Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Heterocumulenic Carbene Nitric Oxide Radical OCCNO•

Bo Lu,[a] Chao Song,[a] Weiyu Qian,[a] Zhuang Wu,[a] Attila G. Császár[c] and Xiaoqing Zeng[a,b]*

[a]College of Chemistry, Chemical Engineering and Materials Science, Soochow University, 215123 Suzhou (China), E-mail: xqzeng@suda.edu.cn
[b]Department of Chemistry, Fudan University, 200433 Shanghai (China)
E-mail: xqzeng@fudan.edu.cn
[c]MTA-ELTE Complex Chemical Systems Research Group, Laboratory of Molecular Structure and Dynamics, Institute of Chemistry, ELTE Eötvös Loránd University, Pázmány Péter sétány 1/A, H-1117 Budapest (Hungary).

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Experimental and computational details

Synthesis of OCCCO and $OC^{13}CCO$

Carbon suboxide, OCCCO, was prepared according to literature[1] by heating a mixture of malonic acid (0.1068 g) and P_2O_5 (1.0568 g) at 140 °C. The gaseous products were condensed in a liquid nitrogen trap and then purified by trap-to-trap distillation (−120, −130, and −196 °C). Pure carbon suboxide, OCCCO, was retained in the middle trap. $OC^{13}CCO$ was prepared and purified the same way as OCCCO, with the ^{13}C substitute of malonic acid (2-13C, 99.0%, Cambridge Isotope Laboratories, Inc.).

NO (≥ 99.96%, Messer), ^{15}NO (≥ 98.0%, Cambridge Isotope Laboratories, Inc.), Ar (≥ 99.999%, Messer), N_2 (≥ 99.999%, Messer) and Ne (≥ 99.999%, Messer) gases were used without further purification.

Matrix infrared spectroscopy

Matrix IR spectra were recorded on a FT-IR spectrometer (Bruker 70V) in a reflectance mode using a transfer optic. A KBr beam splitter and a wide-band MCT detector were used in the mid-IR region (4000–500 cm^{-1}). Typically, 200 scans at a resolution of 0.5 cm^{-1} were co-added for each spectrum. Gaseous OCCCO was mixed with NO and inert gas (1:5:1000) at room temperature. Then the mixtures (1:5:1000, sample: NO: inert gas) were passed through an aluminum oxide furnace (o.d. 2.0 mm, i.d. 1.0 mm), deposited (2 mmol h^{-1}) in a high vacuum (~10^{-6} pa) onto the Rh-plated Cu block matrix support (15 K for Ar- and N_2- matrix; 2.8 K for Ne- matrix) using a closed-cycle helium cryostat (Sumitomo Heavy Industries, SRDK-408D2-F50H) inside the vacuum chamber. Temperatures at the second stage of the cold head were controlled and monitored using a LakeShore 335 digital cryogenic temperature controller a Silicon Diode (DT-670). Photolysis experiments were performed using a Nd^{3+}:YAG laser (MPL-F-266, 10 mW), a LED lamp (830 nm, FU830AD100-BXS22130, 100 mW) and a UV flashlight (365 nm, Boyu T648, 24 W).

Quantum chemical calculation methods

Structures and IR frequencies of stationary points, including transition states, of the species investigated were computed using the unrestricted forms oft he density functionals B3LYP,[2] M06-2X,[3] BP86[4], B2PLYP,[5] B3PW91,[6] wb97xD,[7] PBE1PBE,[8] and TPSs,[9] and utilizing the 6-311+G(3df),[10] cc-pVTZ,[11] Def2-TZVP,[12] Def2-QZVP[12] basis sets. To avoid the nonzero-force dilemma,[13] the force fields were determined at very tightly optimized equilibrium structures. Anharmonic force fields[14] have been determined in a normal-coordinate representation via numerical differentiation of quadratic force constants, evaluated analytically at a number of distorted structures. Second-order vibrational perturbation theory[15] has been used to compute anharmonic corrections to the harmonic wavenumbers. Coupled cluster theory computations, including single and double (CCSD),[16] occasionally single, double, and triple (CCSDT) excitations, and CCSD augmented with a perturbational estimate of the effects of connected triple excitations (CCSD(T)),[17] used both the unrestricted (U) and the restricted open-shell (RO) versions of CC theory.[18] Occasionally the frozen-core approximation, keeping the 1s orbitals of the C, N and O atoms doubly occupied during the correlated-level computations, has been used during the wave-function-theory models. The single-point-energy computations required for the focal-point analysis (FPA)[19] of bond dissociation energies were computed at the aug-cc-pwCVQZ ROCCSD(T) optimized geometries. Additionally, anharmonic frequency computations using second-order vibrational perturbation theory (VPT2) has been employed for OCCNO• at the CCSD(T)-F12a/cc-pVTZ-F12[20] level with the MOLPRO package of *ab initio* programs.[21] The UCCSD(T) and ROCCSD(T) computations, employing, where available, analytic first[22] and second[23] derivatives, were performed with the CFOUR electronic-structure program package.[24] Local minima were confirmed by harmonic vibrational analysis and transition states were further confirmed by intrinsic reaction coordinate (IRC) calculations.[25] Time-dependent (TD) DFT (BP86/6-311+G(3df)) calculations[26] were performed for the prediction of UV-Vis transitions. These

computations were performed using the Gaussian09 software package.[27] The CCSD(T)/cc-pVTZ//B3LYP/6-311+G(3df) computations were performed with the help of the ORCA program.[28] The natural spin densities and Wiberg bond indices (WBI) were computed at the BP86/6-311+G(3df) level with the Natural Bond Orbital (NBO) method.[29] The wavefunction files (.wfn), obtained at the BP86/6-311++G(3df,3pd) level, were used as input for the Multiwfn program[30] to perform the QTAIM analysis.[31] The characteristics of the bond critical points (BCP) were obtained in terms of the electron density (ρ_{CP}) and its Laplacian ($\nabla^2\rho_{CP}$), the total electron energy density (H_{BCP}), the potential electron energy density (V_{BCP}), and the Lagragian kinetic energy (G_{BCP}).

