Table 1S. Total energies.

Species	energy[a] B3LYP/ 6-31+G(d,p)	MP2(FULL)/ 6-31+G(d,p)	B3LYP/ 6-311+G(3df,2p)	MP2/ 6-311+G(3df,2p)	MP2/ 6-311G(d,p)	QCISD(T)/ 6-311G(d,p)	G2(MP2)	ZPVE[b]	H_{298}[c]
Formaldonitrone (**1**)									
1	-169.814 669		-169.869 074	-169.503 710	-169.388 902	-169.428 378	-169.544 549	114.60	11.26
		-169.347 245	-169.868 486	-169.504 037	-169.389 549	-169.428 569	-169.545 296	112.27	11.50
1(VN)[d]			-169.865 619	-169.500 269	-169.385 367	-169.425 825	-169.542 090		
$\mathbf{1}^{+\bullet}$	-169.470 737		-169.523 769	-169.142 202	-169.044 265	-169.101 022	-169.196 157	112.87	11.39
				-169.153 080	-169.056 846		-169.194 454		
		-168.997 006		-169.142 929	-169.047 053	-169.100 145	-169.192 837	113.88	11.39
		-169.005 368		-169.151 759	-169.055 401		-169.193 319		
$\mathbf{1}^{+\bullet}$(VI)[e]			-169.521 445	-169.139 664	-169.043 522	-169.097 940	-169.191 281		
				-169.150 669	-169.054 057		-169.191 751		
Formaldoxime (**2**)									
anti-**2**	-169.829 405		-169.883 044	-169.518 268	-169.409 775	-169.451 210	-169.561 857	112.49	11.89
anti-**2**(VN)[d]			-169.846 079	-169.479 450	-169.368 889	-169.409 431	-169.522 145		
syn-**2**	-169.820 340		-169.875 190	-169.510 186	-169.401 497	-169.442 683	-169.554 037	111.15	11.77
$\mathbf{2}^{+\bullet}$	-169.466 287		-169.521 010	-169.138 118	-169.040 231	-169.095 606	-169.191 661	110.33	12.16
				-169.148 743	-169.050 823		-169.191 694		
$\mathbf{2}^{+\bullet}$(VI)[e]			-169.481 603	-169.095 271	-168.998 623	-169.059 109	-169.153 925		
(from anti-**2**)				-169.108 842	-169.012 083		-169.154 036		
$\mathbf{2}^{+\bullet}$(VI)[e]			-169.480 944	-169.096 576	-168.997 735	-169.054 032	-169.151 040		
(from syn-**2**)				-169.105 031	-169.006 178		-169.151 052		
Nitrosomethane (**3**)									
3	-169.809 090		-169.861 701	-169.497 856	-169.392 564	-169.434 814	-169.543 466	109.33	12.49
3(VN)[d]			-169.841 113	-169.473 448	-169.365 807	-169.408 785	-169.519 785		
$\mathbf{3}^{+\bullet}$	-169.468 853		-169.524 642	-169.158 559	-169.063 367	-169.108 710	-169.202 678	108.74	12.93
			-169.165 727	-169.070 592		-169.202 620			
CH_2-O-NH (**5**)									
5	-169.749 224		-169.803 622	-169.434 296	-169.322 057	-169.368 928	-169.484 225	110.12	11.85

5(VN)[d]			-169.799 449						
5$^{+\bullet}$	-169.436 417		-169.4898621	-169.117 235	-169.021 709	-169.071 346	-169.165 948	107.94	12.46
				-169.120 569	-169.024 811		-169.166 180		
		-168.971 921	-169.4894059	-169.117 408	-169.021 952	-169.071 438	-169.165 970	107.94	12.46
		-168.974 832		-169.120 538	-169.024 864		-169.166 187		
Oxaziridine (**6**)									
6	-169.794 477		-169.848 839	-169.490 408	-169.378 858	-169.417 932	-169.530 541	115.37	10.73
6(VN)[d]			-169.806 855	-169.445 486	-169.331 519	-169.370 185	-169.485 210		
6$^{+\bullet}$	-169.438 868		-169.492 763	-169.129 413	-169.029 901	-169.072 769	-169.169 212	113.58	11.03
				-169.133 098	-169.033 235		-169.169 562		
6$^{+\bullet}$(VI)[e]			-169.458 893	-169.073 124	-168.974 660	-169.039 627	-169.135 021		
				-169.077 508	-168.978 853		-169.135 213		
TS(1→2)	-169.740 966		-169.794 455	-169.429 193	-169.314 975	-169.355 659	-169.477 668	97.69	
TS(1→3)	-169.728 914		-169.782 242	-169.414 405	-169.301 825	-169.343 618	-169.463 827	98.12	
TS(1$^{+\bullet}$**→2**$^{+\bullet}$**)**		-168.895 134	-169.430 750	-169.045 780	-168.946 800	-169.004 0145	-169.106 673	95.86	
		-168.909 712		-169.060 863	-168.961 615		-169.106 941		
TS(1$^{+\bullet}$**→3**$^{+\bullet}$**)**	-169.398 324		-169.453 516	-169.067 785	-168.969 832	-169.027 094	-169.127 489	99.11	
				-169.071 407	-168.973 097		-169.127 846		
		-168.916 228	-169.453 219	-169.068 130	-168.970 186	-169.026 895	-169.127 281	99.11	
		-168.919 443		-169.071 635	-168.973 342		-169.127 631		
TS(1$^{+\bullet}$**→6**$^{+\bullet}$**)**	-169.420 171		-169.473 168	-169.092 041	-168.993 040	-169.051 152	-169.149 231	107.94	
				-169.102 304	-169.002 743		-169.149 791		
1,2-Oxazolidine (**4**)									
4	-248.456304		-248.527 739	-247.951 558	-247.792 475	-247.868 403	-248.001 201	265.92	15.04
4(VN)[d]			-248.490 297						
4$^{+\bullet}$	-248.175 702		-248.246 455	-247.661 743	-247.513 236	-247.592 991	-247.710 774	264.95	15.88
				-247.665 585	-247.516 708		-247.711 144		
		-247.453 122	-248.246 225						
		-247.456 629							
4$^{+\bullet}$(VI)[e]			-248.205 559	-247.604 423					
				-247.608 911					
7$^{+\bullet}$	-248.117 913		-248.190 879	-247.600 043	-247.448 623	-247.532 739	-247.657 916	253.19	19.88
				-247.604 008	-247.452 873		-247.657 630		
8$^{+\bullet}$	-248.119 046		-248.192 067	-247.601 381	-247.450 413	-247.533 052	-247.658 418	251.50	20.63
				-247.603 876	-247.452 879		-247.658 446		
9$^{+\bullet}$	-248.140 379		-248.213 035	-247.613 608	-247.466 929	-247.551 253	-247.673 677	247.97	21.74

