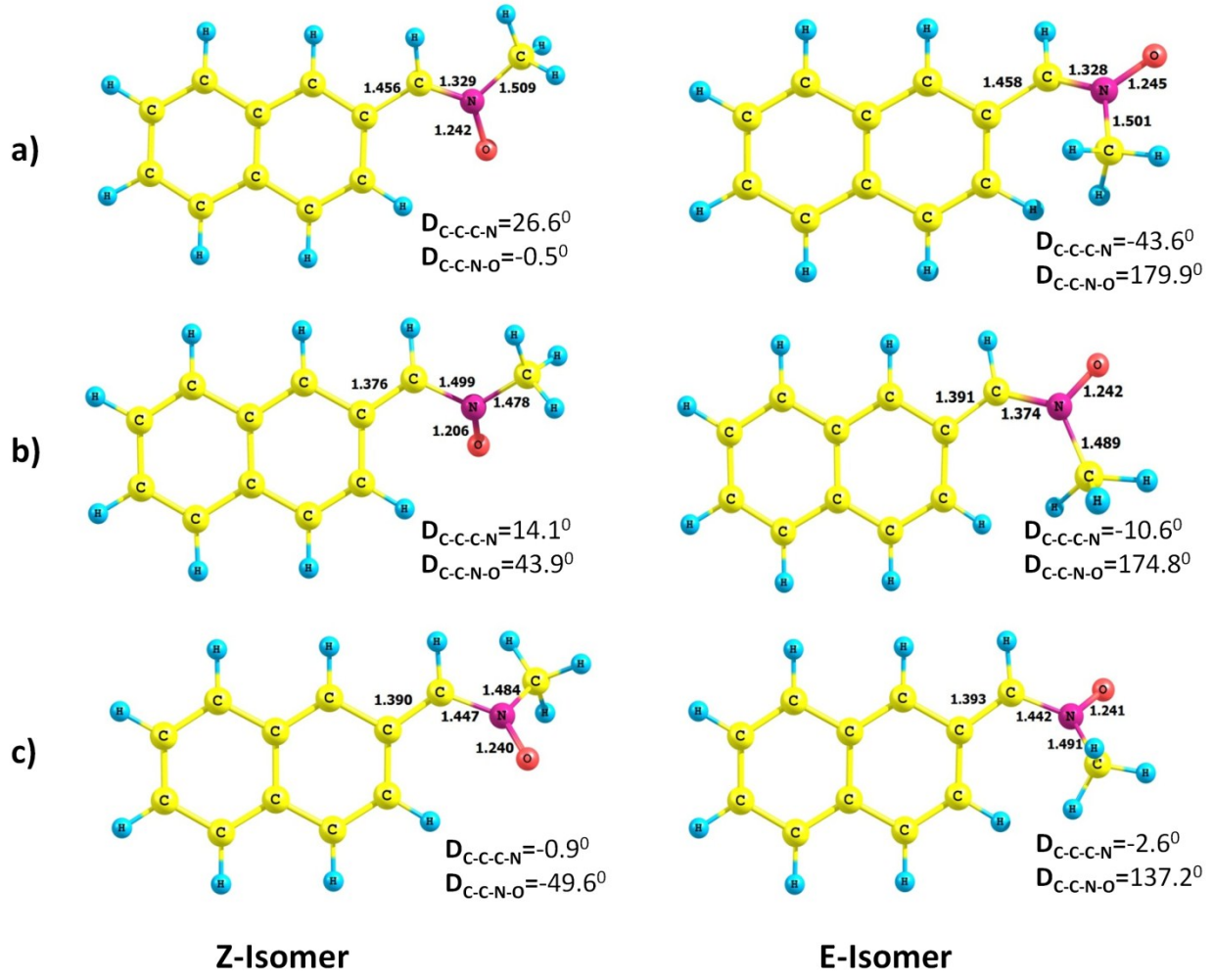


Fig. S2: a) Ground state **b)** Excited state and **c)** Biradical excited state geometries with structural parameters obtained at the PM3/CI level of calculations.

ESP-derived atomic charges using Merz-Kollman Scheme

The ESP-derived atomic charges (Table S1) clearly reveals the lowering of the negative charge on oxygen as we move from ground state to the excited state, which further reduces in the low-

lying conical intersection geometries (**CI_1**, **CI_2** and **CI_4**). This initial electronic transfer from oxygen to nitrogen can be noticed in both the isomers.

Table S1: Atomic charges of the atoms of various important points on potential energy surfaces determined from Electrostatic potential (using Merz-Kollman scheme) at CASSCF/6-31G(d)

Molecular geometries	C	N	C	O
G.S. (Z-Isomer)	-0.2204	0.4999	-0.3921	-0.6323
E.S. (Z-Isomer)	-0.1211	0.2019	-0.3243	-0.2847
G.S. (E-Isomer)	-0.2808	0.4702	-0.3237	-0.5731
E.S. (E-Isomer)	-0.2505	0.2395	-0.1331	-0.3243
TS_{ex1}	-0.3162	0.3314	-0.4135	-0.3065
TS_{ex2}	-0.2916	0.4270	-0.4595	0.3006
TS_{ex3}	-0.2554	0.3189	-0.3516	-0.3232
CI_1	0.0744	-0.0598	-0.4078	-0.1587
CI_2	0.0953	-0.1356	-0.3258	-0.1405
CI_3	-0.0469	0.2364	-.02011	-0.4317
CI_4	0.0954	-0.1806	-0.1955	-0.1446
TS_{gs1}	-0.0386	0.2318	-0.3382	-0.2821
TS_{gs2}	0.2877	-0.1422	-0.2568	-0.3675
TS_{gs5}	-0.1523	0.3468	-0.3742	-0.3471
Ox_1	0.3959	-0.2920	-0.0552	-0.2945
Ox_1	0.2487	-0.2456	-0.2131	-0.2723
Ox_3	0.2503	-0.2513	-0.1328	-0.2774

Transition states

Two transition states (**TS_{ex1}** and **TS_{ex2}**) have been optimized in the excited state for the Z-isomer at the CASSCF level of calculations (Figure S3). The planar **TS_{ex2}** has a negative frequency of 126 cm^{-1} and the vectors corresponding to this frequency indicates a stretch of the oxygen atom towards the front side. It seems that following this frequency we can reach the conical intersection geometry **CI_2** which subsequently leads to **Ox_2**. The other optimized TS geometry (**TS_{ex1}**) has a slightly higher negative frequency (175 cm^{-1}) and not directly connected to this

photochemical path. A transition state with almost similar geometrical parameters ($\mathbf{TS_{ex3}}$) with an opposite C-N-O twist has been obtained from the E-isomer which possesses a negative frequency of 139 cm^{-1}. All these excited state TS geometries are situated marginally (1-2 kcal/mol) above the optimized excited state geometries.