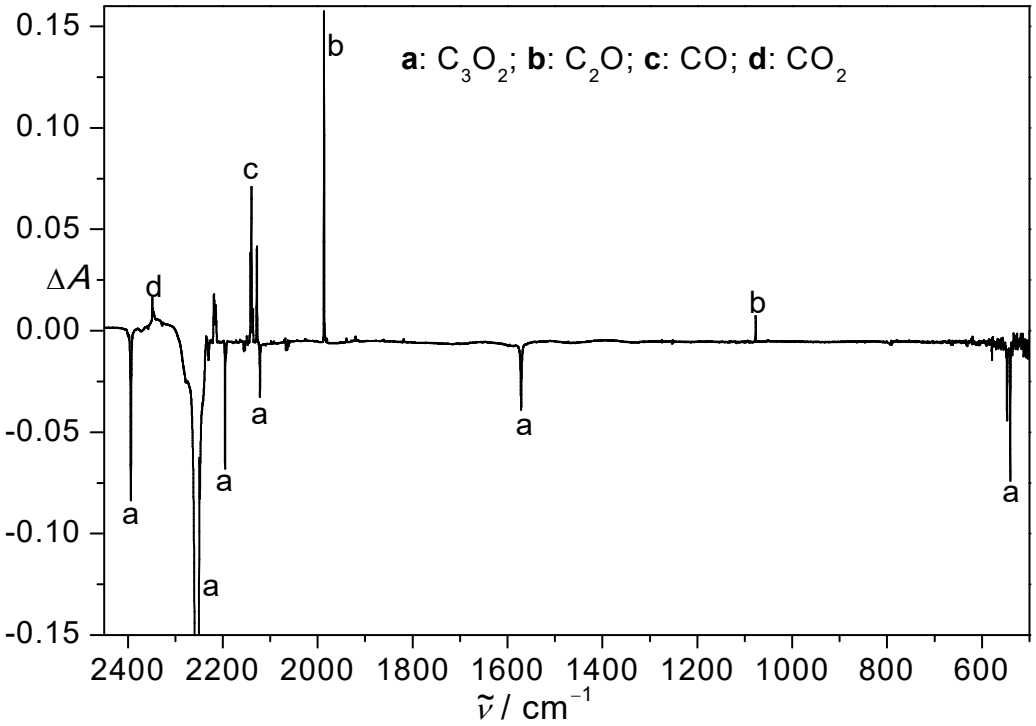

Figure S1. IR difference spectrum reflecting the generation of C_2O in N_2 matrix upon 266 nm laser irradiation (65 min) at 15 K.