				-247.616 709	-247.469 981		-247.673 726		
TS1($4^{+\bullet}\rightarrow 7^{+\bullet}$)	-248.108 812		-248.181 666	-247.580 825	-247.429 289	-247.521 248	-247.645 991	254.63	
				-247.594 832	-247.443 336		-247.645 951		
TS2	-248.089 091		-248.161 641	-247.568 739	-247.418 455	-247.502 395	-247.626 122	254.01	
				-247.571 112	-247.420 739		-247.626 212		
TS3	-248.079 691		-248.153 081	-247.557 013	-247.406 034	-247.491 584	-247.617 186	250.91	
				-247.560 023	-247.408 982		-247.617 249		
Aziridine ($10^{+\bullet}$)	-133.600 136		-133.636 041	-133.288 379	-133.211 584	-133.265 995	-133.317 416	172.14	12.05
				-133.290 897	-133.213 840		-133.317 678		
		-133.188 223		-133.291 378	-133.213 672	-133.264 522	-133.316 853	172.14	12.05
		-133.190 520		-133.294 066	-133.216 008		-133.317 207		
CH_3NO_2	-245.028 722		-245.108 974	-244.621 418	-244.464 004	-244.503 973	-244.673 537	125.63	14.18
CH_2=N-O$^{\bullet}$	-169.192 466		-169.246 281	-168.859 334	-168.754 571	-168.812 652	-168.926 926	80.55	11.32
				-168.876 614	-168.771 109		-168.854 976		
CH2=N=O^{+}	-168.853 992		-168.912 004	-168.558 778	-168.461 273	-168.499 183	-168.606 368	79.61	11.77
HC=N-OH^{+}	-168.866 036		-168.924 513	-168.578 786	-168.479 717	-168.511 375	-168.619 654	80.84	12.35
HC=NH-O$^{\bullet}$	-169.118 235		-169.171 538	-168.787 455	-168.678 503	-168.735 527	-168.854 976	77.96	12.08
CH_2=NH	-94.640 609		-94.669 181	-94.435 970	-94.375 572	-94.409 374	-94.461 322	100.95	10.19
CH_2=NH$^{+\bullet}$	-94.276 323		-94.304 296	-94.059 808	-94.009 087	-94.053 401	-94.094451	91.53	10.18
				-94.068 046	-94.017 569		-94.094 206		
HC=NH$^{\bullet}$	-93.978 254		-94.006 855	-93.770 406	-93.711 921	-93.750 363	-93.809 114	65.44	
				-93.776 253	-93.718 113		-93.808 770		
HC=NH^{+}	-93.709 696		-93.740 789	-93.530 148	-93.480 097	-93.504 656	-93.554 371	66.52	
NO_2	-205.083 886		-205.155 295	-204.781 537	-204.657 014	-204.675 382	-204.831 659	22.15	10.22
				-204.785 595	-204.660 792		-204.831 938		
H-N=O	-130.479 992		-130.523 801	-130.272 615	-130.193 215	-130.210 000	-130.305 974	35.32	9.94
H-N=O$^{+\bullet}$	-130.101 116		-130.148 404	-129.889 979	-129.821 289	-129.857 484	-129.938 242	34.45	10.00
				-129.901 541	-129.832 914		-129.938 178		
^{3}N-OH	-130.448 642		-130.491 088	-130.226 071	-130.150 135	-130.179 649	-130.267 045	36.55	10.03
				-130.229 382	-130.153 070		-130.267 422		
NO	-129.895 477		-129.939 578	-129.690 166	-129.614 646	-129.641 492	-129.737 855	11.41	8.68
				-129.697 062	-129.622 090		-129.737 306		
NO^{+}	-129.532 153		-129.583 837	-129.369 422	-129.305 334	-129.316 240	-129.399 886	14.29	8.60
C_2H_4	-78.599 645		-78.621 049	-78.393 292	-78.344 262	-78.384 158	-78.414 086	128.92	
CH_3-CH=OH^{+}	-154.150 904		-154.198 702	-153.837 675	-153.747 460	-153.794 882	-153.864 267	172.84	13.21
$CH_3CH_2NH_2^{+\bullet}$	-134.872 200		-134.907 893	-134.541 729	-134.464 477	-134.527 329	-134.562 063	230.28	15.28
				-134.544 901	-134.467 503		-134.562 209		