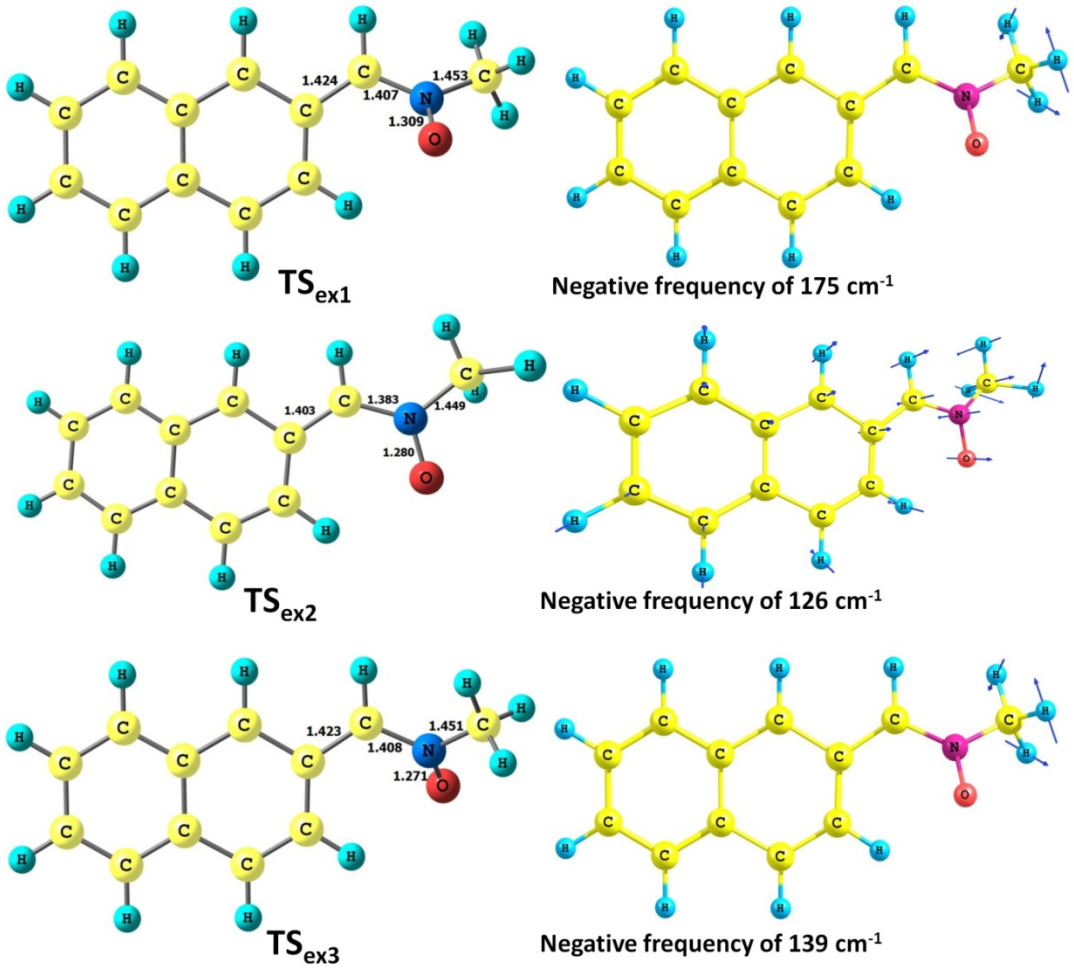


Fig. S3: Optimized transition states geometries ($\mathbf{TS_{ex1-3}}$) on excited state surface with displacement vectors of their respective negative frequencies.

IRC run has been given on the $\mathbf{TS_{gs5}}$ transition state (situated on the ground state surface) both in the forward and reverse directions. The corresponding IRC plot is shown below (Figure S4).

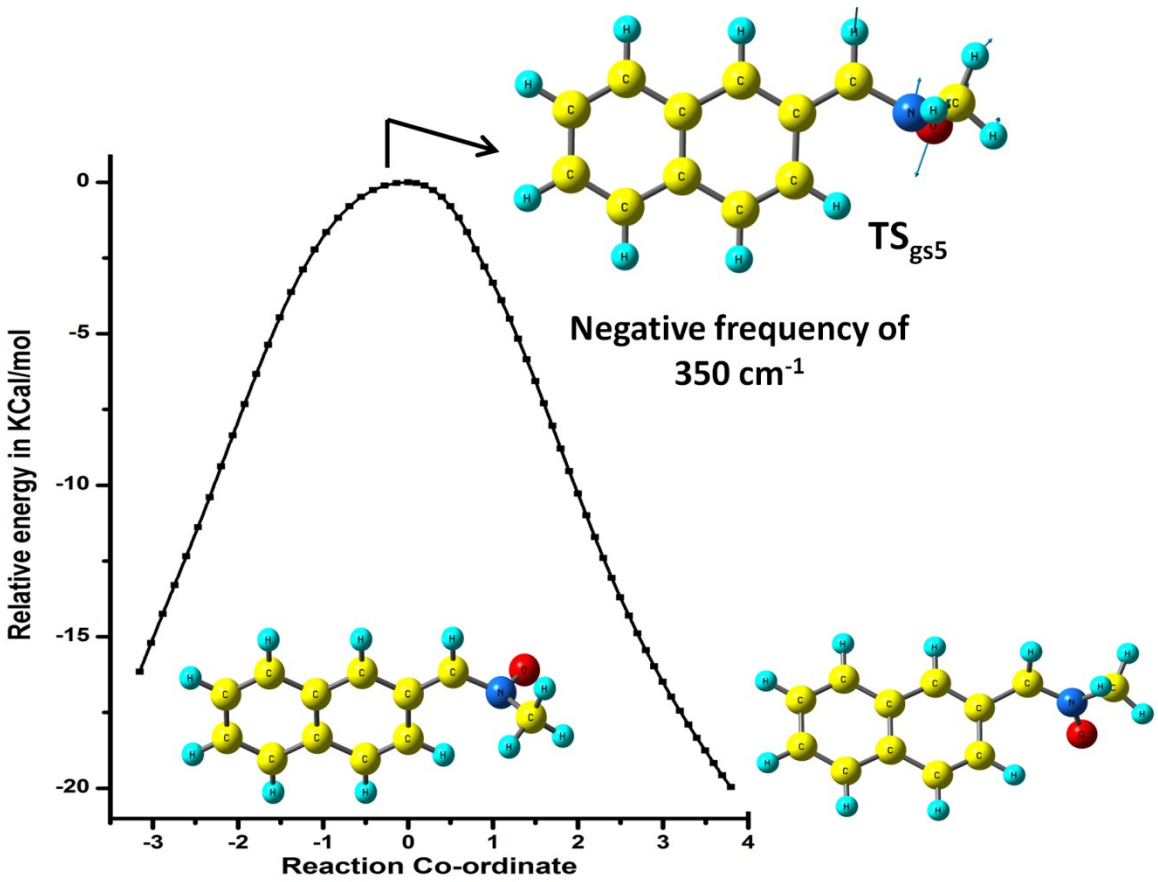


Fig. S4: Intrinsic reaction coordinate (IRC) path of $\mathbf{TS_{gs5}}$ along forward and reverse directions.

Table S2: Absolute (E) and Relative energy values (ΔE) (with respect to the relaxed excited states) at various important transition states geometries. Negative frequencies of the transition states are also shown.

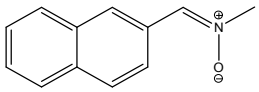
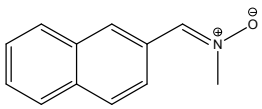
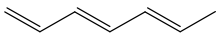
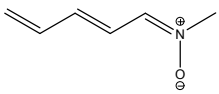
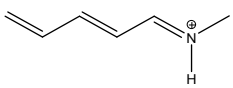
Molecular Geometry	Negative frequency in cm^{-1}	CASSCF		CASMP2		2-Layer ONIOM	
		E in hartree	ΔE in kcal mol^{-1}	E in hartree	ΔE in kcal mol^{-1}	E in hartree	ΔE in kcal mol^{-1}
E.S.(Z isomer)	-	-589.94434	0	-591.80033	0	-589.43709	0
E.S.(E isomer)	-	-589.94401	0.20	-591.79905	0.80	-	-
TS_{ex1}	-175	-589.94073	2.26	-591.79853	1.13	-	-
TS_{ex2}	-126	-589.94251	1.14	-591.80074	-0.26	-	-
TS_{ex3}	-139	-589.94250	1.15	-591.79989	0.28	-	-
TS_{gs1}	-422	-590.04572	-63.61	-591.86748	-42.13	-	-
TS_{gs2}	-1305	-590.04252	-61.60	-591.87407	-46.28	-	-
TS_{gs3}	-332	-	-	-	-	-589.53241	-59.80
TS_{gs4}	-323	-	-	-	-	-589.53050	-60.60
TS_{gs5}	-350	-590.04737	-64.65	-591.88832	-55.21	-	-
TS_{gs6}	-240	-	-	-	-	-589.52925	-57.83

Dominant configurations of S_1 and S_2 states

Analysis of the dominating configurations at the Franck-Condon (FC) geometry reveals that the S_1 state is completely dominated by the HOMO→LUMO excitation (Table S3) in case of 2,4-pentadien-1-iminium ion (85%) and partly dominated in conjugated N-methyl nitrone system (42%). In contrast, this configuration dominates the S_2 state of the 1,3,5-hexatriene (92%) and our presently studied α-naphthyl N-methyl nitrone system (72%) at the FC geometry. The S_1 states of these latter systems are mostly contributed by configurations arising due to the HOMO→LUMO+1, HOMO-1→LUMO excitations. The conjugated non-polar polyene has also a major contribution from the $HOMO^2$→$LUMO^2$ configuration for this first excited singlet state

at the FC geometry. Interestingly, unlike in the iminium ion, this doubly excited configuration becomes a key player in the S_1 state of the nitrones and the polyene as the optimized geometry of this state is approached. This optimized excited state in the α-naphthyl N-methyl nitrone is almost equally contributed by configurations due to $HOMO^2$-$LUMO^2$, HOMO-LUMO+1, HOMO-1-LUMO excitations (Table S3).