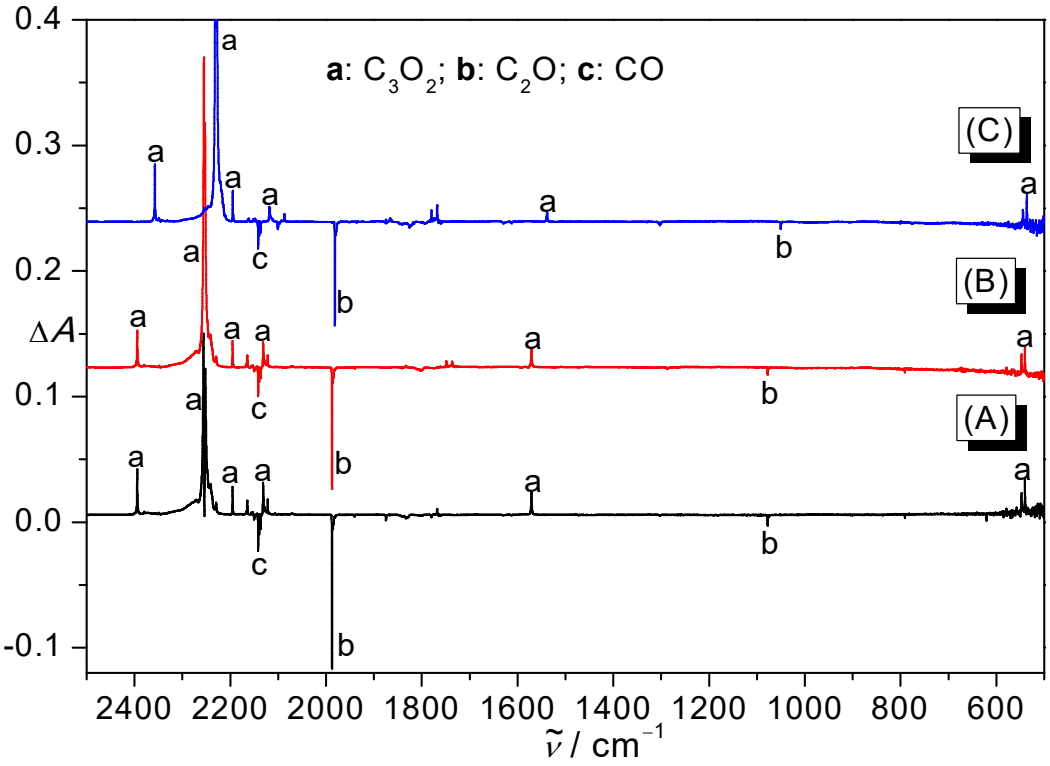

Figure S2. A) IR difference spectrum reflecting the reformation of OCCCO in N_2 matrix upon 830 nm LED irradiation (1 min) at 15 K. B) IR difference spectrum reflecting the reformation of OCCCO by using ^{15}NO in N_2 matrix upon 830 nm LED irradiation (1 min) at 15 K. C) IR difference spectrum reflecting the reformation of $OC^{13}CCO$ in N_2 matrix upon 830 nm LED irradiation (1 min) at 15 K.

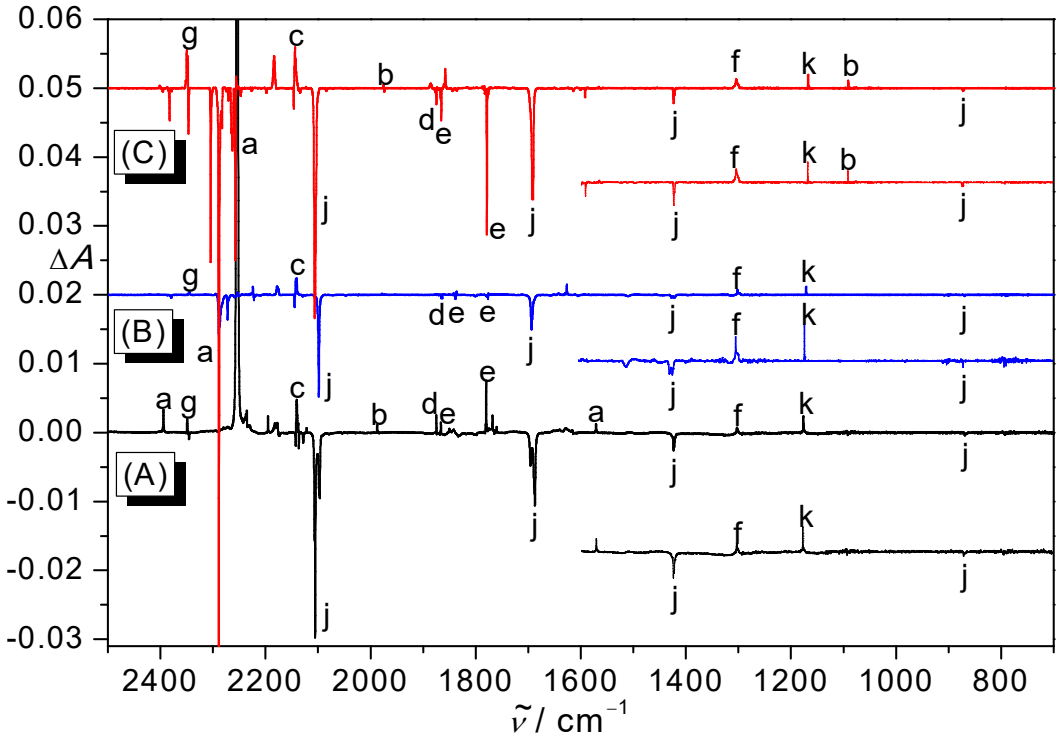

Figure S3. A) IR difference spectrum reflecting the depletion of OCCNO• in N_2-matrix upon 365 nm LED irradiation (2.5 min) at 15 K. B) IR difference spectrum reflecting the depletion of OCCNO• in Ar-matrix upon 365 nm LED irradiation (2 min) at 15 K. C) IR difference spectrum reflecting the depletion of OCCNO• in Ne-matrix upon 365 nm LED irradiation (2 min) at 2.8 K. For clarity, each spectrum in the range of 1600–700 cm^{-1} are displayed after 3-times-expansion along the Δ*A* axis. The bands of C_3O_2 (a), C_2O (b), CO (c), NO• (d), N_2O_2 (e), N_2O_3 (f), CO_2 (g), OCCNO• (j), CNO• (K) are labeled.