CH_2=O	-114.511 523	-114.549 208	-114.306 324	-114.235 150	-114.261 157	-114.336 602	67.55	10.03
CH_3	-39.847 334	-39.857 691	-39.731 269	-39.707 215	-39.732 297	-39.7428 233	75.40	10.54
			-39.733 263	-39.709 167		-39.7428 651		
CH_3^+	-39.484 716	-39.493 705	-39.374 999	-39.356 158	-39.381 153	-39.384 785	79.31	10.55
$^3CH_2$								
CO	-113.317 323	-113.356 431	-113.136 727	-113.074 751	-113.093 899	-113.176 042	12.69	8.65
OH	-75.739 014	-75.765 574	-75.617 394	-75.572 738	-75.589 196	-75.640 921	21.32	8.68
			-75.619 374	-75.574 263		-75.641 375		
H	-0.500 273	-0.502 156	-0.499 810	-0.499 810	-0.499 810	-0.500 000		6.2

[a]In units of hartree: 1 hartree = 2525. kJ mol-1. Upper lines: spin-unprojected (UMP2) energies, lower lines spin-projected (PMP2) energies. [b]From corrected harmonic frequencies in kJ mol-1. [c]298 K enthalpy corrections in kJ mol-1. [d]Vertically neutralized species. Single-point calculations on optimized ion geometries. [e]Vertically ionized species. Single-point calculations on optimized neutral geometries.

Table 2S. Optimized Geometries and Uncorrected Harmonic Frequencies CH_2=NH-O (**1**), B3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.056418	.346426	.000120
2	8	0	-1.187585	-.229122	-0.00005
3	1	0	-.083066	1.377324	-.000400
4	6	0	1.130490	-.193636	-.000171
5	1	0	1.988238	.464809	.000487
6	1	0	1.207492	-1.272321	.000137

Rotational constants (GHZ): 75.3009072 11.6982363 10.1252472

Harmonic frequencies (cm^{-1}):

569.8778	697.9624	797.6523
984.9995	1075.6390	1306.5399
1444.9235	1501.6451	1666.8901
3194.3011	3314.6671	3335.6463

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	23.96706	154.27464	178.24169

Table 3S. Optimized Geometries and Uncorrected Harmonic Frequencies CH_2=NH-O (**1**), UMP2(FULL)/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.063684	.346216	-.000265
2	8	0	-1.187328	-.231009	.000113
3	1	0	-.090540	1.373390	.000449
4	6	0	1.139919	-.193277	.000003
5	1	0	1.980450	.477050	.000491
6	1	0	1.214988	-1.266220	-.000003

Rotational constants (GHZ): 75.3528866 11.6313487 10.0760298

Harmonic frequencies (cm^{-1}):

573.6039	636.8323	727.1841
980.0249	1099.0940	1320.8987
1504.6404	1518.9694	1683.6802
3278.1259	3408.6843	3430.1726

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	23.95052	155.16182	179.11233
X	.99983	-.01828	.00002
Y	.01828	.99983	.00013
Z	-.00002	-.00013	1.00000

Table 4S. Optimized Geometries and Uncorrected Harmonic Frequencies CH_2=NH-$O^{+\bullet}$ (**$1^{+\bullet}$**), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.058785	.398493	-.000036
2	8	0	-1.156283	-.258693	-.000001
3	1	0	-.135533	1.429200	.000194
4	6	0	1.111047	-.208664	.000007
5	1	0	2.013142	.400522	-.000083
6	1	0	1.117870	-1.297641	.000107

Rotational constants (GHZ): 65.5572766 12.1977230 10.2482197
Harmonic frequencies (cm^{-1}):

553.2036	557.3874	948.9656
1055.5137	1077.7985	1204.0391
1339.8272	1493.7900	1563.3146
3146.2024	3286.8692	3369.2330

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	27.52923	147.95722	175.48645

Table 5S. Optimized Geometries and Uncorrected Harmonic Frequencies CH_2=NH-$O^{+\bullet}$ (**1**$^{+\bullet}$), UMP2(FULL)/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.034337	.411640	-.000023
2	8	0	-1.162370	-.255544	.000083
3	1	0	-.105563	1.433701	.000080
4	6	0	1.094219	-.220385	-.000110
5	1	0	2.011263	.354407	.000047
6	1	0	1.068301	-1.302928	.000030

Rotational constants (GHZ): 64.0917709 12.3084311 10.3254851
Harmonic frequencies (cm^{-1}):

555.6604	610.5230	1004.1610
1025.3151	1205.3736	1225.5970
1438.8221	1529.5932	1712.6654
3240.8844	3381.8637	3519.3534

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	28.15870	146.62643	174.78513
X	.99972	-.02385	.00007
Y	.02385	.99972	.00000
Z	-.00007	.00000	1.00000

Table 6S. Optimized Geometries and Uncorrected Harmonic Frequencies anti-CH_2=N-OH (anti-**2**), B3LYP/6-31+G(d,p)

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.142258	-.025727	.000000
2	7	0	.000000	.538250	.000000
3	8	0	-1.036347	-.408956	.000000
4	1	0	-1.835107	.136398	.000000
5	1	0	1.266672	-1.109419	.000000
6	1	0	2.005662	.631283	.000000

Rotational constants (GHZ): 68.8570423 11.7763595 10.0564439
Harmonic frequencies (cm^{-1}):

425.6420	533.7833	794.9651
920.7745	977.8657	1179.5908
1345.8579	1450.7327	1717.5496
3117.0120	3247.3570	3819.0464

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	26.20997	153.25120	179.46117

Table 7S. Optimized Geometries and Uncorrected Harmonic Frequencies syn-CH_2=N-OH (syn-**2**), B3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.120377	-.049595	.000000
2	7	0	.000000	.557656	.000000
3	8	0	-1.134834	-.231674	.000000
4	1	0	-.879116	-1.176291	.000000
5	1	0	1.221129	-1.141407	.000000
6	1	0	2.014400	.565074	.000000