Table S3: A comparison of dominant configurations of S_1 and S_2 states at Frank Condon geometries and at optimized first singlet excited state (S_1) geometries of different systems

Systems	**At Frank Condon geometry**		**At optimized S_1 state geometry**	
	S_1 state	**S_2 state**	**S_1 state**	**S_2 state**
	H→L+1 (0.66) H-1→L (0.56) H→L (0.15)	H→L (0.87) H-1→L (0.20)	H-1→L (0.48) H→L+1 (0.47) H^2→L^2 (0.45)	H→L (0.60) H-4→L (0.58) H→L+1 (0.15)
	H→L+1 (0.57) H-1→L (0.56) H-2→L (0.33)	H→L (0.84) H→L+1 (0.19)	H-1→L (0.46) H→L+1 (0.48) H^2→L^2 (0.47)	H-4→L (0.64) H→L (0.52) H→L+1 (0.18)
	H^2→L^2 (0.53) H→L+1 (0.52) H→L+4 (0.45)	H→L (0.96)	H^2→L^2 (0.60) H→L+1 (0.47) H→L+4 (0.40)	H→L (0.94)
	H→L (0.65) H-1→L (0.43) H^2→L^2 (0.38)	H-2→L (0.88)	H^2→L^2 (0.60) H-1→L (0.49) H→L+2 (0.33) H→L (0.17)	H-2→L (0.86)
	H→L (0.92)	H-1→L (0.64) H^2→L^2 (0.46) H→L+4 (0.28)	H→L (0.87) H^2→L^2 (0.29)	H-1→L (0.55) H→L+1 (0.46) H^2→L^2 (0.42) H→L (0.24)

Experimental studies have revealed that the photoproduct oxaziridines are also fluorescent in nature which results in increase and fluctuation of fluorescence intensity of the parent nitrone system during their irradiation. GUGA CISD-based radiative transition studies have also been carried out on the ground state oxaziridine systems and the results (Table S4) are found to be quite similar to the nitrone systems. The S_0-S_1 transition is found to be weaker than the S_0-S_2 and S_2-S_1 transitions; however, the transition moment and oscillator strength values of the latter-mentioned transitions have decreased significantly in comparison to those in nitrones while these parameters of the lowest transition (S_0-S_1) has reduced slightly.

Table S4: Important radiative transition properties of the oxaziridine geometries at their respective ground state equilibrium geometries

Systems	Transition moment (Debye)			Oscillator strength		
	S_0-S_1	S_0-S_2	S_2-S_1	S_0-S_1	S_0-S_2	S_2-S_1
Ox_1	0.151	1.6159	0.405	0.000	0.115	0.000
Ox_2	0.203	1.554	0.333	0.001	0.107	0.000
Ox_3	0.207	1.568	0.330	0.001	0.108	0.000

Cartesian coordinates of optimized geometries at CASSCF (14, 12)/6-31G*

Z-Isomer

Ground state optimized geometry
Energy (CASSCF) = -590.18078; No imaginary frequency

6	-1.475293000	-0.611764000	0.000001000
6	-1.743322000	0.757374000	0.000001000
6	-0.649797000	1.673332000	0.000001000
6	0.650152000	1.242033000	-0.000001000
6	0.932636000	-0.160046000	0.000000000
6	-0.122296000	-1.051563000	0.000000000
6	-2.561656000	-1.538946000	0.000002000
6	-3.857808000	-1.094587000	0.000004000
6	-4.130967000	0.300252000	0.000004000
6	-3.098933000	1.202480000	0.000003000

6	2.279667000	-0.734931000	-0.000002000
7	3.411145000	-0.089143000	0.000002000
6	4.679018000	-0.817541000	-0.000001000
8	3.552220000	1.167974000	0.000006000
1	-0.858780000	2.728496000	0.000001000
1	1.462754000	1.935648000	-0.000001000
1	0.068439000	-2.111240000	-0.000001000
1	-2.347479000	-2.593302000	0.000001000
1	-4.671799000	-1.797048000	0.000005000
1	-5.150059000	0.643044000	0.000005000
1	-3.298927000	2.259336000	0.000003000
1	2.361078000	-1.803097000	-0.000007000
1	5.224145000	-0.511700000	-0.879924000
1	5.224143000	-0.511711000	0.879926000
1	4.523542000	-1.886111000	-0.000008000

Excited state optimized geometry
Energy (CASSCF) = -590.04631; No imaginary frequency

6	1.483846000	-0.650349000	0.000000000
6	1.767494000	0.784738000	0.000000000
6	0.682034000	1.686283000	0.000000000
6	-0.668688000	1.253976000	0.000001000
6	-0.985174000	-0.141490000	0.000004000
6	0.154755000	-1.081614000	0.000002000
6	2.554494000	-1.542919000	-0.000002000
6	3.876188000	-1.099505000	-0.000005000
6	4.163714000	0.276355000	-0.000001000
6	3.117322000	1.206447000	0.000000000
6	-2.249393000	-0.703777000	0.000006000
7	-3.462967000	-0.064093000	0.000000000
6	-4.709790000	-0.815880000	0.000002000
8	-3.588005000	1.181802000	-0.000010000
1	0.884088000	2.742189000	-0.000001000
1	-1.455447000	1.975698000	0.000000000
1	-0.049758000	-2.137050000	0.000002000
1	2.350558000	-2.599505000	-0.000004000
1	4.677621000	-1.815510000	-0.000007000
1	5.183714000	0.614020000	-0.000002000
1	3.333938000	2.259868000	0.000000000
1	-2.338659000	-1.771218000	0.000011000

1	-5.277190000	-0.550305000	0.881294000
1	-5.277185000	-0.550318000	-0.881297000
1	-4.513361000	-1.877561000	0.000011000

E-Isomer

Ground state optimized geometry

Energy (CASSCF) = -590.17567; No imaginary frequency

6	2.867369000	0.736156000	-1.918856000
7	3.578994000	0.318081000	-0.904937000
6	4.006431000	-1.073564000	-0.734487000
8	3.941233000	1.071426000	0.029832000
1	3.540521000	-1.727410000	-1.451805000
1	5.081880000	-1.105069000	-0.829956000
1	3.731283000	-1.351946000	0.270259000
1	2.587812000	1.768974000	-1.851031000
1	-2.123513000	-1.671305000	-6.324178000
6	0.698813000	-0.850634000	-4.597694000
6	1.643644000	-1.498548000	-5.394749000
6	1.210436000	-2.218863000	-6.547999000
6	-0.119279000	-2.279291000	-6.874295000
6	-1.082028000	-1.620448000	-6.062480000
6	-0.682464000	-0.923501000	-4.952378000
6	1.131532000	-0.133777000	-3.443699000
6	2.460443000	-0.069638000	-3.092692000
6	3.420512000	-0.719340000	-3.926953000
6	3.022303000	-1.415316000	-5.036786000
1	1.944764000	-2.714052000	-7.158450000
1	-0.439429000	-2.823693000	-7.744310000
1	-1.405754000	-0.422156000	-4.333905000
1	0.393827000	0.361286000	-2.836599000
1	4.465641000	-0.644303000	-3.686133000
1	3.753017000	-1.898226000	-5.661093000