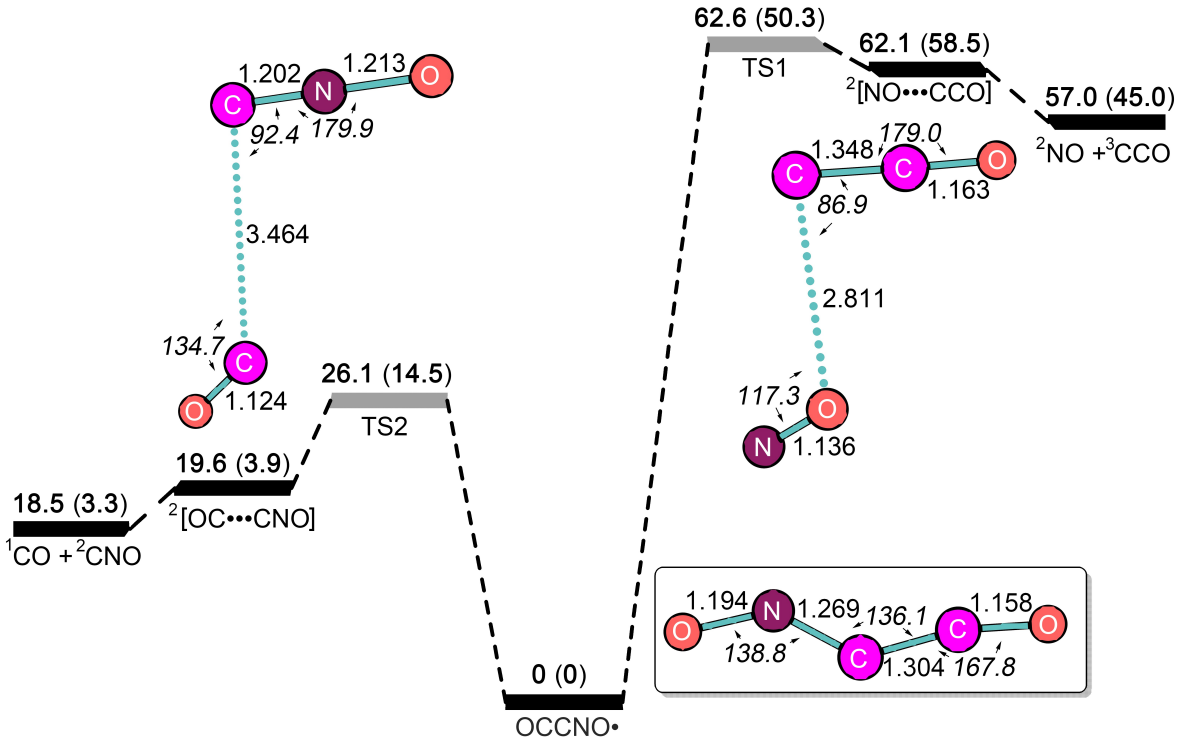

Figure S4. Calculated energy profile (ΔG^0, kcal mol^{-1}) for the decomposition of OCCNO at the B3LYP/6-311+G(3df) and CCSD(T)/cc-pVTZ//B3LYP/6-311+G(3df) (in parentheses) levels. Zero-point vibrational energy (ZPVE) corrections have been included. The structural parameters (bond lengths in Å, angles in degrees in italics) calculated at the B3LYP/6-311+G(3df) level are given. It should be noted that the UCCSD(T)/cc-pVTZ calculation suffers from spin contamination. The calculated T_1 diagnostics value of 0.054 indicates the strong multireference character of OCCNO•.

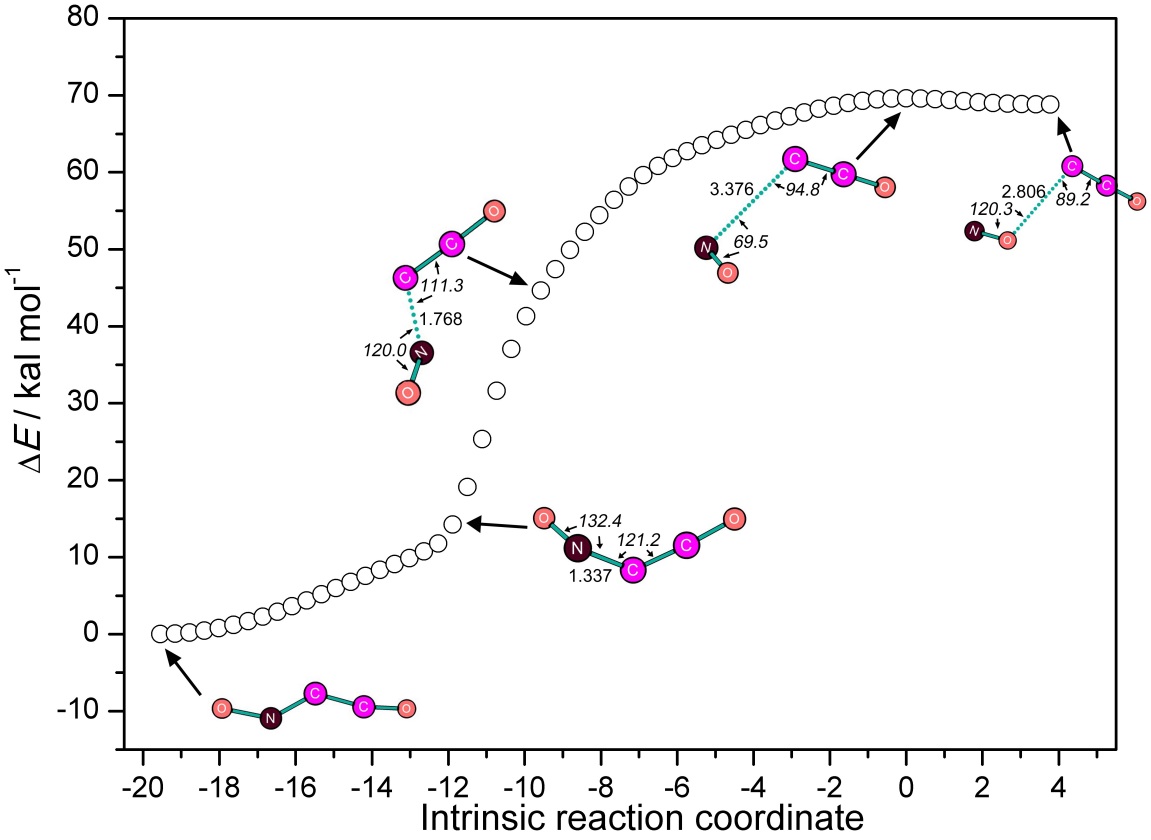

Figure S5. Calculated IRC for the decomposition of OCCNO• into OCC•••NO complex at the UB3LYP/6-311+G(3df) level. Molecular structures (bond lengths in Å, angles in degrees in italics) calculated at the UB3LYP/6-311+G(3df) level are depicted.