Rotational constants (GHZ): 66.1808779 11.8966811 10.0839833
Harmonic frequencies (cm^{-1}):

459.5989	564.8762	776.4222
944.6780	947.4213	1168.3977
1381.0522	1467.7131	1690.3600
3057.3927	3234.2914	3605.0585

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	27.26983	151.70123	178.97106

Table 8S. Optimized Geometries and Uncorrected Harmonic Frequencies CH_2=N-OH cation-radical (**2**$^{+\bullet}$), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.198888	.123539	.010368
2	7	0	-.035139	-.367386	.016840
3	8	0	1.136589	.171469	-.106152
4	1	0	1.731222	-.171098	.605696
5	1	0	-1.350965	1.195552	.182112

6	1	0	-2.033669	-.565739	-.118685

Rotational constants (GHZ): 103.3844984 10.6403733 9.8595150
Harmonic frequencies (cm^{-1}):

376.4536	456.4263	725.0246
1036.7105	1050.9599	1166.6754
1326.4374	1428.2787	1740.1988
3076.0784	3221.2915	3549.2908

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	17.45659	169.61258	183.04563

Table 9S. Optimized Geometries and Uncorrected Harmonic Frequencies Nitrosomethane (**3**), B3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	.000000	.568593	.000000
2	8	0	1.163126	.232912	.000000
3	6	0	-.949839	-.569484	.000000
4	1	0	-.430043	-1.531904	.000000
5	1	0	-1.587965	-.447320	.882656
6	1	0	-1.587965	-.447320	-.882656

Rotational constants (GHZ): 61.3775096 11.414122443 10.2350764
Harmonic frequencies (cm^{-1}):

A"	A'	A'
169.9071	576.9442	855.3788
A"	A'	A'
973.3619	1158.1107	1378.3438
A"	A'	A'
1453.8929	1457.3827	1668.8056
A'	A"	A'
3028.9192	3114.0137	3145.5972

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	29.40395	158.14078	176.32904

Table 10S. Optimized Geometries and Uncorrected Harmonic Frequencies Nitrosomethane cation-radical (**3**$^{+\bullet}$), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.226742	-.380454	.000000
2	8	0	-1.224771	.176969	.000000
3	6	0	1.164033	.118187	.000000
4	1	0	1.153743	1.211518	-.000008
5	1	0	1.623706	-.336600	.889268
6	1	0	1.623711	-.336616	-.889258

Rotational constants (GHZ): 84.4024457 10.3554834 9.7936249
Harmonic frequencies (cm^{-1}):

147.9367	455.2827	705.9425
1028.2051	1093.3386	1348.4466
1374.5063	1436.4019	2005.7956
3014.3341	3097.9943	3170.8188

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	21.38257	174.27879	184.27714
X	.99997	.00824	.00000
Y	-.00824	.99997	.00000
Z	.00000	.00000	1.00000

Table 11S. Optimized Geometries and Uncorrected Harmonic Frequencies CH_2-O-NH (**5**) B3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.137194	.158414	.000000
2	8	0	.006570	-.413459	-.000004
3	7	0	1.157871	.299067	.000005
4	1	0	-1.984688	-.511773	-.000007
5	1	0	-1.189877	1.242271	.000011
6	1	0	1.840071	-.466780	-.000002

Rotational constants (GHZ): 80.5010330 11.7230371 10.2328665
Harmonic frequencies (cm^{-1}):

506.6941	550.8759	712.8378
785.6131	954.9356	1236.5238
1359.5456	1490.6188	1602.9766
3163.0369	3323.0039	3431.4613

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	22.41886	153.94826	176.36712
X	.99936	-.03585	.00000
Y	.03585	.99936	-.00001
Z	.00000	.00001	1.00000

Table 12S. Optimized Geometries and Uncorrected Harmonic Frequencies CH_2-O-$NH^{+\bullet}$ Cation-Radical ($\mathbf{5}^{+\bullet}$) UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.104658	.192447	-.000014
2	8	0	-.029639	-.474562	.000002
3	7	0	1.154118	.314055	-.000009
4	1	0	-2.018363	-.403641	.000025
5	1	0	-1.065009	1.285544	.000056
6	1	0	1.869610	-.438473	.000048

Rotational constants (GHZ): 68.3646984 12.0033891 10.2106209
Harmonic frequencies (cm^{-1}):

341.2904	494.9426	604.2222
747.2117	1181.0664	1231.1938
1359.5857	1473.4128	1591.0780
3103.5795	3262.3323	3350.0540

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	26.39873	150.35263	176.75136
X	.99921	-.03968	.00000
Y	.03968	.99921	.00001
Z	.00000	-.00001	1.00000

Table 13S. Optimized Geometries and Uncorrected Harmonic Frequencies Oxaziridine (**6**) B3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.691861	-.331144	.017476
2	7	0	.040940	.865393	.019730
3	8	0	.730919	-.453990	-.160922
4	1	0	-1.144769	-.611920	.970202
5	1	0	-1.294912	-.523820	-.869097
6	1	0	1.146893	-.622607	.762655

Rotational constants (GHZ): 26.3273251 24.3624159 14.5291776
Harmonic frequencies (cm^{-1}):

758.3973	898.0579	969.2919
1086.9822	1216.3704	1253.7986
1277.0242	1348.6874	1548.1017
3084.6058	3181.2833	3406.3416

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	68.55012	74.07891	124.21496