Excited state optimized geometry

Energy (CASSCF) = -590.04387; No imaginary frequency

6	-1.478273000	-0.742782000	-0.315694000
6	-1.766877000	0.630064000	-0.666338000
6	-0.681454000	1.563654000	-0.684479000
6	0.624474000	1.181400000	-0.391892000

6	0.940634000	-0.153015000	-0.061716000
6	-0.182679000	-1.118048000	-0.021459000
6	-2.571618000	-1.673930000	-0.288990000
6	-3.875863000	-1.262439000	-0.595454000
6	-4.128566000	0.060662000	-0.930804000
6	-3.056973000	0.999676000	-0.961041000
6	2.234037000	-0.613894000	0.239392000
7	3.394021000	0.175901000	0.108754000
6	3.864754000	0.639604000	-1.186966000
8	4.294682000	0.004592000	0.985837000
1	-0.891992000	2.590416000	-0.922995000
1	1.397282000	1.926914000	-0.386123000
1	0.031624000	-2.139545000	0.236435000
1	-2.374133000	-2.697717000	-0.028024000
1	-4.678788000	-1.976690000	-0.568989000
1	-5.124854000	0.385567000	-1.166532000
1	-3.265307000	2.023091000	-1.219210000
1	2.394096000	-1.580640000	0.675918000
1	4.492392000	1.505189000	-1.030958000
1	4.441215000	-0.135719000	-1.681616000
1	3.025470000	0.905294000	-1.811114000

Cartesian coordinates of optimized geometries at ONIOM (CASSCF (4, 4)/6-31G*: RHF/4-31G)

Z-Isomer

Ground state optimized geometry

Energy (ONIOM) = -589.57514; No imaginary frequency

6	-1.468433000	-0.625844000	0.000003000
6	-1.730458000	0.758456000	0.000004000
6	-0.637285000	1.656917000	0.000006000
6	0.645943000	1.217039000	0.000007000
6	0.917470000	-0.178126000	0.000000000
6	-0.128801000	-1.062259000	0.000002000
6	-2.557424000	-1.534169000	0.000000000
6	-3.836333000	-1.081885000	0.000000000
6	-4.098952000	0.306436000	0.000002000

6	-3.076328000	1.199249000	0.000004000
6	2.259696000	-0.744022000	-0.000002000
7	3.381199000	-0.104187000	-0.000007000
6	4.660098000	-0.799437000	-0.000002000
8	3.509290000	1.209442000	-0.000013000
1	-0.837582000	2.710478000	0.000005000
1	1.470522000	1.891911000	0.000004000
1	0.060995000	-2.119486000	0.000000000
1	-2.352857000	-2.587436000	-0.000002000
1	-4.655358000	-1.772901000	-0.000002000
1	-5.114501000	0.648881000	0.000003000
1	-3.273772000	2.253378000	0.000006000
1	2.340387000	-1.814288000	0.000003000
1	5.197396000	-0.479220000	-0.879433000
1	5.197393000	-0.479220000	0.879431000
1	4.529520000	-1.872462000	-0.000002000

Excited state optimized geometry
Energy (ONIOM) = -589.57514; No imaginary frequency

6	-1.499256000	-0.634641000	-0.000014000
6	-1.745553000	0.753382000	-0.000084000
6	-0.643565000	1.641454000	-0.000222000
6	0.635002000	1.189220000	-0.000270000
6	0.889920000	-0.209234000	-0.000213000
6	-0.166233000	-1.085741000	-0.000100000
6	-2.597860000	-1.531970000	0.000132000
6	-3.871513000	-1.066127000	0.000205000
6	-4.118319000	0.325384000	0.000127000
6	-3.086746000	1.207869000	-0.000013000
6	2.210371000	-0.791076000	-0.000328000
7	3.443529000	-0.153753000	-0.000323000
6	4.746349000	-0.732561000	0.000037000
8	3.491589000	1.239517000	0.001113000
1	-0.833921000	2.696677000	-0.000277000
1	1.472127000	1.848493000	-0.000346000
1	0.013454000	-2.144476000	-0.000077000
1	-2.404240000	-2.587262000	0.000189000
1	-4.698137000	-1.747853000	0.000319000

1	-5.130072000	0.678804000	0.000180000
1	-3.273380000	2.263824000	-0.000073000
1	2.309762000	-1.856756000	-0.000308000
1	5.314367000	-0.448578000	-0.883390000
1	5.313560000	-0.449337000	0.884234000
1	4.630589000	-1.808016000	-0.000483000

E-Isomer

Ground state optimized geometry

Energy (ONIOM) = -589.56218; No imaginary frequency

6	-2.321901000	-0.642996000	-0.550986000
7	-3.391139000	-0.239381000	0.059726000
6	-3.392209000	0.746126000	1.183504000
8	-4.550246000	-0.688876000	-0.219600000
1	-3.982550000	0.284954000	1.958189000
1	-2.395734000	0.965927000	1.528366000
1	-3.891382000	1.635805000	0.830321000
1	-2.510702000	-1.421473000	-1.264671000
1	4.546679000	-1.838563000	0.349937000
6	1.411034000	-0.633305000	-0.072473000
6	1.705262000	0.743818000	-0.084224000
6	3.050203000	1.160618000	0.062996000
6	4.044754000	0.249183000	0.215915000
6	3.750396000	-1.131909000	0.228802000
6	2.470374000	-1.560648000	0.088180000
6	0.068247000	-1.049334000	-0.218688000
6	-0.947798000	-0.149324000	-0.357490000
6	-0.637177000	1.235465000	-0.391893000
6	0.642389000	1.662977000	-0.255373000
1	3.270681000	2.210209000	0.051366000
1	5.060569000	0.571538000	0.327308000
1	2.243318000	-2.608856000	0.097094000
1	-0.147317000	-2.100610000	-0.210636000
1	-1.423871000	1.944140000	-0.554722000
1	0.865819000	2.711327000	-0.290340000

Cartesian coordinates of optimized geometries at CASSCF (4, 4)/6-31G*

Z-Isomer

Ground state optimized geometry
Energy (CASSCF) = -590.12072; No imaginary frequency

6	-1.473149000	-0.620607000	-0.000004000
6	-1.739976000	0.761686000	0.000001000
6	-0.646311000	1.666497000	0.000000000
6	0.639128000	1.230931000	-0.000005000
6	0.915613000	-0.167604000	-0.000009000
6	-0.125831000	-1.054152000	-0.000009000
6	-2.560208000	-1.536061000	-0.000002000
6	-3.841752000	-1.088019000	0.000004000
6	-4.110538000	0.303552000	0.000010000
6	-3.090473000	1.200532000	0.000008000
6	2.268984000	-0.740486000	-0.000007000
7	3.405986000	-0.087875000	-0.000005000
6	4.673306000	-0.811586000	0.000003000
8	3.540513000	1.181544000	-0.000004000
1	-0.849512000	2.723052000	0.000006000
1	1.459139000	1.916516000	0.000000000
1	0.067085000	-2.113756000	-0.000009000
1	-2.352264000	-2.591978000	-0.000006000
1	-4.660162000	-1.785420000	0.000005000
1	-5.130402000	0.644493000	0.000015000
1	-3.293403000	2.257066000	0.000013000
1	2.351212000	-1.809183000	-0.000002000
1	5.215582000	-0.500298000	-0.879657000
1	5.215571000	-0.500302000	0.879672000
1	4.523688000	-1.881303000	0.000000000

Excited state optimized geometry
Energy (CASSCF) = -589.94434; No imaginary frequency