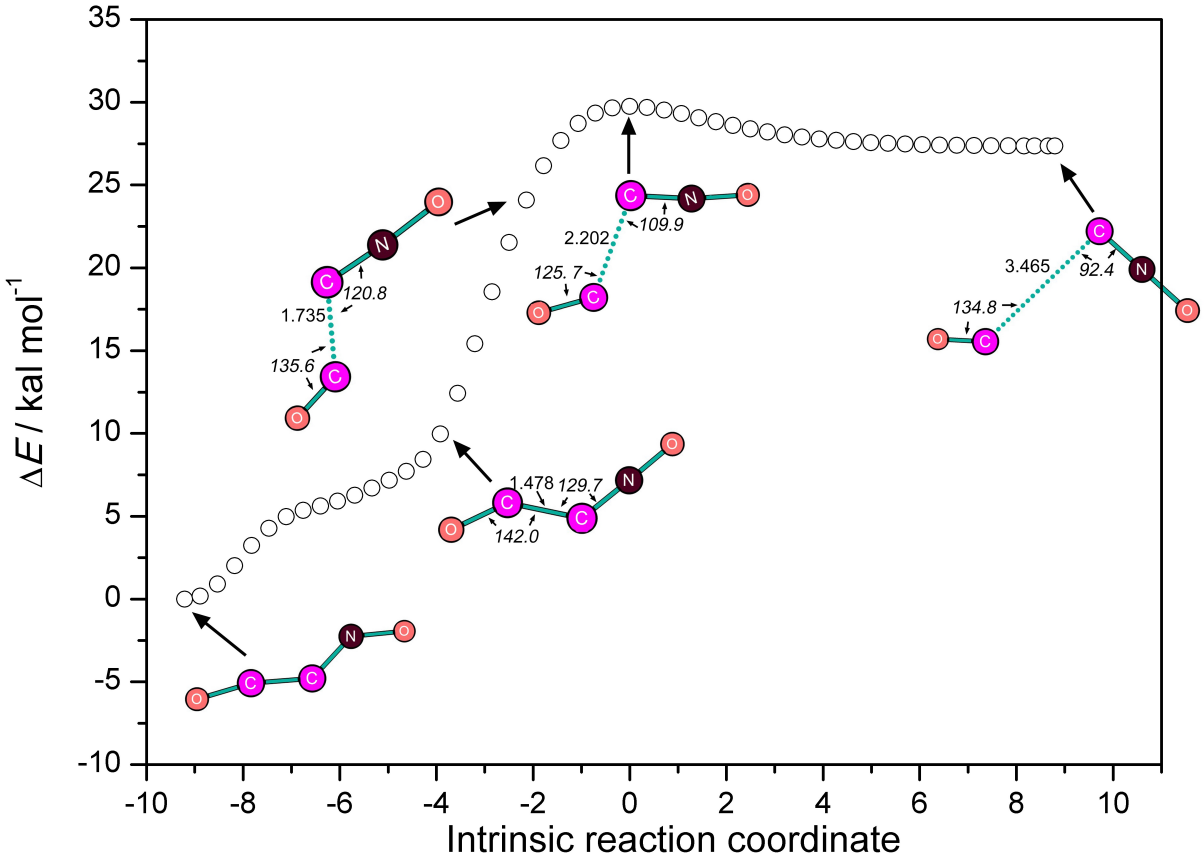

Figure S6. Calculated IRC for the decomposition of OCCNO• into ONC•••CO complex at the UB3LYP/6-311+G(3df) level. Molecular structures (bond lengths in Å, angles in degrees in italics) calculated at the UB3LYP/6-311+G(3df) level are depicted.