Table 14S. Optimized Geometries and Uncorrected Harmonic Frequencies $[Oxaziridine]^{+\bullet}$ Cation-Radical ($\mathbf{6}^{+\bullet}$) UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.843820	-.121311	.021594
2	8	0	.387374	.748114	.021758
3	7	0	.499006	-.557078	-.113749
4	1	0	-1.324686	-.186136	.995026
5	1	0	-1.417502	-.071346	-.899722
6	1	0	1.213071	-1.100012	.397316

Rotational constants (GHZ): 30.2966822 23.0184674 14.6961169
Harmonic frequencies (cm^{-1}):

647.5284	724.5083	986.3986
1051.3317	1134.6162	1181.7885

1254.0733 1380.6470 1517.8472
3146.3534 3288.6406 3403.3831
Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	59.56894	78.40405	122.80395

Table 15S. Optimized Geometries and Uncorrected Harmonic Frequencies **TS(1 → 2)**, UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.171000	.156452	-.000029
2	7	0	-.025530	-.403234	-.000002
3	8	0	1.193837	.263211	.000008
4	1	0	.932397	-.996955	-.000016
5	1	0	-1.222832	1.244527	.000032
6	1	0	-2.055553	-.469327	.000111

Rotational constants (GHZ): 78.8666997 11.0256048 9.6732759
Harmonic frequencie (cm^{-1}):

	381.5091	481.5322	
755.4885	907.2014	950.7872	
1229.5736	1415.4156	1621.6932	
2812.8382	3132.9568	3270.8041	-1949.2359

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	22.88344	163.68637	186.56980
X	.99931	-.03711	-.00001
Y	.03711	.99931	.00000
Z	.00001	.00000	1.00000

Table 16S. Optimized Geometries and Uncorrected Harmonic Frequencies **TS(1 → 3)**, UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.095713	.205731	.004780
2	7	0	.112179	-.427441	-.114950
3	8	0	1.182602	.208500	.014259
4	1	0	-.566658	-.821274	.837327
5	1	0	-1.153408	1.287947	.148906
6	1	0	-1.951724	-.376974	-.324335

Rotational constants (GHZ): 69.5369826 11.7113787 10.4320880
Harmonic frequencies (cm^{-1}):

	539.7706	691.5041	
939.8848	1086.8355	1181.4357	
1242.6038	1467.5035	1492.8182	
2055.8007	3088.9009	3247.3401	-1712.2953

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	25.95369	154.10151	172.99904
X	.99997	-.00814	-.00111
Y	.00804	.99752	-.06990
Z	.00168	.06989	.99755

Table 17S. Optimized Geometries and Uncorrected Harmonic Frequencies TS($\mathbf{1}^{+\bullet} \rightarrow \mathbf{2}^{+\bullet}$), UMP2(FULL)/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.195559	-.100288	.000200
2	7	0	-.005641	.242078	-.000568
3	8	0	1.209070	-.213272	.000152
4	1	0	.919606	1.097727	.001027
5	1	0	-1.431270	-1.161037	.000080
6	1	0	-1.948054	.676670	.000453

Harmonic frequencies (cm^{-1}):

-s	457.3639	599.3654	
759.3817	1073.5572	1152.1917	
1202.8469	1483.2871	2170.3882	
2346.7595	3221.8518	3355.4376	-2325.4969

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	16.62268	168.50109	185.12373
X	.99953	.03078	.00001
Y	-.03078	.99953	.00029
Z	.00000	-.00029	1.00000

Table 18S. Optimized Geometries and Uncorrected Harmonic Frequencies TS($\mathbf{1}^{+\bullet} \rightarrow \mathbf{3}^{+\bullet}$), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.128643	.176647	-.020049
2	7	0	.111959	-.335987	-.114091
3	8	0	1.207833	.172588	.012345
4	1	0	-.463470	-.806483	.861313
5	1	0	-1.277944	1.229794	.235071
6	1	0	-1.933104	-.511983	-.276216

Rotational constants (GHZ): 85.2498046 11.1888127 10.3086530

Harmonic frequencies (cm^{-1}):

	452.6142	728.8427	
996.8030	1129.4416	1159.2315	
1232.9435	1471.3661	1594.0490	
2085.8275	3098.6680	3256.1511	-1411.4866

Principal axes and moments of inertia in atomic units:

	1	2	3

EIGENVALUES --	21.17003	161.29872	175.07051
X	.99997	-.00544	-.00501
Y	.00509	.99765	-.06827
Z	.00537	.06824	.99765

Table 19S. Optimized Geometries and Uncorrected Harmonic Frequencies TS($1^{+\bullet} \rightarrow 6^{+\bullet}$), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.176611	.597525	-.144305
2	8	0	-.868990	-.492795	.079931
3	6	0	.977202	-.145370	.007325
4	1	0	1.235861	-.807846	-.816084
5	1	0	1.568470	-.071448	.923273
6	1	0	-.479341	1.511194	.219550

Rotational constants (GHZ): 36.4633681 16.7358369 12.5451612

Harmonic frequencies (cm^{-1}):

	634.5420	690.4384	
1067.7099	1104.9897	1203.4671	
1343.0187	1383.0474	1488.5371	
3118.2994	3275.0118	3430.2660	-631.7404

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	49.49464	107.83692	143.85954
X	.99374	-.11148	.00717
Y	.11041	.98992	.08876
Z	-.01699	-.08741	.99603

Table 20S. Optimized Geometries and Uncorrected Harmonic Frequencies 1,2-Oxazolidine (**4**), B3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.385224	1.203948	-.022309
2	6	0	-1.235042	-.091647	-.095476
3	6	0	1.047031	.649440	.141935
4	8	0	-.348496	-1.150124	.268770
5	7	0	.905257	-.732578	-.357522
6	1	0	-.489788	1.792337	-.937880
7	1	0	-.661903	1.837845	.824326
8	1	0	-2.063628	-.121347	.615870
9	1	0	-1.615443	-.256768	-1.112139
10	1	0	1.786728	1.176022	-.467649
11	1	0	1.354331	.684662	1.197005
12	1	0	1.580278	-1.354164	.088054