6	-1.545442000	-0.675896000	0.101206000
6	-1.749413000	0.707901000	-0.099809000
6	-0.588195000	1.579683000	-0.184858000
6	0.722156000	1.085470000	-0.073580000
6	0.971109000	-0.241599000	0.115803000
6	-0.190079000	-1.170846000	0.213976000
6	-2.645143000	-1.516222000	0.185103000
6	-3.937744000	-1.013565000	0.073018000

6	-4.136460000	0.337574000	-0.123751000
6	-3.042163000	1.193000000	-0.209119000
6	2.279221000	-0.802248000	0.210853000
7	3.451781000	-0.020471000	0.208299000
6	4.677513000	-0.597911000	-0.304425000
8	3.578847000	0.882266000	1.098652000
1	-0.746976000	2.630831000	-0.336956000
1	1.540032000	1.776298000	-0.137458000
1	-0.018951000	-2.214935000	0.393444000
1	-2.494291000	-2.570602000	0.339202000
1	-4.777983000	-1.681078000	0.140802000
1	-5.132636000	0.732644000	-0.210744000
1	-3.199309000	2.246697000	-0.361339000
1	2.420649000	-1.865222000	0.272412000
1	5.418572000	0.185470000	-0.353926000
1	5.042740000	-1.394754000	0.339046000
1	4.503991000	-0.995247000	-1.295839000

E-Isomer

Ground state optimized geometry

Energy (CASSCF) = -590.08524; No imaginary frequency

6	2.450739000	0.396630000	-1.560693000
7	3.238146000	-0.017579000	-0.602954000
6	3.905073000	-1.322915000	-0.611108000
8	3.474733000	0.660216000	0.425258000
1	3.682888000	-1.781136000	0.339493000
1	3.564034000	-1.942768000	-1.422636000
1	4.968840000	-1.149990000	-0.681940000
1	1.999547000	1.349711000	-1.366212000
1	-2.033468000	-2.430021000	-6.215730000
6	0.582491000	-1.249381000	-4.406685000
6	1.626870000	-1.565017000	-5.296749000
6	1.316093000	-2.199838000	-6.528155000
6	0.030379000	-2.501735000	-6.845882000
6	-1.020773000	-2.185289000	-5.950270000
6	-0.752310000	-1.576938000	-4.766057000
6	0.893539000	-0.617753000	-3.174712000
6	2.178033000	-0.314512000	-2.833117000
6	3.224333000	-0.621312000	-3.748721000
6	2.957399000	-1.228821000	-4.932362000

1	2.115926000	-2.438231000	-7.207066000
1	-0.197717000	-2.982649000	-7.780051000
1	-1.548882000	-1.335254000	-4.084526000
1	0.089882000	-0.380438000	-2.499349000
1	4.235000000	-0.352891000	-3.498277000
1	3.757080000	-1.452975000	-5.616201000

Excited state optimized geometry
Energy (CASSCF) = -589.94401; No imaginary frequency

6	-1.527861000	-0.739013000	-0.327914000
6	-1.796431000	0.612968000	-0.642151000
6	-0.696408000	1.566971000	-0.638145000
6	0.619947000	1.175610000	-0.347650000
6	0.931685000	-0.118406000	-0.045868000
6	-0.167130000	-1.125181000	-0.017067000
6	-2.569140000	-1.653609000	-0.325289000
6	-3.868797000	-1.257108000	-0.627037000
6	-4.130619000	0.061823000	-0.933632000
6	-3.094501000	0.991702000	-0.939982000
6	2.247633000	-0.572848000	0.255621000
7	3.387692000	0.245052000	0.100251000
6	3.894298000	0.580064000	-1.220836000
8	4.264721000	0.155143000	1.020192000
1	-0.910630000	2.596588000	-0.855091000
1	1.391656000	1.923064000	-0.341524000
1	0.058832000	-2.147556000	0.216586000
1	-2.367574000	-2.683191000	-0.085578000
1	-4.663732000	-1.980964000	-0.619489000
1	-5.131975000	0.375977000	-1.167330000
1	-3.302862000	2.020181000	-1.178476000
1	2.420963000	-1.538145000	0.690678000
1	4.557136000	1.427479000	-1.122354000
1	4.439953000	-0.254444000	-1.651307000
1	3.070447000	0.835448000	-1.870668000

Cartesian coordinates of optimized geometries at B3LYP/6-311G**

Z-Isomer
Ground state optimized geometry
Energy (DFT) = -593.97019; No imaginary frequency

6	-1.473692000	-0.634733000	0.000001000
6	-1.745382000	0.770680000	0.000002000
6	-0.647812000	1.670373000	0.000002000
6	0.649140000	1.227980000	0.000001000
6	0.932868000	-0.173418000	0.000000000
6	-0.130966000	-1.069087000	0.000000000
6	-2.566207000	-1.544310000	0.000001000
6	-3.860506000	-1.087285000	0.000002000
6	-4.127795000	0.302825000	0.000003000
6	-3.093918000	1.208061000	0.000003000
6	2.268646000	-0.730759000	-0.000001000
7	3.405665000	-0.064660000	-0.000001000
6	4.685274000	-0.812319000	-0.000002000
8	3.544259000	1.198764000	0.000000000
1	-0.850270000	2.736605000	0.000003000
1	1.480223000	1.916400000	0.000001000
1	0.065145000	-2.137417000	-0.000001000
1	-2.359784000	-2.609717000	0.000000000
1	-4.685854000	-1.790390000	0.000002000
1	-5.154999000	0.649761000	0.000004000
1	-3.296712000	2.274024000	0.000004000
1	2.369482000	-1.806895000	-0.000002000
1	5.237701000	-0.504438000	-0.887167000
1	5.237701000	-0.504441000	0.887164000
1	4.519619000	-1.888366000	-0.000004000

E-Isomer

Ground state optimized geometry

Energy (DFT) = -593.95906; No imaginary frequency

6	2.673718000	0.578318000	-1.799322000
7	3.573569000	0.331389000	-0.868568000
6	4.357278000	-0.926472000	-0.803542000
8	3.813225000	1.133873000	0.085800000
1	3.921850000	-1.706351000	-1.422601000
1	5.381811000	-0.711190000	-1.108441000
1	4.351976000	-1.210908000	0.246174000
1	2.118260000	1.486682000	-1.600197000
1	-2.103965000	-1.435807000	-6.570090000

6	0.633148000	-0.826249000	-4.625091000
6	1.597223000	-1.582900000	-5.363097000
6	1.185647000	-2.269944000	-6.532459000
6	-0.121042000	-2.216886000	-6.954682000
6	-1.076561000	-1.469906000	-6.225610000
6	-0.709040000	-0.790699000	-5.090336000
6	1.043432000	-0.143973000	-3.457238000
6	2.350695000	-0.194396000	-2.992457000
6	3.307293000	-0.924788000	-3.762660000
6	2.937936000	-1.596506000	-4.898718000
1	1.920953000	-2.839928000	-7.090830000
1	-0.425790000	-2.747082000	-7.849773000
1	-1.441395000	-0.217515000	-4.531589000
1	0.303623000	0.425547000	-2.903674000
1	4.349852000	-0.914279000	-3.472980000
1	3.684291000	-2.135188000	-5.473392000

Cartesian coordinates of optimized geometries at RHF/6-311G**

Z-Isomer

Ground state optimized geometry

Energy (RHF) = -590.18904; No imaginary frequency

6	-1.462765000	-0.617345000	0.000001000
6	-1.733555000	0.763046000	0.000002000
6	-0.643492000	1.670638000	0.000002000
6	0.642459000	1.239294000	0.000001000
6	0.924106000	-0.158497000	0.000000000
6	-0.116317000	-1.047436000	0.000000000
6	-2.547076000	-1.535958000	0.000002000
6	-3.828602000	-1.091855000	0.000003000
6	-4.101307000	0.298942000	0.000004000
6	-3.084726000	1.198140000	0.000003000
6	2.273720000	-0.727331000	-0.000002000
7	3.380609000	-0.092732000	0.000000000
6	4.649299000	-0.819882000	-0.000002000
8	3.523204000	1.164361000	0.000003000
1	-0.849390000	2.726582000	0.000002000
1	1.460086000	1.927429000	0.000001000
1	0.079804000	-2.106267000	-0.000001000
1	-2.336341000	-2.591214000	0.000001000