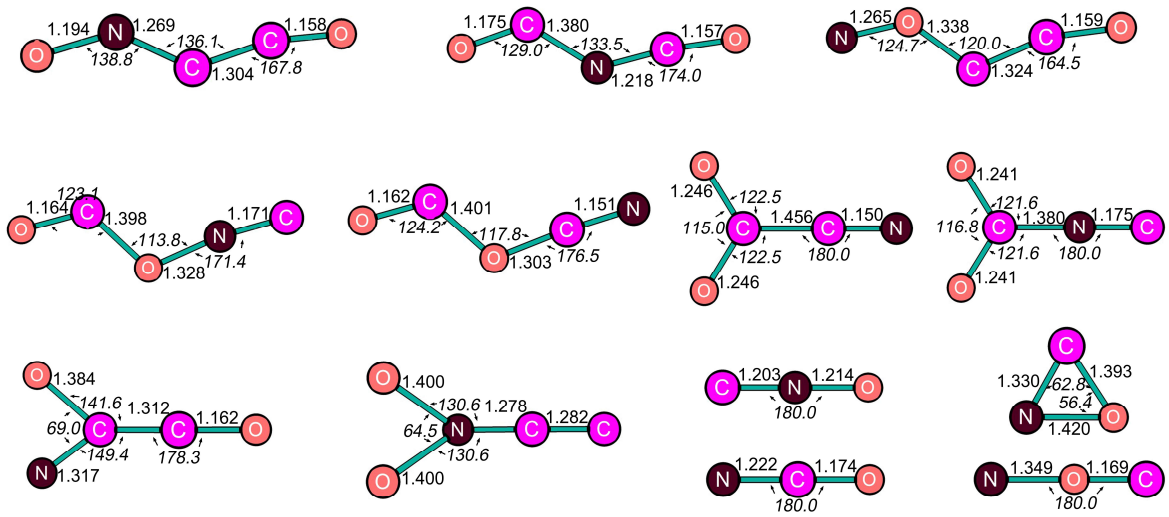

Figure S7. Isomers of OCCNO• and CNO•. Molecular structures (bond lengths in Å, angles in degrees in italics) are those computed at the UB3LYP/6-311+G(3df) level.

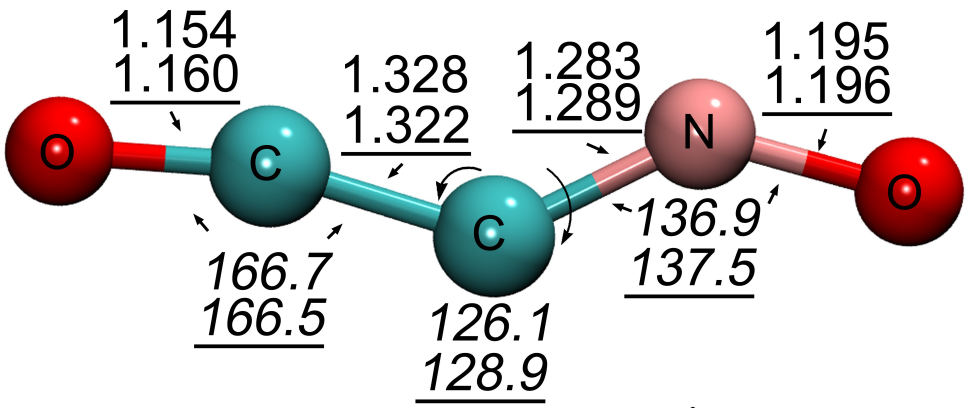

Figure S8. Calculated molecular structure (bond lengths in Å, angles in degrees in italics) of OCCNO• at the UCCSD(T)/aug-cc-pVQZ and ROCCSD(T)/aug-cc-pVQZ (underlined) level.

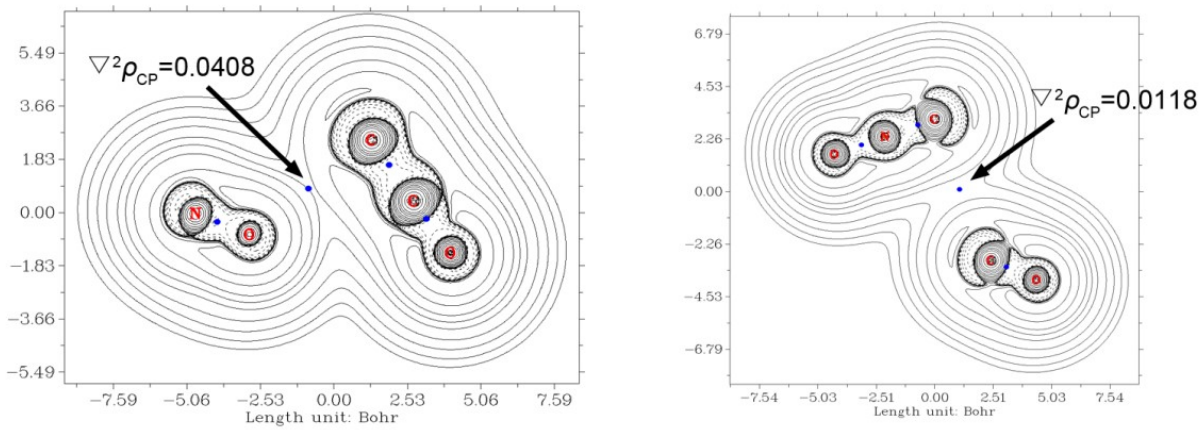

Figure S9. Calculated contour maps of Laplacian of OCC•••NO (left) and ONC•••CO (right) complexes. The bond critical points have been indicated by blue dots. According to Bader's AIM theory,[30] the negative and positive values of $\nabla^2\rho_{BCP}$ correspond to the covalent bond and closed-shell interactions (*i.e.*, H-bond, Van der Waals (vdW) interactions, and ionic bond), respectively. Therefore, the calculated positive Laplacian values for the bond critical points connecting the fragments in OCC•••NO (+0.0408) and ONC•••CO (+0.0118) indicate Van der Waals (vdW) interactions.