Rotational constants (GHZ): 7.2990837 7.1789838 4.0968873

Harmonic frequencies (cm^{-1}):

125.0920 334.0544 635.3126
681.1772 810.7159 851.0340
916.3843 932.8019 945.0179
977.4948 1058.6897 1090.5738
1154.0440 1216.7150 1247.5743
1254.3006 1308.1345 1343.5149
1370.9864 1421.3019 1496.8630
1506.9538 1523.0033 3008.3034
3029.3782 3077.2762 3103.7044
3116.1063 3131.3205 3499.6085

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	247.25585	251.39229	440.51521
X	.82065	-.57087	.02516
Y	.57098	.82096	.00353
Z	-.02267	.01147	.99968

Table 21S. Optimized Geometries and Uncorrected Harmonic Frequencies 1,2-Oxazolidine Cation-Radical(**4**$^{+\bullet}$), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.653994	1.061304	-.180872
2	6	0	-1.209008	-.324591	.142160
3	6	0	.843946	.921573	.143607
4	8	0	-.043156	-1.240484	-.069061
5	7	0	1.049472	-.510950	-.069960
6	1	0	-.797537	1.305211	-1.235839
7	1	0	-1.126620	1.834686	.426844
8	1	0	-1.494453	-.473362	1.186885
9	1	0	-1.982974	-.698603	-.526989
10	1	0	1.510605	1.482194	-.516809
11	1	0	1.092410	1.156383	1.187752
12	1	0	1.911850	-1.055703	-.109001

Rotational constants (GHZ): 7.4292407 7.2362773 4.0247703

Harmonic frequencies (cm^{-1}):

188.3081 208.8096 397.5731
629.1799 747.7464 782.3549
884.4751 892.8917 917.6951
943.0945 1042.5748 1115.5269
1189.1661 1223.4156 1233.1546
1265.9689 1328.7107 1354.9597
1384.4230 1470.2835 1488.9075
1499.1494 1514.6033 3043.2891
3103.9703 3108.2328 3133.9349
3165.7010 3192.6113 3546.9049

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	242.92404	249.40188	448.40849
X	-.24130	.97045	.00138
Y	.97044	.24130	-.00484
Z	.00503	-.00017	.99999

Table 22S. Optimized Geometries and Uncorrected Harmonic Frequencies syn-anti-CH_2=NH-O-CH_2-CH_2 Cation-Radical ($7^{+\bullet}$), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-.050544	-.715316	-.000015
2	7	0	1.281674	-.510370	.000004
3	6	0	1.947453	.585594	-.000005
4	6	0	-.929516	.521644	.000011
5	6	0	-2.318632	.033612	.000003
6	1	0	1.750336	-1.419655	.000045
7	1	0	1.452464	1.548331	-.000040
8	1	0	3.029755	.506902	.000029
9	1	0	-.673202	1.080520	-.905846
10	1	0	-.673156	1.080489	.905871
11	1	0	-2.824729	-.173272	.935315
12	1	0	-2.824668	-.173295	-.935335

Rotational constants (GHZ): 17.0287210 2.8342727 2.5124077

Harmonic frequencies (cm^{-1}):

92.8768	133.4423	196.0814
228.8509	377.8175	566.8400
663.4391	669.6849	784.8988
843.6269	960.6373	976.5619
1010.5325	1113.5832	1151.4680
1232.6245	1272.1009	1368.0841
1446.8656	1473.6529	1498.5056
1510.4696	1697.1366	3056.7700
3128.5011	3184.5744	3189.0013
3304.2448	3314.6080	3508.5134

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	105.98219	636.75635	718.33133
X	.99999	.00535	.00000
Y	-.00535	.99999	.00000
Z	.00000	.00000	1.00000

Table 23S. Optimized Geometries and Uncorrected Harmonic Frequencies anti-anti-CH_2=NH-O-CH_2-CH_2 Cation-Radical ($8^{+\bullet}$), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	.026983	-.364746	-.145344
2	7	0	1.197210	.311175	-.113295
3	6	0	2.313671	-.278743	.094270
4	6	0	-1.183713	.512627	.195712
5	6	0	-2.376929	-.309202	-.046729
6	1	0	1.144244	1.312212	-.329737
7	1	0	2.314595	-1.343360	.308070

8	1	0	3.223559	.309842	.034628
9	1	0	-1.121415	1.378124	-.474409
10	1	0	-1.059418	.803170	1.241115
11	1	0	-2.843534	-.851736	.766646
12	1	0	-2.772532	-.416596	-1.050011

Rotational constants (GHZ): 24.5178817 2.4162984 2.2944310

Harmonic frequencies (cm^{-1}):

69.1946	78.2017	140.1545
217.3851	404.2921	481.5394
659.1776	684.8175	785.5977
833.8439	955.9218	970.2045
1046.9413	1119.6051	1147.2254
1210.1230	1264.0997	1365.9084
1421.3264	1473.1058	1488.8617
1509.6391	1721.8863	3054.7743
3143.8458	3173.6634	3182.6415
3301.2164	3302.2519	3456.1782

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	73.60918	746.90328	786.57461
X	.99999	.00303	.00176
Y	-.00291	.99804	-.06254
Z	-.00194	.06253	.99804

