OXAZIRIDINE (C-CH_3NO), C-CH_2NO RADICALS AND CL, NH_2 AND METHYL DERIVATIVES OF OXAZIRIDINE; STRUCTURES AND QUANTUM CHEMICAL PARAMETERS (Supplementary material)

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Supplementary material contains Tables S1 to S9 and Figures S1 to S4.

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Table S1

Structure of oxaziridine, radicals and their corresponding cations calculated using B3LYP/6-311++G (d, p) method [16].

Oxaziridine			*Radical 1*		*Radical 2*		*Radical 3*	
	B3lyp	*Ref [16]*		*B3lyp*		*B3lyp*		*B3lyp*
Bond lengths (Å)			*Bond lengths (Å)*		*Bond lengths (Å)*		*Bond lengths (Å)*	
C1-O2	1.398	1.403	C1-O2	1.426	C1-O2	1.347	C1-O2	1.348
C1-H3	1.090	1.089	C1-H3	1.087	C1-H3	1.091	C1-H3	1.092
C1-H4	1.088	1.091	C1-H4	1.087	C1-N4	1.414	C1-N4	1.409
C1-N5	1.436	1.439	C1-N5	1.429	N4- H5	1.025	N4- H5	1.028
N5-H6	1.025	1.026	O2-N5	1.383	O2-N4	1.544	O2-N4	1.541
O2-N5	1.496	1.500						
Bond angles(º)			*Bond angles(º)*		*Bond angles(º)*		*Bond angles(º)*	
H3-C1-O2	115.8		O2-C1-H3	115.6	H3-C1-O2	122.9	H3-C1-O2	123.0
O2-C1-H4	116.3	115.8	O2-C1-H4	115.7	O2-C1-N4	68.0	O2-C1-N4	67.9
N5-C1-H3	119.7	116.2	H3-C1-H4	117.3	C1-N4-H5	107.7	C1-N4-H5	109.5
C1-N5-H6	107.7	107.6	N5-C1-H3	118.3	O2-N4-H5	102.6	O2-N4-H5	103.1
O2-N5-H6	103.1		N5-C1-H4	118.3	N4-O2-C1	58.1	N4-O2-C1	57.9
H3-C1-H4	115.8		O2-C1-N5	58.0	C1-N4-O2	54.0	C1-N4-O2	54.1
N5-O2-C1	59.4		N5-O2-C1	61.1				
O2-C1-N5	63.7		C1-N5-O2	60.9				
C1-N5-O2	56.9							
Torsion angles(º)			*Torsion angles(º)*		*Torsion angles(º)*		*Torsion angles(º)*	
H4-C1-N5-H6	-157.5		N5-O2-C1-H3	108.7	H3-C1-N4-H5	-151.5	H3-C1-N4-H5	-23.2
H3-C1-N5-H6	-11.67		N5-O2-C1-H4	-108.7				
Oxaziridine Cation			*Rad.1 Cation*		*Rad.2 Cation*		*Rad.3 Cation*	
	B3lyp	*Ref [16]*		*B3lyp*		*B3lyp*		*B3lyp*
Bond lengths (Å)			*Bond lengths (Å)*		*Bond lengths (Å)*		*Bond lengths (Å)*	
C1-O2	1.502	1.507	C1-O2	1.529	C1-O2	1.239	C1-O2	1.239
C1-H3	1.085	1.086	C1-H3	1.086	C1-H3	1.092	C1-H3	1.092
C1-H4	1.084	1.088	C1-H4	1.086	C1-N4	1.338	C1-N4	1.338
C1-N5	1.416	1.439	C1-N5	1.442	N4- H5	1.037	N4- H5	1.037
N5-H6	1.032	1.032	O2-N5	1.223	O2-N4	1.677	O2-N4	1.677
O2-N5	1.311	1.317						
Bond angles(º)			*Bond angles(º)*		*Bond angles(º)*		*Bond angles(º)*	
H3-C1-O2	113.3		O2-C1-H3	112.8	H3-C1-O2	136.0	H3-C1-O2	136.0
O2-C1-H4	114.0	113.3	O2-C1-H4	112.8	O2-C1-N4	81.1	O2-C1-N4	81.1
N5-C1-H3	119.0	113.9	H3-C1-H4	124.7	C1-N4-H5	115.8	C1-N4-H5	115.8
C1-N5-H6	140.3	140.3	N5-C1-H3	116.6	O2-N4-H5	106.4	O2-N4-H5	106.4
O2-N5-H6	122.1		N5-C1-H4	116.6	N4-O2-C1	52.0	N4-O2-C1	52.0
H3-C1-H4	121.9		O2-C1-N5	48.5	C1-N4-O2	46.9	C1-N4-O2	46.9
N5-O2-C1	56.0		N5-O2-C1	62.0				
O2-C1-N5	53.3		C1-N5-O2	69.5				
C1-N5-O2	66.7							
Torsion angles(º)			*Torsion angles(º)*		*Torsion angles(º)*		*Torsion angles(º)*	
H4-C1-N5-H6	-145.5		N5-O2-C1-H3	106.1	H3-C1-N4-H5	-96.2	H3-C1-N4-H5	-96.2
H3-C1-N5-H6	14.1		N5-O2-C1-H4	-106.0				

Table S2

Atomic charges on C, N and O atoms from NBO calculation calculated using B3LYP level of theory and 6-311++G (d, p) basis set.