Table S1. Focal-point analysis (FPA) of the C-C bond dissociation energy of OCCNO• based on the restricted open-shell coupled-cluster formalism (in cm^{-1})[a]

	ΔE_e(HF)	δ[MP2]	δ[CCSD]	δ[CCSD(T)]	δ[CCSDT]	ΔE_e[CCSDT]
aug-cc-pwCVDZ	–6132.3	+17310.9	–8907.1	+2747.9	–146.2	+4873.2
aug-cc-pwCVTZ	–6545.0	+18572.4	–8878.0	+2971.9	[–146.2]	[+5975.1]
aug-cc-pwCVQZ	–6500.7	+18868.2	–8881.8	+3020.5	[–146.2]	[+6360.0]
aug-cc-pwCV5Z	–6517.1	+18959.7	–8892.7	+3032.9	[–146.2]	[+6436.6]
CBS	[–6520.0]	[+19055.7]	[–8904.1]	[+3046.3]	[–146.2]	**[+6531.7]**
extrapolation	$a + b(n+1)\exp(-9\sqrt{n})$ (n = 4, 5)	$a + b\,n^{-3}$ (n = 4, 5)	$a + b\,n^{-3}$ (n = 4, 5)	$a + b\,n^{-3}$ (n = 4, 5)		

ΔE_0(final) = ΔE_e[CCSDT/CBS] + Δ_{ZPVE}[UCCSD(T)(FC)/cc-pVTZ] =+6531.7 – 1010.2 = +**5522(650)** cm^{-1}

[a]The symbol δ denotes the increment in the relative energy (ΔE_e) with respect to the preceding level of theory in the hierarchy HF → MP2 → CCSD → CCSD(T) → CCSDT. Square brackets signify results obtained from basis set extrapolation so radditivity assumptions. Final predictions are bold faced.

Table S2. Focal-point analysis (FPA) of the C-C bond dissociation energy of OCCNO• based on the unrestricted open-shell coupled-cluster formalism (in cm^{-1})[a]

	ΔE_e(HF)	δ[MP2]	δ[CCSD]	δ[CCSD(T)]	δ[CCSDT]	ΔE_e[CCSDT]
aug-cc-pwCVDZ	–3975.3	+6611.9	–591.0	+2061.4	+732.6	+4839.7
aug-cc-pwCVTZ	–7156.3	+15884.2	–5776.0	+2928.4	–	+5880.3
aug-cc-pwCVQZ	–7107.9	+16246.1	–5843.9	+2981.9	–	+6276.4
aug-cc-pwCV5Z	–7123.0	+16354.8	–5871.6	+2996.5	–	+6356.7
CBS	[–7125.6]	[+16468.9]	[–5900.8]	[+3011.9]	–	**[+6454.3]**
extrapolation	$a + b(n+1)\exp(-9\sqrt{n})$ (n = 4, 5)	$a + b\,n^{-3}$ (n = 4, 5)				

ΔE_0(final) = ΔE_e[CCSDT/CBS] + Δ_{ZPVE}[UCCSD(T)(FC)/cc-pVTZ] =+6454.3 – 1010.2 = +**5444(650)** cm^{-1}

[a]See footnote [a] in Table S1.

Table S3. Focal-point analysis (FPA) of the C-N bond dissociation energy of OCCNO• based on the restricted open-shell coupled-cluster formalism (in cm^{-1})[a]

	ΔE_e(HF)	δ[MP2]	δ[CCSD]	δ[CCSD(T)]	δ[CCSDT]	ΔE_e[CCSDT]
aug-cc-pwCVDZ	+4694.5	19506.2	–7527.6	+3184.6	–204.6	+19653.1
aug-cc-pwCVTZ	+5204.7	+21003.6	–7741.2	+3435.5	[–204.6]	[+21698.0]
aug-cc-pwCVQZ	+5267.1	+21539.7	–7774.5	+3489.0	[–204.6]	[+22316.7]
aug-cc-pwCV5Z	+5253.6	+21714.4	–7809.1	+3504.6	[–204.6]	[+22458.9]
CBS	[+5251.3]	[+21897.7]	[–7845.3]	[+3520.9]	[–204.6]	**[+22619.9]**
extrapolation	$a + b(n+1)\exp(-9\sqrt{n})$ (n = 4, 5)	$a + b\,n^{-3}$ (n = 4, 5)	$a + b\,n^{-3}$ (n = 4, 5)	$a + b\,n^{-3}$ (n = 4, 5)		

ΔE_0(final) = ΔE_e[CCSDT/CBS] + Δ_{ZPVE}[UCCSD(T)(FC)/cc-pVTZ] =+22619.9 – 1244.6 = +**21375(700)** cm^{-1}

[a]See footnote [a] in Table S1.

Table S4. Focal-point analysis (FPA) of the C-N bond dissociation energy of OCCNO• based on the unrestricted open-shell coupled-cluster formalism (in cm^{-1})[a]

	ΔE_e(HF)	δ[MP2]	δ[CCSD]	δ[CCSD(T)]	δ[CCSDT]	ΔE_e[CCSDT]
aug-cc-pwCVDZ	+5615.7	+11375.4	–635.5	+2706.0	+557.5	+19619.1
aug-cc-pwCVTZ	+3286.8	+21089.1	–6199.8	+3559.4	–	+21735.5
aug-cc-pwCVQZ	+3344.5	+21787.1	–6383.7	+3616.8	–	+22366.7
aug-cc-pwCV5Z	+3330.1	+22012.1	[–6465.7]	+3636.2	–	+22512.7
CBS	[+3327.6]	[+22248.2]	[–6551.7]	[+3654.5]	–	**[+22678.5]**
extrapolation	$a + b(n+1)\exp(-9\sqrt{n})$ (n = 4, 5)	$a + b\,n^{-3}$ (n = 4, 5)				

ΔE_0(final) = ΔE_e[CCSDT/CBS] + Δ_{ZPVE}[UCCSD(T)(FC)/cc-pVTZ] =+22678.5 – 1244.6 = +**21434(700)** cm^{-1}

[a]See footnote [a] in Table S1.