Table 24S. Optimized Geometries and Uncorrected Harmonic Frequencies [Aziridine]$^{+\bullet}$-Ethylene Complex (**9**$^{+\bullet}$), UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.699444	-.135659	.613153
2	8	0	1.367819	.141380	-.393947
3	6	0	2.452152	-.057440	.123668
4	6	0	-1.585156	.780917	-.062677
5	6	0	-1.585732	-.698676	-.377606
6	1	0	-.719681	-.346004	1.611408
7	1	0	2.550902	-.400724	1.165625
8	1	0	3.372438	.108501	-.460543
9	1	0	-1.104993	1.431979	-.790212
10	1	0	-2.362594	1.235796	.546175
11	1	0	-1.107319	-.997800	-1.307689
12	1	0	-2.362775	-1.361973	-.005571

Rotational constants (GHZ): 13.6264739 2.3182108 2.2758082

Harmonic frequencies (cm^{-1}):

42.8227	105.2640	112.1920
141.9544	278.2019	293.1213
672.5303	779.6652	861.9554
875.3428	937.2552	1110.0248
1112.2370	1147.2912	1179.7685
1191.0558	1191.7919	1210.0933
1259.5081	1467.0779	1489.4784
1492.8423	1755.0886	2988.1494

3090.2432	3132.3320	3137.3847
3228.4888	3239.6060	3527.1227

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	132.44374	778.50606	793.01111
X	.99997	-.00277	.00706
Y	.00316	.99846	-.05534
Z	-.00689	.05536	.99844

Table 25S. Optimized Geometries and Uncorrected Harmonic Frequencies Aziridine cation-radical (**10**$^{+\bullet}$) UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	.021826	.788371	.000000
2	6	0	.021826	-.375191	.796328
3	6	0	.021826	-.375191	-.796328
4	1	0	-.692732	1.523156	.000000
5	1	0	-.845495	-.539986	1.432083
6	1	0	.984510	-.729744	1.165693
7	1	0	-.845495	-.539986	-1.432083
8	1	0	.984510	-.729744	-1.165693

Rotational constants (GHZ): 25.3326480 19.5970792 13.1796542

Harmonic frequencies (cm^{-1}):

A'	A'	A"
360.1096	801.1694	870.7588
A'	A"	A"
873.7063	931.4695	1041.3708
A'	A"	A'
1050.6836	1106.5086	1174.8184
A"	A'	A"
1269.4229	1279.0673	1452.7714
A'	A"	A'
1486.3826	3107.9674	3125.3724
A"	A'	A'
3227.4631	3238.5443	3486.8850

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	71.24171	92.09235	136.93388
X	.00000	-.12494	.99216
Y	.00000	.99216	.12494
Z	1.00000	.00000	.00000

Table 26S. Optimized Geometries and Uncorrected Harmonic Frequencies Transition state for ring opening in 1,2-oxazolidine cation-radical (**4**$^{+\bullet}$)to syn-anti-CH_2=NH-O-CH_2-CH_2 cation-radical (**7**$^{+\bullet}$), **TS1**, UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.085120	.963819	-.366282
2	6	0	-1.176298	-.378395	.278168
3	6	0	1.145621	.846277	.309785
4	8	0	.034515	-1.174805	-.038433
5	7	0	1.117252	-.370031	-.176646
6	1	0	-.965875	1.034969	-1.444385
7	1	0	-1.505719	1.826963	.141374
8	1	0	-1.285317	-.327941	1.364642
9	1	0	-1.978460	-.996593	-.138447
10	1	0	1.931775	1.500887	-.053971
11	1	0	.657737	1.072136	1.250260
12	1	0	1.743751	-.711963	-.905516

Rotational constants (GHZ): 7.7382169 5.5746079 3.7473384

Harmonic frequencies (cm^{-1}):

	215.6594	318.4783	
477.5060	524.7851	639.2165	
671.1898	793.2669	830.6729	
840.6266	917.0441	939.9385	
992.3763	1031.2467	1134.6494	
1208.9663	1234.1390	1360.7608	
1376.6763	1469.6232	1480.8037	
1506.3944	1589.5688	3081.4464	
3139.2360	3159.5166	3174.7979	
3270.4304	3291.0666	3536.4311	-406.6267

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	233.22442	323.74316	481.60614
X	.99917	.03726	-.01648
Y	-.03713	.99928	.00790
Z	.01677	-.00728	.99983

Table 27S. Optimized Geometries and Uncorrected Harmonic Frequencies Transition state for ring opening in 1,2-oxazolidine cation-radical (**4**$^{+\bullet}$) by cleavage of OCH_2--CH_2 bond, **TS2**, UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.076906	1.085956	.027118
2	6	0	1.297883	.747638	.104017
3	6	0	-1.206113	-.386202	-.189829
4	8	0	1.093444	-.443371	-.331881
5	7	0	-.016536	-1.045309	.413150
6	1	0	-1.126466	1.483855	1.037415
7	1	0	-1.254679	1.778222	-.791417
8	1	0	1.918104	1.371535	-.535665
9	1	0	1.095502	.982319	1.146388
10	1	0	-2.068428	-.771219	.374734
11	1	0	-1.329101	-.637470	-1.248191
12	1	0	.044090	-2.027467	.131903

Rotational constants (GHZ): 7.8858359 5.3536287 3.6365053

Harmonic frequencies (cm^{-1}):

	221.6207	375.6563	
460.8575	466.3924	575.2027	
711.1469	734.2321	837.0299	
874.0384	968.0407	1003.7312	
1039.3936	1081.1070	1137.0563	
1203.5123	1235.3191	1339.6860	
1385.0332	1453.7249	1466.2399	
1492.2793	1550.6351	3036.7038	
3108.5445	3135.1458	3158.5412	
3271.0914	3283.3075	3492.6530	-129.8438

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	228.85857	337.10615	496.28448
X	.99764	.06750	.01292
Y	-.06772	.99755	.01764
Z	-.01169	-.01847	.99976