1	-4.644844000	-1.791776000	0.000003000
1	-5.122053000	0.637283000	0.000004000
1	-3.290706000	2.253986000	0.000004000
1	2.350146000	-1.796694000	-0.000004000
1	5.193067000	-0.508211000	-0.880051000
1	5.193066000	-0.508217000	0.880051000
1	4.493434000	-1.889049000	-0.000005000

E-Isomer

Ground state optimized geometry

Energy (RHF) = -590.17804; No imaginary frequency

6	2.851067000	0.704262000	-1.913294000
7	3.559215000	0.314637000	-0.928650000
6	4.034249000	-1.059944000	-0.754763000
8	3.899752000	1.080209000	0.019171000
1	3.615924000	-1.731038000	-1.486353000
1	5.113438000	-1.039353000	-0.812464000
1	3.742000000	-1.344044000	0.244546000
1	2.535186000	1.728447000	-1.839517000
1	-2.106840000	-1.641695000	-6.329180000
6	0.694358000	-0.847306000	-4.591899000
6	1.644891000	-1.508030000	-5.390500000
6	1.207833000	-2.217818000	-6.538939000
6	-0.109271000	-2.262444000	-6.863562000
6	-1.067092000	-1.598011000	-6.059075000
6	-0.676628000	-0.910405000	-4.956357000
6	1.131466000	-0.137948000	-3.444767000
6	2.446794000	-0.095923000	-3.092628000
6	3.403555000	-0.749232000	-3.919161000
6	3.013724000	-1.432309000	-5.023279000
1	1.937160000	-2.720596000	-7.149307000
1	-0.433519000	-2.802526000	-7.734883000
1	-1.402239000	-0.404449000	-4.344215000
1	0.398638000	0.369429000	-2.841609000
1	4.447268000	-0.681889000	-3.671530000
1	3.747061000	-1.917185000	-5.643158000

Cartesian coordinates of other important optimized geometries

Conical intersection geometries

CI_1
(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -590.00090

6	-1.184656000	-0.455087000	-0.139916000
6	-1.844022000	0.748532000	0.179227000
6	-1.060254000	1.904117000	0.443277000
6	0.292608000	1.850049000	0.401397000
6	0.970609000	0.634941000	0.085737000
6	0.231502000	-0.483853000	-0.183453000
6	-1.963651000	-1.615514000	-0.398874000
6	-3.319853000	-1.569614000	-0.337775000
6	-3.980244000	-0.358846000	-0.015348000
6	-3.261581000	0.767193000	0.234335000
6	2.424159000	0.645254000	0.053732000
7	3.159984000	-0.516504000	-0.163313000
6	4.511532000	-0.346942000	-0.647186000
8	3.160019000	-1.062106000	1.082982000
1	-1.557705000	2.827200000	0.684499000
1	0.871610000	2.732609000	0.611412000
1	0.727959000	-1.406639000	-0.420365000
1	-1.460022000	-2.534783000	-0.641337000
1	-3.900606000	-2.453525000	-0.532066000
1	-5.054348000	-0.337439000	0.031678000
1	-3.760248000	1.688426000	0.480623000
1	2.954478000	1.530295000	0.371464000
1	5.103513000	0.296232000	0.000877000
1	4.980561000	-1.319320000	-0.710107000
1	4.460780000	0.087079000	-1.637763000

CI_2
(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -589.99772

6	-1.188317000	-0.421003000	-0.050980000
6	-1.890589000	0.779560000	0.162377000
6	-1.144830000	1.967636000	0.396008000
6	0.210952000	1.969046000	0.382564000
6	0.932999000	0.764124000	0.127871000
6	0.231418000	-0.396128000	-0.064340000

6	-1.922383000	-1.616338000	-0.274450000
6	-3.281355000	-1.600341000	-0.304153000
6	-3.986132000	-0.387972000	-0.111639000
6	-3.308289000	0.767894000	0.119433000
6	2.391952000	0.726457000	0.013164000
7	3.217162000	1.745796000	0.471760000
6	4.638820000	1.509256000	0.561574000
8	2.929779000	2.730639000	-0.462305000
1	-1.677516000	2.887888000	0.564059000
1	0.748673000	2.885244000	0.533390000
1	0.755932000	-1.317916000	-0.254922000
1	-1.386740000	-2.537562000	-0.425622000
1	-3.829229000	-2.509300000	-0.478598000
1	-5.060924000	-0.387773000	-0.150821000
1	-3.840808000	1.691853000	0.264263000
1	2.855243000	-0.129560000	-0.459269000
1	5.065054000	1.188684000	-0.385604000
1	5.115150000	2.425427000	0.882088000
1	4.799412000	0.745418000	1.312332000

CI_3
(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -589.92472

6	-1.173269000	-0.701206000	-0.285400000
6	-1.418239000	0.681419000	-0.339599000
6	-0.303429000	1.593031000	-0.616396000
6	0.951402000	1.177415000	-0.719875000
6	1.289104000	-0.242518000	-0.525863000
6	0.170073000	-1.202070000	-0.475103000
6	-2.255630000	-1.578885000	-0.206955000
6	-3.547464000	-1.104164000	-0.132824000
6	-3.785262000	0.265893000	-0.149918000
6	-2.726846000	1.145401000	-0.256269000
6	1.719202000	-0.648894000	0.716289000
7	2.216709000	-2.004808000	0.967499000
6	2.664118000	-2.892834000	-0.088213000
8	2.387709000	-2.365629000	2.159103000
1	-0.536939000	2.634239000	-0.748460000
1	1.749374000	1.865588000	-0.923219000

1	0.282574000	-2.214794000	-0.800202000
1	-2.067773000	-2.637370000	-0.207934000
1	-4.371021000	-1.792209000	-0.077837000
1	-4.791510000	0.639099000	-0.103259000
1	-2.911611000	2.203840000	-0.305527000
1	1.882560000	0.018410000	1.562348000
1	3.567311000	-3.380086000	0.239812000
1	1.919907000	-3.650315000	-0.309840000
1	2.855626000	-2.314937000	-0.983379000

CI_4
(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -590.01051

6	-1.171284000	-0.445430000	-0.128037000
6	-1.840755000	0.760714000	0.154032000
6	-1.066992000	1.933697000	0.378183000
6	0.285997000	1.904490000	0.329026000
6	0.973697000	0.685308000	0.053979000
6	0.245756000	-0.451535000	-0.167862000
6	-1.935468000	-1.620948000	-0.353258000
6	-3.292707000	-1.587633000	-0.294635000
6	-3.964856000	-0.375551000	-0.007122000
6	-3.257600000	0.765319000	0.209950000
6	2.424415000	0.628655000	-0.015092000
7	3.219696000	1.733507000	0.348810000
6	4.549071000	1.775851000	-0.219018000
8	3.283971000	1.632647000	1.710930000
1	-1.577212000	2.856219000	0.593638000
1	0.858780000	2.794540000	0.504433000
1	0.750173000	-1.380301000	-0.373342000
1	-1.422356000	-2.541703000	-0.569664000
1	-3.863937000	-2.482652000	-0.464748000
1	-5.039070000	-0.363853000	0.039176000
1	-3.766441000	1.687598000	0.429557000
1	2.908043000	-0.328033000	-0.135742000
1	4.453479000	1.884882000	-1.291968000
1	5.067947000	2.637153000	0.179396000
1	5.122315000	0.877777000	0.003419000

Transition States on excited state surface

TS_{ex1}

(CASSCF (4, 4)/6-31G* level of theory)