Structure	*C*	*O*	*N*
1	0.104	-0.419	-0.334
2	0.031	-0.344	-0.030
3	0.247	-0.382	-0.355
4	0.264	-0.384	-0.352
5	0.229	-0.394	-0.320
6	0.219	-0.395	-0.318
7	0.098	-0.358	-0.152
8	0.212	-0.347	-0.164
9	0.215	-0.360	-0.189
10	0.289	-0.391	-0.312
11	0.273	-0.362	-0.190
12	0.256	-0.429	-0.334
13	0.256	-0.429	-0.345
14	0.115	-0.424	-0.221
15	0.268	-0.436	-0.229
16	0.273	-0.437	-0.223
17	0.382	-0.439	-0.341
18	0.401	-0.453	-0.229
19	0.400	-0.446	-0.338
20	0.405	-0.428	-0.352
21	0.120	-0.507	-0.078
22	0.681	-0.450	-0.362
23	0.423	-0.660	-0.081
24	0.409	-0.567	-0.090
25	0.695	-0.687	-0.082

Table S3

HOMO and LUMO energy calculated using B3LYP/6-311++G(d,p).

Structure		*HOMO*	*LUMO*	$\lvert \varepsilon_{HOMO} - \varepsilon_{LUMO} \rvert$*(a.u)*	$\lvert \varepsilon_{HOMO} - \varepsilon_{LUMO} \rvert$*(eV)*
1		-0.27725	-0.01485	0.26240	7.14
2	α	-0.26441	-0.00640	0.25801	7.02
	β	-0.34121	-0.09747	0.24374	6.63
3	α	-0.23618	-0.03616	0.20002	5.44
	β	-0.29604	-0.08922	0.20682	5.63
4	α	-0.23490	-0.03582	0.19908	5.42
	β	-0.29651	-0.08498	0.21153	5.76
5		-0.30005	-0.03029	0.26976	7.34
6		-0.30595	-0.02904	0.27691	7.54
7		-0.29704	-0.08020	0.21684	5.90
8		-0.31679	-0.09387	0.22292	6.07
9		-0.30450	-0.08717	0.21733	5.91
10		-0.31627	-0.05155	0.26472	7.20
11		-0.31728	-0.09750	0.21978	5.98
12		-0.27033	-0.01281	0.25752	7.01
13		-0.27300	-0.01402	0.25898	7.05
14		-0.26317	-0.00845	0.25472	6.93
15		-0.25903	-0.00860	0.25043	6.81
16		-0.25189	-0.01155	0.24034	6.54
17		-0.26570	-0.01498	0.25072	6.82
18		-0.24766	-0.01233	0.23533	6.40
19		-0.25804	-0.01804	0.24000	6.53
20		-0.25814	-0.02235	0.23579	6.42
21		-0.27093	-0.02900	0.24193	6.58
22		-0.26037	-0.02011	0.24026	6.54
23		-0.23782	-0.08651	0.15131	4.12
24		-0.25659	-0.05476	0.20183	5.49
25		-0.23626	-0.08794	0.14832	4.04

Table S4

Selected natural bond orbital occupancies of oxaziridine and related radicals (a.u.) calculated using B3LYP/6-311++G (d, p) basis set. Only ring bonds (C-O, N-O and C-N) have been presented.

Oxaziridine (structure 1)		*Radical 1 (structure 2)*		
		Spin	*α*	*β*
BD (1) C - O	1.98513	BD (1) C - O	0.99319	0.99300
BD (1) O - N	1.97718	BD (1) O - N	0.99144	0.99134
BD (1) C - N	1.98439	BD (2) O - N		0.97258
BD*(1) C - O	0.01374	BD (1) C - N	0.99452	0.99424
BD*(1) O - N	0.02295	BD*(1) C - O	0.00894	0.01014
BD*(1) C - N	0.00802	BD*(1) O - N	0.00683	0.00624
		BD*(2) O – N		0.00730
		BD*(1) C – N	0.00345	0.00361