Table 28S. Optimized Geometries and Uncorrected Harmonic Frequencies Transition state for ring opening in 1,2-oxazolidine cation-radical ($\mathbf{4}^{+\bullet}$) by cleavage of OCH_2--CH_2 bond, **TS3**, UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.298715	.895679	-.346334
2	6	0	-1.226854	.863084	.270464
3	6	0	1.108275	-.396757	.370453
4	8	0	-1.238081	-.311246	-.229607
5	7	0	-.032887	-1.093382	-.213309
6	1	0	1.182899	.929640	-1.426163
7	1	0	1.777610	1.731674	.153197
8	1	0	-.569726	1.155226	1.081160
9	1	0	-2.049636	1.492372	-.061455
10	1	0	1.953725	-1.073643	.158816
11	1	0	1.064164	-.274657	1.462768
12	1	0	-.304994	-1.989015	.194201

Rotational constants (GHZ): 8.1186446 4.9259785 3.5315744

Harmonic frequencies (cm^{-1}):

	288.8121	327.1877	
410.7317	449.5332	530.3913	
592.0970	667.7147	754.6955	
887.6392	917.3561	956.3462	
984.3231	1067.4080	1118.5996	
1204.8560	1233.8742	1362.4660	
1377.9541	1452.0806	1463.8847	
1480.4599	1557.0292	3000.7476	
3042.4613	3157.1008	3165.0194	
3284.3599	3299.4060	3526.1889	-164.7149

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	222.29587	366.37211	511.03019
X	.99954	-.03049	-.00007
Y	.03048	.99933	-.02007

Z	.00069	.02006	.99980

Table 29S. Optimized Geometries and Uncorrected Harmonic Frequencies $CH_2=N=O^+$ Cation, B3LYP/6-31+G)d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.079322	.000086	-.000122
2	8	0	-1.224849	-.000079	.000146
3	6	0	1.165062	-.000080	-.000610
4	1	0	1.681312	.967696	.001673
5	1	0	1.682366	-.967189	.001674

Rotational constants (GHZ): 267.8857232 11.0291100 10.5929910

Harmonic frequencies (cm^{-1}):

442.4272	452.9224	824.1217
1029.0506	1227.4229	1387.1113
2229.5305	3058.9210	3169.3209

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	6.73698	163.63434	170.37125
X	1.00000	.00000	.00013
Y	.00000	1.00000	.00000
Z	-.00013	.00000	1.00000

Table 30S. Optimized Geometries and Uncorrected Harmonic Frequencies CH_3-CH=OH^+ Cation, B3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.108860	.431029	-.000082
2	6	0	1.214534	-.163083	-.000055
3	8	0	-1.139548	-.311666	-.000013
4	1	0	-2.000328	.158235	.000178
5	1	0	-.247359	1.517669	.000030
6	1	0	1.768197	.232311	-.868522
7	1	0	1.195026	-1.253127	-.000949
8	1	0	1.766803	.230561	.870185

Rotational constants (GHZ): 52.6161269 9.7423594 8.6489139

Harmonic frequencies (cm^{-1}):

154.0814	489.9015	655.9734
926.8468	937.2495	1100.4188
1138.6161	1292.7167	1343.2179
1422.2129	1435.6378	1437.3985
1652.7067	3002.1084	3039.9887
3139.1879	3184.0971	3654.0376

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	34.30015	185.24683	208.66680

X	.99952	-.03103	.00001
Y	.03103	.99952	.00002
Z	-.00001	-.00002	1.00000

Table 31S. Optimized Geometries and Uncorrected Harmonic Frequencies
Ethylamine Cation-Radical, UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.075185	.602339	-.000006
2	6	0	-1.257114	-.286540	.000005
3	7	0	1.203054	-.247408	-.000001
4	1	0	1.600666	-.612135	-.868204
5	1	0	1.600697	-.612079	.868212
6	1	0	.073472	1.210587	.908180
7	1	0	.073462	1.210573	-.908202
8	1	0	-2.070446	.444601	-.000031
9	1	0	-1.303825	-.902210	.898751
10	1	0	-1.303832	-.902277	-.898698

Rotational constants (GHZ): 30.5331155 8.8670442 7.9055469
Harmonic frequencies (cm^{-1}):

179.3172	235.5231	328.8141
705.7904	788.5353	829.6062
941.6235	943.7634	1077.2573
1164.2564	1256.2158	1347.6510
1383.3479	1453.2908	1481.9319
1505.7133	1639.6159	3066.9793
3077.0888	3155.0055	3169.1415
3195.0914	3466.1787	3586.6696

Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	59.10767	203.53357	228.28796
X	.99996	-.00843	.00000
Y	.00843	.99996	.00000
Z	.00000	.00000	1.00000

Table 32S. Optimized Geometries and Uncorrected Harmonic Frequencies
CH_2=N-O Radical, UB3LYP/6-31+G(d,p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.012144	.392217	.000184
2	6	0	-1.198015	-.106589	-.000284
3	8	0	1.081930	-.295541	-.000079
4	1	0	.087807	1.415319	.000135
5	1	0	-1.470149	-1.156976	.000921

Rotational constants (GHZ): 72.7189695 13.2312173 11.1943978
Harmonic frequencies (cm^{-1}):

314.8154 447.3610 934.8374
1018.5250 1197.4252 1434.5187
1588.5200 3231.5987 3367.0518
Principal axes and moments of inertia in atomic units:

	1	2	3
EIGENVALUES --	24.81802	136.40024	161.21825
X	.99833	.05775	-.00004
Y	-.05775	.99833	-.00013
Z	.00003	.00013	1.00000