Energy (CASSCF) = -589.94073; Imaginary frequency at -175 cm^{-1}

6	-1.553637000	-0.645331000	-0.047471000
6	-1.743668000	0.749195000	0.090351000
6	-0.574200000	1.612086000	0.165351000
6	0.732962000	1.097552000	0.104483000
6	0.971484000	-0.242407000	-0.023378000
6	-0.201323000	-1.163770000	-0.108722000
6	-2.663813000	-1.476803000	-0.121145000
6	-3.953166000	-0.954655000	-0.059956000
6	-4.138603000	0.408670000	0.075341000
6	-3.034922000	1.254472000	0.149664000
6	2.267443000	-0.831745000	-0.067561000
7	3.464307000	-0.092680000	-0.071298000
6	4.644365000	-0.493129000	0.676679000
8	3.608213000	0.905013000	-0.906247000
1	-0.724214000	2.668713000	0.269972000
1	1.555657000	1.780524000	0.154165000
1	-0.038983000	-2.215633000	-0.238922000
1	-2.522914000	-2.536359000	-0.227088000
1	-4.798607000	-1.612603000	-0.118667000
1	-5.129223000	0.817940000	0.122591000
1	-3.181445000	2.313389000	0.253453000
1	2.380101000	-1.898164000	-0.069222000
1	5.492948000	-0.566564000	0.011677000
1	4.865414000	0.226877000	1.453707000
1	4.467872000	-1.454268000	1.135588000

TS_{ex2}

(CASSCF (4, 4)/6-31G* level of theory)

Energy (CASSCF) = -589.94251; Imaginary frequency at -126 cm^{-1}

6	-1.518007000	-0.634518000	-0.000004000
6	-1.786179000	0.755772000	-0.000008000
6	-0.673297000	1.694131000	-0.000008000
6	0.654997000	1.271617000	-0.000012000
6	0.969223000	-0.072509000	-0.000008000
6	-0.138940000	-1.068233000	-0.000005000

6	-2.571486000	-1.536527000	0.000002000
6	-3.891026000	-1.096682000	0.000006000
6	-4.154075000	0.257699000	0.000007000
6	-3.107862000	1.175541000	0.000006000
6	2.230260000	-0.687478000	-0.000004000
7	3.483652000	-0.103207000	0.000000000
6	4.719406000	-0.859858000	0.000001000
8	3.596588000	1.171407000	0.000014000
1	-0.897141000	2.744491000	-0.000004000
1	1.433538000	2.004331000	-0.000006000
1	0.087068000	-2.117121000	0.000006000
1	-2.360706000	-2.592399000	0.000004000
1	-4.696356000	-1.809003000	0.000012000
1	-5.170388000	0.610039000	0.000013000
1	-3.324482000	2.229576000	0.000008000
1	2.276020000	-1.757034000	0.000000000
1	5.298663000	-0.618930000	-0.882246000
1	5.298637000	-0.618980000	0.882279000
1	4.498802000	-1.917513000	-0.000033000

TS_{ex3}
(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -589.94250; Imaginary frequency at -139 cm^{-1}

6	-1.550815000	-0.645136000	0.041826000
6	-1.748900000	0.747935000	-0.089823000
6	-0.583324000	1.615287000	-0.170698000
6	0.725048000	1.109533000	-0.121140000
6	0.969640000	-0.227663000	-0.000384000
6	-0.196651000	-1.153894000	0.090015000
6	-2.654042000	-1.480913000	0.121291000
6	-3.945580000	-0.965039000	0.071895000
6	-4.138618000	0.394811000	-0.057164000
6	-3.040240000	1.245972000	-0.137253000
6	2.269288000	-0.807248000	0.029524000
7	3.453907000	-0.046693000	0.039180000
6	4.661406000	-0.508837000	-0.618719000
8	3.596241000	0.866124000	0.911676000
1	-0.739044000	2.673171000	-0.270267000
1	1.545406000	1.797926000	-0.176348000
1	-0.028286000	-2.206183000	0.215993000

1	-2.507046000	-2.542225000	0.222699000
1	-4.788826000	-1.629184000	0.135156000
1	-5.133626000	0.800469000	-0.095463000
1	-3.193509000	2.306531000	-0.236577000
1	2.393702000	-1.873406000	0.041082000
1	4.954974000	0.186337000	-1.396451000
1	5.461796000	-0.588469000	0.104890000
1	4.483914000	-1.475957000	-1.068601000

Transition States on ground state surface

TS_{gs1}

(CASSCF (4, 4)/6-31G* level of theory)

Energy (CASSCF) = -590.04572; Imaginary frequency at -422 cm^{-1}

6	1.175660000	-0.464659000	0.005744000
6	1.879220000	0.755567000	0.008727000
6	1.137296000	1.969253000	-0.017901000
6	-0.215723000	1.956908000	-0.043228000
6	-0.940595000	0.726051000	-0.042889000
6	-0.242219000	-0.450901000	-0.021178000
6	1.910644000	-1.679951000	0.028883000
6	3.269292000	-1.669719000	0.055088000
6	3.974308000	-0.442312000	0.059217000
6	3.296638000	0.736195000	0.036301000
6	-2.387108000	0.769536000	-0.062347000
7	-3.167977000	-0.415285000	-0.046223000
6	-4.128048000	-0.594631000	1.023917000
8	-3.549988000	-0.867796000	-1.215974000
1	1.669885000	2.904141000	-0.018090000
1	-0.762066000	2.883679000	-0.064587000
1	-0.771612000	-1.385223000	-0.029675000
1	1.372943000	-2.611789000	0.024179000
1	3.817032000	-2.594912000	0.072055000
1	5.049372000	-0.448700000	0.079786000
1	3.829828000	1.670872000	0.038368000
1	-2.906617000	1.710016000	-0.123352000
1	-4.932000000	0.136379000	0.974779000
1	-4.546010000	-1.587283000	0.940904000
1	-3.621197000	-0.495836000	1.974977000

TS_{gs2}

(CASSCF (4, 4)/6-31G* level of theory)

Energy (CASSCF) = -590.04252; Imaginary frequency at -1305 cm^{-1}

6	1.447599000	-0.616838000	0.043114000
6	1.721951000	0.756504000	-0.091245000
6	0.629480000	1.672634000	-0.170222000
6	-0.651122000	1.248167000	-0.114433000
6	-0.936495000	-0.147572000	0.004914000
6	0.092330000	-1.040678000	0.082340000
6	2.524262000	-1.534520000	0.128132000
6	3.811759000	-1.097331000	0.081700000
6	4.087315000	0.282179000	-0.052315000
6	3.070364000	1.184012000	-0.135919000
6	-2.291830000	-0.686318000	-0.039287000
7	-3.378332000	0.012897000	-0.243945000
6	-4.659463000	-0.609597000	-0.461886000
8	-3.337268000	0.805081000	0.975664000
1	0.843924000	2.722762000	-0.261087000
1	-1.469992000	1.937876000	-0.132387000
1	-0.111012000	-2.094113000	0.172242000
1	2.309149000	-2.583813000	0.231052000
1	4.624989000	-1.797404000	0.147206000
1	5.108662000	0.616455000	-0.087756000
1	3.281263000	2.233985000	-0.236906000
1	-2.359591000	-1.768428000	-0.007075000
1	-4.950487000	-1.226999000	0.382784000
1	-5.390038000	0.175377000	-0.591821000
1	-4.617287000	-1.210481000	-1.363304000

TS_{gs3}

[ONIOM {CASSCF (4, 4)/6-31G*: RHF/4-31G} level of theory]

Energy (ONIOM) = -589.53241; Imaginary frequency at -332 cm^{-1}

6	-1.183870000	-0.477739000	0.007624000
6	-1.856983000	0.764243000	-0.027647000
6	-1.098207000	1.969805000	-0.030730000
6	0.250049000	1.934994000	-0.003074000
6	0.940436000	0.686271000	0.010354000
6	0.220404000	-0.491566000	0.028302000
6	-1.936940000	-1.677778000	0.025523000
6	-3.293679000	-1.641435000	0.003099000
6	-3.963199000	-0.400607000	-0.034784000