Radical 2 (structure 3)			*Radical 3 (structure 4)*		
Spin	*α*	*β*	*Spin*	*α*	*β*
BD (1) C - O	0.99240	0.99507	BD (1) C - O	0.99233	0.98646
BD (2) C - O		0.98108	BD (2) C - O		0.98261
BD (1) O - N	0.98739	0.98321	BD (1) O - N	0.98745	0.98255
BD (1) C - N	0.99088	0.98911	BD (1) C - N	0.99123	0.99145
BD*(1) C - O	0.00579	0.00562	BD*(1) C - O	0.00559	0.00861
BD*(2) C - O		0.04363	BD*(2) C - O		0.04443
BD*(1) O - N	0.01445	0.02413	BD*(1) O - N	0.01429	0.02355
BD*(1) C - N	0.00364	0.00424	BD*(1) C - N	0.00392	0.00354

Table S5

Selected natural bond orbital occupancies (a.u.) of compounds (structures 5-25) calculated using B3LYP/6-311++G (d, p) basis set. Only ring bonds (C-O, N-O and C-N) have been presented.

	Structure 5	*Structure 6*	*Structure 7*	*Structure 8*	*Structure 9*
BD (1) C - O	1.98624	1.98613	1.98420	1.98506	1.98530
BD (1) O - N	1.96892	1.96922	1.98121	1.97272	1.97513
BD (1) C - N	1.98344	1.98368	1.98628	1.98508	1.98529
BD*(1) C - O	0.04670	0.05145	0.01402	0.05537	0.05370
BD*(1) O - N	0.02277	0.02240	0.04655	0.05493	0.06143
BD*(1) C - N	0.03697	0.03714	0.01387	0.04906	0.06139
	Structure 10	*Structure 11*	*Structure 12*	*Structure 13*	*Structure 14*
BD (1) C - O	1.98781	1.98622	1.98185	1.98230	1.98166
BD (1) O - N	1.95967	1.96585	1.97570	1.97616	1.97175
BD (1) C - N	1.98324	1.98409	1.98038	1.98005	1.98017
BD*(1) C - O	0.08643	0.09434	0.03075	0.03229	0.01496
BD*(1) O - N	0.02071	0.06635	0.02365	0.02372	0.04600
BD*(1) C - N	0.06978	0.09901	0.02258	0.02260	0.01378
	Structure 15	*Structure 16*	*Structure 17*	*Structure 18*	*Structure 19*
BD (1) C - O	1.97894	1.97817	1.97905	1.97580	1.98453
BD (1) O - N	1.97063	1.97024	1.97441	1.97053	1.97379
BD (1) C - N	1.97629	1.97812	1.97625	1.97386	1.98273
BD*(1) C - O	0.03383	0.03198	0.04968	0.05103	0.07579
BD*(1) O - N	0.04681	0.04703	0.02372	0.04661	0.02329
BD*(1) C - N	0.02760	0.03011	0.03723	0.04394	0.04123
	Structure 20	*Structure 21*	*Structure 22*		
BD (1) C - O	1.98405	1.98364	1.98277		
BD (1) O - N	1.97361	1.96576	1.96992		
BD (1) C - N	1.98332	1.97633	1.98002		
BD*(1) C - O	0.04616	0.01478	0.10272		
BD*(1) O - N	0.02411	0.21708	0.02338		
BD*(1) C - N	0.06810	0.01355	0.08428		
	Structure 23		*Structure 24*		*Structure 25*
BD (1) C1 - O2	1.99510	BD (1) C1 - O2	1.98593	BD (1) C1 - O2	1.95925
BD (1) N4 - N5	1.98808	BD (1) O2 - N4	1.95523	BD (1) N3 - N10	1.98582
BD (2) N4 - N5	1.98367	BD (1) N4 - N5	1.99294	BD (2) N3 - N10	1.98158
BD (1) C1 - N4	1.96699	BD (1) C1 - N4	1.96393	BD (1) C1 – N3	1.96159
BD*(1) C1 - O2	0.05408	BD*(1) C1 - O2	0.06452	BD* (1) C1 - O2	0.06288
BD*(1) N4 - N5	0.07885	BD*(1) O2 - N4	0.31694	BD*(1) N3 - N10	0.10405
BD*(2) N4 - N5	0.31404	BD*(1) N4 - N5	0.00963	BD*(2) N3 - N10	0.27438
BD*(1) C1 - N4	0.13001	BD*(1) C1 - N4	0.04954	BD* (1) C1 – N3	0.15597

Table S6

Selected second order perturbation theory analysis of Fock Matrix in NBO Basis for structures calculated by B3LYP/6-311++G (d, p) method. E (2) (kcal/mol) were reported.

Donor NBO (i)	*Acceptor NBO (j)*	*E(2)*	*Donor NBO (i)*	*Acceptor NBO (j)*	*E(2)*	*Donor NBO (i)*	*Acceptor NBO (j)*	*E(2)*
1			***2 α***			***2β***		
BD (1) C1 - O2	BD*(1) O2 - N5	4.02	BD (1) C1 - O2	BD*(1) O2 - N5	2.10	BD (1) C1 - O2	BD*(1) O2 - N5	2.17
BD (1) O2 - N5	BD*(1) C1 - O2	5.27	BD (1) O2 - N5	BD*(1) C1 - O2	2.58	BD (1) O2 - N5	BD*(1) C1 - O2	2.55
BD (1) O2 - N5	BD*(1) C1 - N5	3.87				BD (2) O2 - N5	BD*(1) C1 - H3	5.40
3α			***3β***			***4α***		
BD (1) C1 - O2	BD*(1) O2 - N5	2.09	BD (2) C1 - O2	BD*(1) O2 – N4	3.59	BD (1) C1 - O2	BD*(1) O2 - N5	2.22
BD (1) O2 – N4	BD*(1) C1 - O2	3.01	LP (1) N4	BD*(2) C1 - O2	4.43	BD (1) O2 – N4	BD*(1) C1 - O2	2.98
4β			***5***			***6***		
BD (2) C1 - O2	BD*(1) O2 – N4	2.64	BD (1) C1 - O2	BD*(1) O2 – N6	3.54	BD (1) C1 - O2	BD*(1) O2 – N5	3.39
BD (1) O2 – N4	BD*(1) C1 - O2	3.20	BD (1) O2 – N6	BD*(1) C1 - O2	5.22	BD (1) O2 – N5	BD*(1) C1 - O2	5.15
LP (1) N4	BD*(2) C1 - O2	3.24	BD (1) O2 – N6	BD*(1) C1 – N6	4.07	BD (1) O2 – N5	BD*(1) C1 – N5	4.04
			LP (3)Cl5	BD*(1) C1 - O2	6.62	LP (3)Cl6	BD*(1) C1 - O2	7.38
7			***8***			***9***		
BD (1) C1 - O2	BD*(1) O2 – N5	3.36	BD (1) C1 - O2	BD*(1) O2 – N4	2.73	BD (1) C1 - O2	BD*(1) O2 – N4	2.88
BD (1) O2 – N5	BD*(1) C1 - O2	4.27	BD (1) O2 – N4	BD*(1) C1 - O2	4.24	BD (1) O2 – N4	BD*(1) C1 - O2	4.17
LP (3)Cl6	BD*(1) O2 – N5	6.12	LP (3)Cl5	BD*(1) C1 - O2	6.22	LP (3)Cl6	BD*(1) O2 – N4	8.61
			LP (3)Cl5	BD*(1) C1 – N4	5.30			
			LP (3)Cl6	BD*(1) O2 – N4	7.35			
10			***11***			***12***		
BD (1) C1 - O2	BD*(1) O2 – N4	2.88	BD (1) C1 - O2	BD*(1) O2 – N3	2.14	BD (1) C1 - O2	BD*(1) O2 – N5	4.11
BD (1) O2 – N4	BD*(1) C1 - O2	4.61	LP (3)Cl4	BD*(1) O2 – N3	9.40	BD (1) O2 – N5	BD*(1) C1 - O2	5.47
LP (3)Cl5	BD*(1) C1 - O2	7.94	LP (2)Cl5	BD*(1) C1 - O2	5.35			
LP (3)Cl5	BD*(1) C1 - O2	6.95	LP (3)Cl5	BD*(1) C1 – N3	8.08			
			LP (3)Cl6	BD*(1) C1 - O2	5.24			
			LP (3)Cl6	BD*(1) C1 – N3	6.29			
13			***14***			***15***		
BD (1) C1 - O2	BD*(1) O2 – N5	4.03	BD (1) C1 - O2	BD*(1) O2 – N5	4.83	BD (1) C1 - O2	BD*(1) O2 – N4	4.85
BD (1) O2 – N5	BD*(1) C1 - O2	5.38	BD (1) O2 – N5	BD*(1) C1 - O2	5.40	BD (1) O2 – N4	BD*(1) C1 - O2	5.60
			BD (1) C6 - H7	BD* (1) O2 – N5	5.53	BD (1) C5 – H6	BD* (1) O2 – N4	5.56