6	-3.267443000	0.769268000	-0.048727000
6	2.347002000	0.636499000	-0.004381000
7	3.055488000	-0.595597000	0.029321000
6	4.049356000	-0.672355000	-1.024324000
8	3.711133000	-0.514268000	1.278807000
1	-1.620508000	2.905174000	-0.047743000
1	0.819172000	2.843691000	0.004876000
1	0.763688000	-1.412982000	0.075655000
1	-1.414527000	-2.613390000	0.057961000
1	-3.862404000	-2.548533000	0.016404000
1	-5.034565000	-0.384879000	-0.050630000
1	-3.783853000	1.708063000	-0.074394000
1	2.931945000	1.538779000	0.083006000
1	4.730730000	0.176274000	-1.013349000
1	4.623761000	-1.579819000	-0.890848000
1	3.543143000	-0.712060000	-1.983339000

TS_{gs4}
[ONIOM {CASSCF (4, 4)/6-31G*: RHF/4-31G} level of theory]
Energy (ONIOM) = -589.53050; Imaginary frequency at -323 cm^{-1}

6	-1.474144000	-0.613695000	0.004348000
6	-1.718748000	0.779247000	0.004551000
6	-0.621006000	1.681751000	-0.017575000
6	0.652122000	1.228935000	-0.032155000
6	0.908994000	-0.171814000	-0.019832000
6	-0.146201000	-1.062299000	-0.016896000
6	-2.570244000	-1.514721000	0.017919000
6	-3.843884000	-1.050818000	0.032131000
6	-4.087033000	0.340880000	0.032820000
6	-3.058255000	1.229179000	0.018699000
6	2.229364000	-0.662866000	0.020367000
7	3.361038000	0.197545000	-0.039550000
6	4.294159000	-0.068760000	1.038886000
8	3.966866000	-0.144922000	-1.266880000
1	-0.822885000	2.733861000	-0.031705000
1	1.494247000	1.885874000	-0.067538000
1	0.048161000	-2.118107000	-0.027655000
1	-2.373235000	-2.568957000	0.015229000
1	-4.670816000	-1.730991000	0.041685000
1	-5.098562000	0.694199000	0.043557000

1	-3.249980000	2.283497000	0.017247000
1	2.418688000	-1.724404000	-0.029080000
1	4.602247000	-1.112455000	1.074405000
1	5.171807000	0.547318000	0.894456000
1	3.827389000	0.196599000	1.981712000

TS_{gs5}
(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -590.04737; Imaginary frequency at -350 cm^{-1}

6	1.515881000	-0.624572000	-0.020970000
6	1.704578000	0.764326000	0.026461000
6	0.542842000	1.625003000	0.026216000
6	-0.701133000	1.133245000	-0.014759000
6	-0.934804000	-0.301816000	-0.057999000
6	0.175379000	-1.144695000	-0.063122000
6	2.640151000	-1.469564000	-0.024236000
6	3.906061000	-0.948385000	0.018597000
6	4.093969000	0.440036000	0.066173000
6	3.010778000	1.279112000	0.069679000
6	-2.239304000	-0.840667000	-0.093521000
7	-3.402473000	-0.024047000	-0.075086000
6	-4.283839000	-0.079036000	1.074288000
8	-3.942337000	0.251120000	-1.193950000
1	0.700591000	2.689075000	0.055295000
1	-1.548983000	1.790941000	-0.025493000
1	0.036577000	-2.210795000	-0.099804000
1	2.495187000	-2.535214000	-0.061469000
1	4.758906000	-1.603280000	0.015339000
1	5.089889000	0.843998000	0.099218000
1	3.152942000	2.345185000	0.105121000
1	-2.392482000	-1.905155000	-0.142847000
1	-4.806563000	-1.030801000	1.131783000
1	-3.706285000	0.059846000	1.979008000
1	-5.007117000	0.717651000	0.980215000

Oxaziridine geometries

Ox_1

(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -590.07421; No imaginary frequency

6	-1.109400000	-0.801321000	0.227791000
6	-1.700398000	0.470607000	0.154821000
6	-0.854588000	1.625342000	0.126807000
6	0.487736000	1.502559000	0.169526000
6	1.100133000	0.209430000	0.238992000
6	0.318828000	-0.906572000	0.268705000
6	-1.939880000	-1.944789000	0.259288000
6	-3.296833000	-1.820708000	0.218672000
6	-3.890075000	-0.543554000	0.145415000
6	-3.110162000	0.573772000	0.114666000
6	2.589784000	0.112647000	0.265767000
7	3.254568000	-0.679686000	-0.687867000
6	4.616869000	-0.296162000	-1.002930000
8	3.168594000	-1.059545000	0.701607000
1	-1.310281000	2.598553000	0.074646000
1	1.110386000	2.380647000	0.153044000
1	0.775057000	-1.877045000	0.326290000
1	-1.484343000	-2.917816000	0.315186000
1	-3.920746000	-2.696124000	0.242406000
1	-4.961384000	-0.456133000	0.114008000
1	-3.560792000	1.549371000	0.059125000
1	3.094041000	1.007763000	0.599274000
1	5.088608000	0.272168000	-0.207147000
1	5.193179000	-1.192313000	-1.188968000
1	4.589258000	0.295248000	-1.910958000

Ox_2
(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -590.07610; No imaginary frequency

6	-0.993651000	0.019126000	1.100402000
6	-1.633292000	1.257326000	1.263630000
6	-0.907093000	2.459646000	0.966110000
6	0.368292000	2.418662000	0.538494000
6	1.032837000	1.156598000	0.370990000
6	0.367117000	0.000405000	0.640939000
6	-1.701056000	-1.167071000	1.389081000

6	-2.994057000	-1.118120000	1.823575000
6	-3.636943000	0.123576000	1.987945000
6	-2.971326000	1.283061000	1.713897000
6	2.447563000	1.117739000	-0.093574000
7	3.343863000	2.106069000	0.343878000
6	4.743824000	1.731548000	0.381989000
8	2.863599000	2.058861000	-1.015221000
1	-1.406570000	3.404322000	1.091412000
1	0.909155000	3.318220000	0.315860000
1	0.852455000	-0.952501000	0.513164000
1	-1.207487000	-2.114978000	1.262099000
1	-3.526204000	-2.026688000	2.041481000
1	-4.655814000	0.153784000	2.330435000
1	-3.461785000	2.232585000	1.838706000
1	2.841315000	0.126525000	-0.260466000
1	5.339518000	2.595672000	0.120941000
1	4.978144000	1.440599000	1.399519000
1	4.979142000	0.918051000	-0.297358000

Ox_3
(CASSCF (4, 4)/6-31G* level of theory)
Energy (CASSCF) = -590.09886; No imaginary frequency

6	1.402434000	-0.604443000	-0.056263000
6	1.714836000	0.763413000	0.055924000
6	0.657555000	1.709697000	0.048796000
6	-0.633113000	1.315062000	-0.060482000
6	-0.950202000	-0.060286000	-0.169411000
6	0.043237000	-0.985720000	-0.171751000
6	2.452518000	-1.553126000	-0.052170000
6	3.746488000	-1.155248000	0.058942000
6	4.060082000	0.215489000	0.171756000
6	3.071737000	1.147736000	0.170001000
6	-2.366675000	-0.485363000	-0.286334000
7	-3.343697000	0.216231000	0.436285000
6	-4.540609000	-0.531161000	0.769072000
8	-3.237450000	0.314079000	-1.085347000
1	0.898563000	2.751483000	0.130366000
1	-1.431963000	2.025989000	-0.067384000
1	-0.188680000	-2.030615000	-0.262783000
1	2.209858000	-2.594623000	-0.138970000

1	4.536752000	-1.879060000	0.061162000
1	5.085255000	0.515663000	0.258458000
1	3.307831000	2.190578000	0.254972000
1	-2.511120000	-1.547572000	-0.418389000
1	-4.418544000	-0.904906000	1.780106000
1	-5.389258000	0.138568000	0.747225000
1	-4.721753000	-1.360132000	0.092670000