Continuation of Table S6

Donor NBO (i)	*Acceptor NBO (j)*	*E(2)*	*Donor NBO (i)*	*Acceptor NBO (j)*	*E(2)*	*Donor NBO (i)*	*Acceptor NBO (j)*	*E(2)*
16			***17***			***18***		
BD (1) C1 - O2	BD*(1) O2 – N4	4.93	BD (1) C1 - O2	BD*(1) O2 – N4	4.03	BD (1) C1 - O2	BD*(1) O2 – N3	4.81
BD (1) O2 – N4	BD*(1) C1 - O2	5.60	BD (1) O2 – N4	BD*(1) C1 - O2	5.36	BD (1) O2 – N3	BD*(1) C1 - O2	5.73
BD (1) C5 – H6	BD* (1) O2 – N4	5.82	BD (1) C5 – H6	BD*(1) C1 - O2	5.09	BD (1) C4 – H6	BD* (1) O2 – N3	5.80
						BD (1) C8 – H9	BD*(1) C1 - O2	5.09
						BD (1) C12 – H13	BD*(1) C1 – N3	5.41
						BD (1) C12 – H14	BD*(1) C1 - O2	5.37
19			***20***			***21***		
BD (1) C1 - O2	BD*(1) O2 – N5	4.35	BD (1) O2 – N5	BD*(1) C1 - O2	5.13	BD (1) C1 - O2	BD*(1) O2 – N5	3.80
BD (1) O2 – N5	BD*(1) C1 - O2	5.53	BD (1) O2 - N4	BD*(1) C1 - O2	5.13	BD (1) O2 – N5	BD*(1) C1 - O2	7.06
LP (1) N6	BD*(1) C1 - O2	15.00	LP (2) O2	BD*(1) C1 - H3	7.91	LP (1) N6	BD* (1) O2 – N5	36.59
			LP (2) O2	BD*(1) C1 - N6	7.54			
			LP (1) N4	BD*(1) C1 - N6	4.75			
			LP (1) N6	BD*(1) C1 - O2	4.06			
			LP (1) N6	BD*(1) C1 - N4	15.14			
22			***23***			***24***		
BD (1) C1 - O2	BD*(1) O2 – N4	3.69	BD (1) C1 - O2	LP (3) O2	7.77	BD (1) C1 - O2	BD*(1) O2 – N4	2.37
BD (1) O2 – N4	BD*(1) C1 - O2	5.11	BD(1) C1 – N4	LP (3) O2	8.53	BD (1) O2 – N4	BD*(1) C1 - O2	7.16
LP (1) N5	BD*(1) C1 - O2	17.23	BD(1) C1 – N4	BD*(1) N5 – H6	5.49	LP (1) N4	BD*(1) N5 – H7	7.65
LP (1) N8	BD*(1) C1 – N4	14.67	LP (3) O2	BD*(1) C1 - O2	15.76	LP (1) N5	BD* (1) O2 – N5	59.30
BD*(1) C1 - O2	BD*(1) C1 – N4	34.83	LP (3) O2	BD*(1) C1 – N4	19.75	LP (1) N8	BD*(1) C1 - O2	13.18
			LP (3) O2	BD*(2) N4 - N5	19.56	BD(1) C1 – N4	BD*(1) O2 – N4	5.28
			LP (1) N4	BD*(1) N5 – H7	8.18			
			LP (1) N8	BD*(1) C1 – N4	10.13			
			LP (1) N8	BD*(1) N5 – H7	6.61			
			BD*(2) N4 - N5	BD*(1) N4 - N5	23.69			
25								
LP (3) O2	BD*(1) C1 - O2	5.90						
LP (3) O2	BD*(1) C1 – N3	15.52						
LP (3) O2	BD*(1) N3 - N10	10.34						
LP (1) N4	BD*(1) C1 - O2	12.98						
LP (1) N7	BD*(1) C1 - N3	10.37						
LP (1) N7	BD*(1) N10 – H12	7.63						
BD*(2) N3 - N10	BD*(1) N3 - N10	41.17						

Table S7

VIE and AIE (eV) for oxaziridine and three radicals calculated using B3LYP/6-311++G (d, p) method (1Hartree=27.2114 eV) [16].

IE B3LYP		*This work*				*Reference [16]*			
		|VIE-AIE|	*IE*			*|VIE-AIE|*			
			B3LYP	*QCISD(T)*	*G2(MP2)*	*B3LYP*	*QCISD(T)*	*G2(MP2)*	
Oxaziridine	AIE	9.71	0.92	9.67	9.69	9.82	0.94	0.96	0.94
	VIE	10.63		10.61	10.65	10.76			
Radical 1	AIE	9.86	0.64						
	VIE	10.50							
Radical 2	AIE	8.10	1.45						
	VIE	9.55							
Radical 3	AIE	8.03	1.50						
	VIE	9.53							

Table S8

Vertical Ionization Energies (eV) calculated using B3LYP/6-311++G (d, p).

Structure	*VIE*	*Structure*	*VIE*
1	10.63	14	9.93
2	10.50	15	9.66
3	9.55	16	9.49
4	9.53	17	9.95
5	10.87	18	9.23
6	11.09	19	9.72
7	10.74	20	9.69
8	11.06	21	9.94
9	10.73	22	9.67
10	11.10	23	8.73
11	10.93	24	9.29
12	10.22	25	8.58
13	10.31		

Table S9

The value of the HOMO-LUMO energy (a.u.), Quantum chemical parameters: Ionization potential (*I*), Electron Affinity (*A*), Electronegativity (χ), Chemical Potential (μ), Global Hardness (η), Global Softness (*S, σ*) and Electrophilicity (ω); for oxaziridine and three radicals calculated using B3LYP method and 6-311++G (d, p) basis set.

Parameter	*Oxaziridine*	*Radical 1*	*Radical 2*	*Radical 3*
I=VIE (a.u.)	0.39 66	0.38587	0.35096	0.35016
A=VEA (a.u.)	0.02241	0.00114	0.00209	0.00399
χ (a.u.)	0.20653	0.19351	0.17652	0.17708
μ (a.u.)	-0.20653	-0.19351	-0.17652	-0.17708
η (a.u.)	0.18413	0.19237	0.17446	0.17309
S or σ $(a.u.)^{-1}$	5.43103	5.19835	5.73277	5.77749
ω (a..)	0.11583	0.09732	0.08932	0.09058

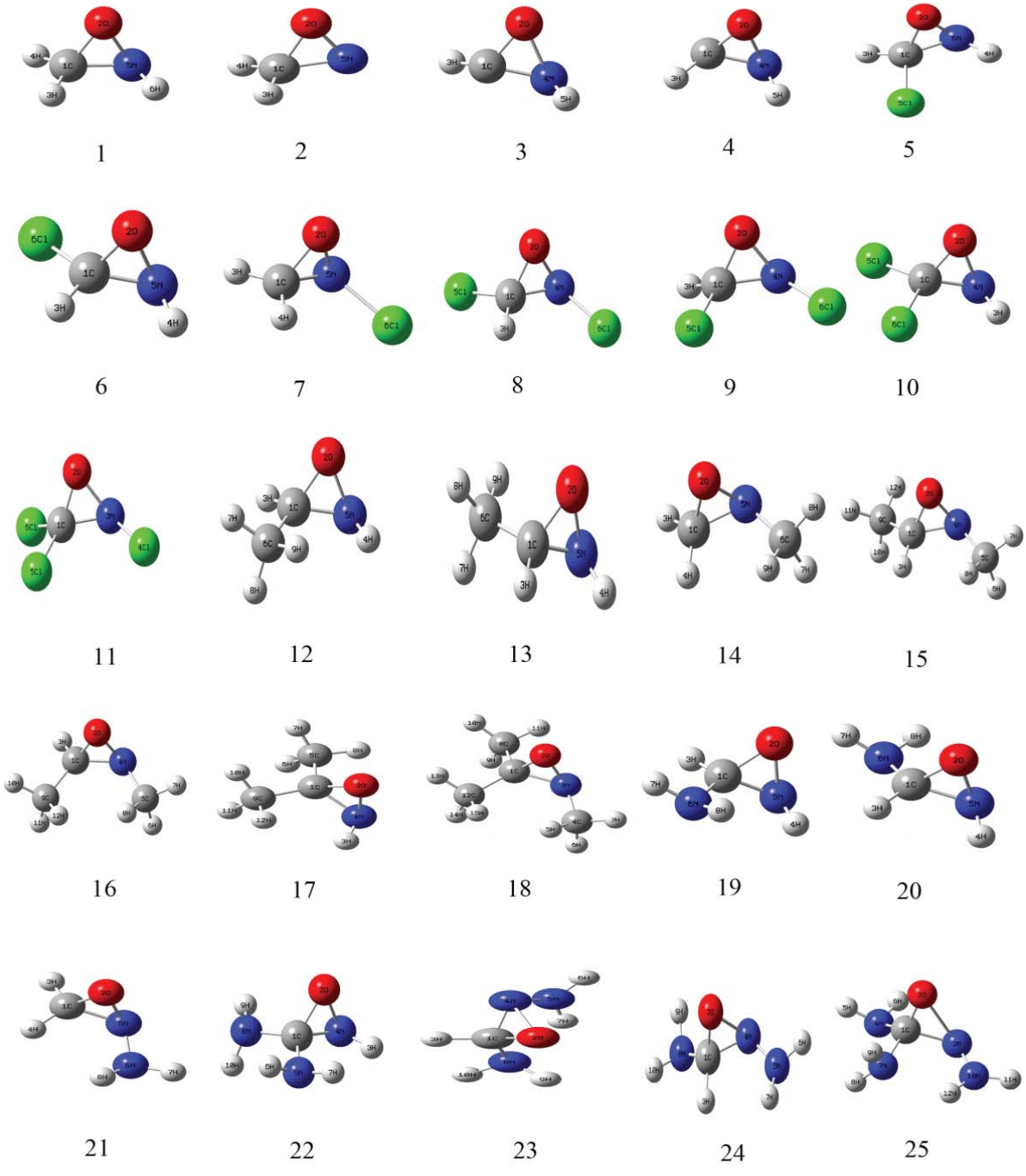

Figure S1. Optimum geometry of (1) oxaziridine [CH_3NO (^1A)] (2) radical 1 [CH_2NO (^2A)] (3) radical 2 [CH_2NO (^2A)] (4) radical 3 [CH_2NO (^2A)] (5) CH_2NOCl (^1A) (6) CH_2NOCl (^1A) (7) CH_2NOCl (^1A) (8) $CHNOCl_2$(^1A) (9) $CHNOCl_2$(^1A) (10) $CHNOCl_2$ (^1A) (11) $CNOCl_3$(^1A) (12) C_2H_5NO (^1A) (13) C_2H_5NO (^1A) (14) C_2H_5NO (^1A) (15) C_3H_7NO (^1A) (16) C_3H_7NO (^1A) (17) C_3H_7NO (^1A) (18) C_4H_9NO (^1A) (19) CH_4N_2O (^1A) (20) CH_4N_2O (^1A) (21) CH_4N_2O (^1A) (22) CH_5N_3O (^1A) (23) CH_5N_3O (^1A) (24) CH_5N_3O (^1A) (25) CH_6N_4O (^1A).

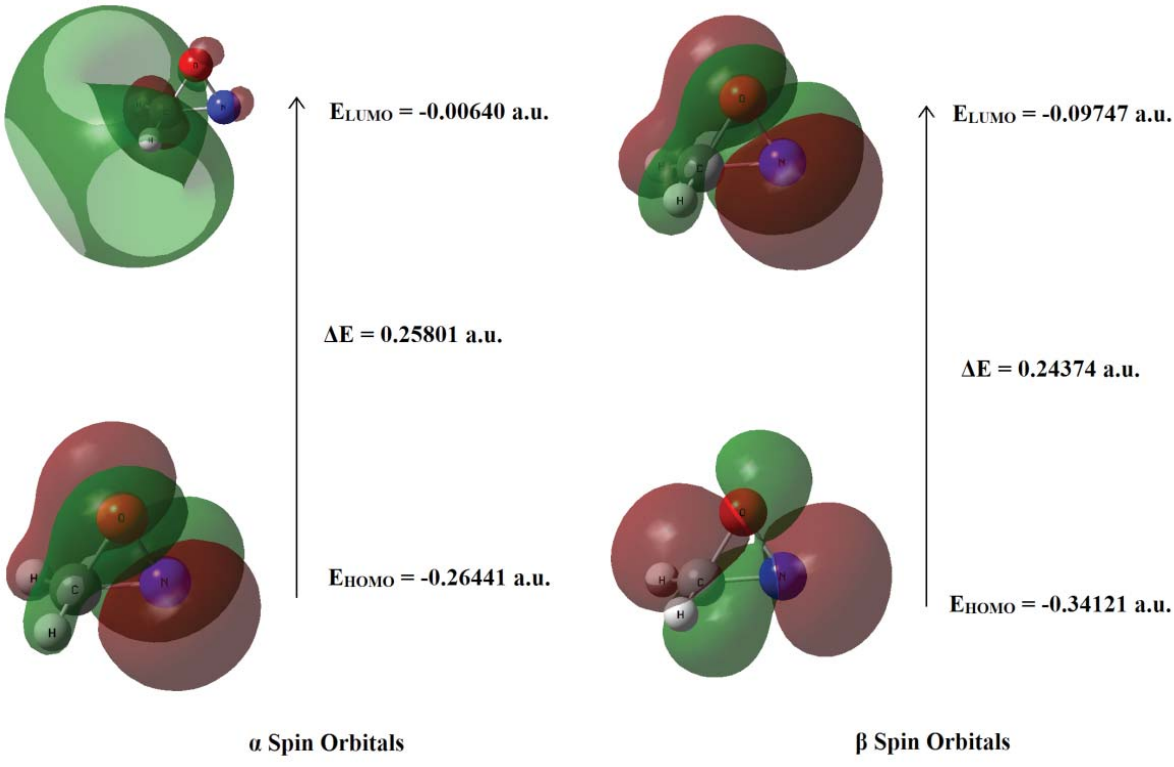

Figure S2. Isodensity plots of the frontier molecular orbitals of radical 1.

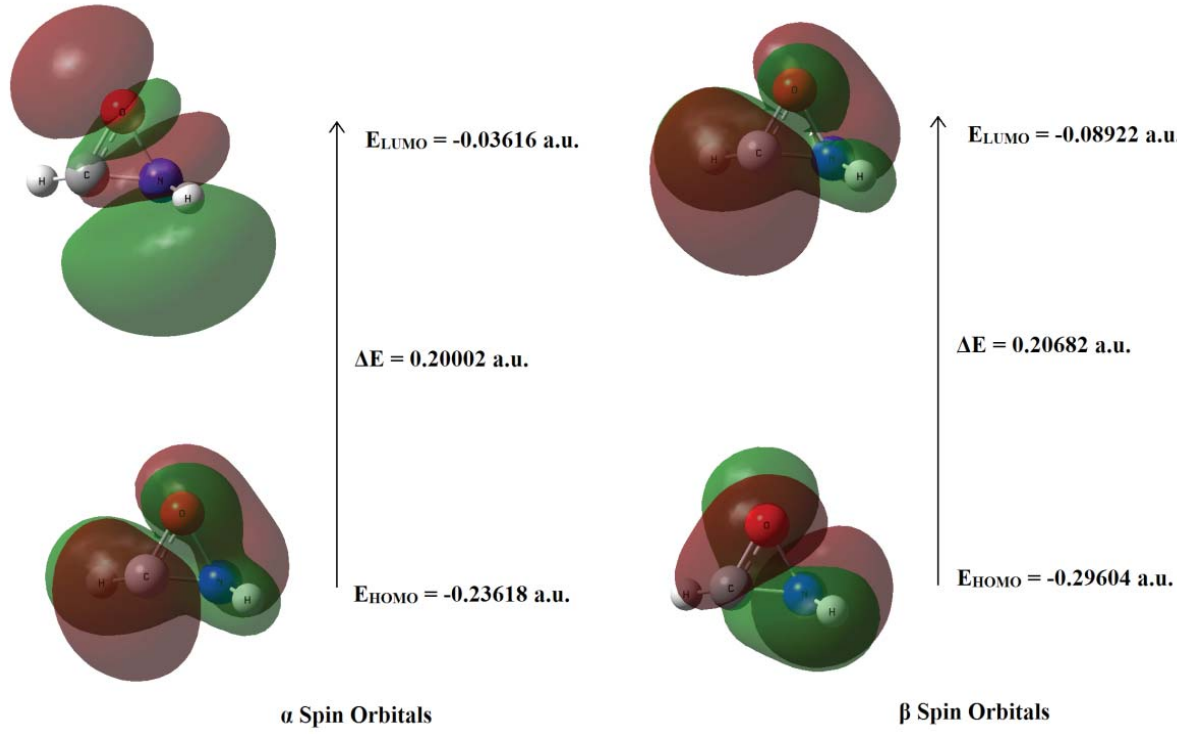

Figure S3. Isodensity plots of the frontier molecular orbitals of radical 2.

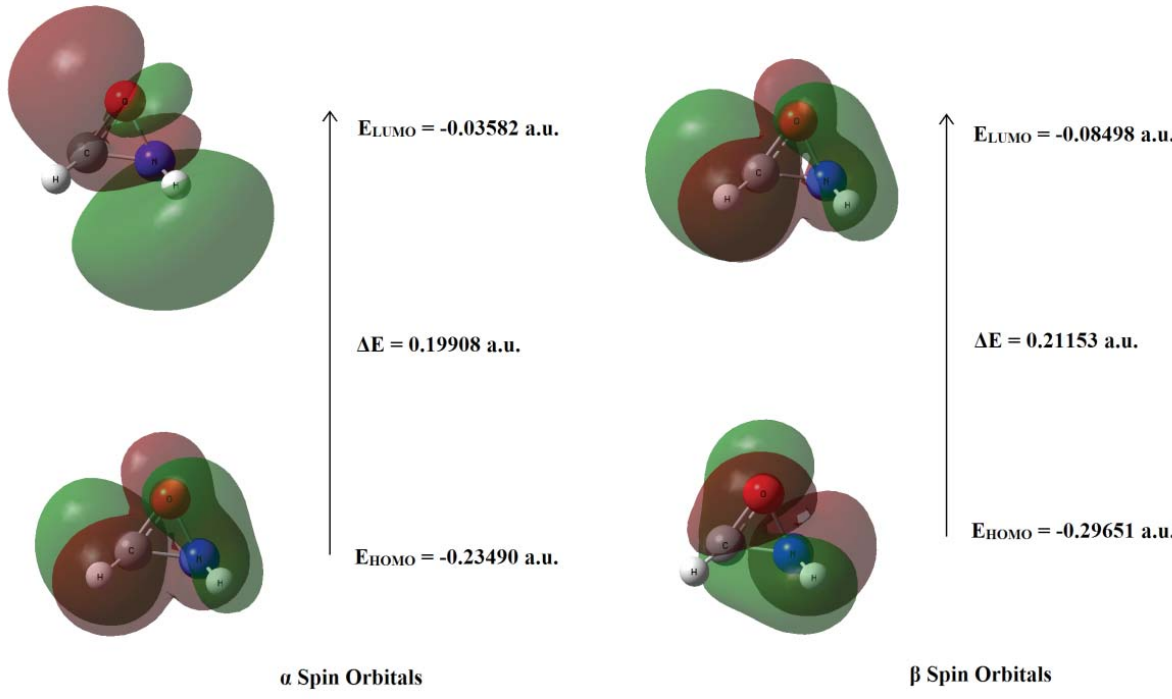

Figure S4. Isodensity plots of the frontier molecular orbitals of radical 3.