Table S5. Vibrational fundamentals (in cm^{-1}) of OCCNO• computed at the CCSD(T)-F12/cc-pVTZ-F12 level.

ν_{harm}	ν_{anharm}[a]
2162	2140
1853	2080
1475	1038
937	930
586	554
550	571
520	506
172	180
169	153

[a] The anharmonic frequencies were calculated with the VPT2 method.

Table S6. Vibrational fundamentals (cm^{-1}) and the corresponding IR intensities (km mol^{-1}, in parentheses) of different isomers of OCCNO•.

OCNCO•			OCOCN•			O_2CNC•			O_2CCN•		
B3LYP[a]	BP86[a]	M06-2X[a]	B3LYP[a]	BP86[a]	M06-2X[a]	B3LYP[a]	BP86[a]	M06-2X[a]	B3LYP[a]	BP86[a]	M06-2X[a]
ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}
2338 (105)	2274 (963)	2377 (1326)	2374 (105)	2268 (69)	2456 (122)	2170 (530)	2211 (684)	2211 (584)	2353 (66)	1244 (81)	2427 (58)
1890 (734)	1822 (630)	1964 (840)	1938 (326)	1865 (286)	2014 (366)	1492 (241)	1573 (313)	1573 (313)	1517 (151)	1437 (80)	1602 (204)
1460 (43)	1401 (18)	1489 (84)	1102 (141)	1049 (92)	1149 (186)	1123 (126)	884 (66)	884 (66)	1067 (166)	1332 (< 1)	837 (43)
890 (74)	853 (53)	913 (92)	886 (217)	813 (189)	959 (215)	869 (53)	767 (366)	767 (366)	825 (33)	795 (17)	699 (27)
662 (23)	587 (17)	651 (24)	545 (10)	501 (12)	585 (4)	734 (38)	730 (45)	730 (45)	713 (21)	697 (13)	642 (115)
621 (21)	573 (13)	647 (27)	524 (1)	496 (4)	545 (1)	533 (10)	533 (9)	533 (9)	588 (17)	567 (4)	528 (5)
543 (9)	520 (10)	550 (8)	503 (5)	481 (3)	529 (7)	518 (6)	411 (290)	411 (290)	512 (3)	478 (1)	404 (796)
166 (3)	166 (2)	157 (4)	190 (8)	179 (7)	198 (9)	163 (5)	174 (4)	174 (4)	263 (22)	250 (19)	270 (24)
114 (2)	114 (2)	115 (3)	159 (8)	153 (6)	169 (9)	144 (1)	143 (3)	143 (3)	191 (5)	179 (7)	154 (55)

[a] The 6-311+G(3df) basis set has been utilized for all these computations.

Table S6. Continued.

OCC(O)N•			O_2NCC•			OCONC•			OCCON•		
B3LYP[a]	BP86[a]	M06-2X[a]	B3LYP[a]	BP86[a]	M06-2X[a]	B3LYP[a]	BP86[a]	M06-2X[a]	B3LYP[a]	BP86[a]	M06-2X[a]
ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}
2215 (850)	2044 (535)	2273 (1065)	1900 (379)	1855 (364)	1994 (254)	2201 (64)	2087 (59)	2286 (64)	2131 (1017)	2070 (905)	2188 (1029)
1567 (10)	1429 (6)	1620 (17)	1189 (20)	1243 (83)	1404 (58)	1930 (258)	1853 (221)	2007 (296)	1359 (12)	1296 (4)	1428 (1)
1072 (62)	998 (19)	1093 (84)	1145 (408)	940 (23)	1058 (11)	986 (58)	912 (14)	1066 (124)	1156 (18)	1264 (174)	1175 (21)
854 (39)	788 (6)	875 (86)	815 (25)	658 (74)	838 (17)	906 (235)	834 (252)	974 (198)	875 (40)	827 (5)	907 (67)
644 (8)	613 (2)	651 (8)	554 (4)	591 (25)	753 (50)	536 (4)	501 (5)	573 (2)	585 (15)	562 (9)	602 (20)
329 (93)	288 (21)	388 (188)	489 (<1)	420 (3)	552 (3)	403 (10)	380 (11)	444 (8)	539 (12)	546 (7)	536 (14)
302 (16)	238 (12)	355 (12)	364 (21)	413 (8)	411 (30)	306 (1)	305 (1)	353 (1)	422 (1)	428 (3)	439 (1)
214 (11)	197 (11)	212 (10)	190 (12)	153 (4)	198 (15)	166 (4)	162 (3)	186 (6)	179 (4)	189 (3)	178 (7)
116 (<1)	126 (1)	116 (< 1)	144 (19)	134 (17)	183 (4)	142 (2)	140 (1)	170 (2)	169 (3)	180 (5)	167 (2)

[a] The 6-311+G(3df) basis set has been utilized for all these computations. For the structures of the molecules, see Figure S7.

Table S7. Computed harmonic and observed anharmonic fundamentals of CNO•.

calculated		observed[c]			isotope shifts				assignment[f]
UBP86[a]	MRCI-F12[b]	matrix			$\Delta\nu(C^{14/15}NO•)$		$\Delta\nu(^{13/12}CNO•)$		
ν_{harm}	ν_{harm}	N_2	Ne	Ar	calc[d]	obs[e]	calc[d]	obs[e]	
1844 (< 1)	1918				39.2		20.7		ν_{asym}(CNO)
1172 (61)	1185	1176.5	1171.2	1167.3	1.5	2.5	19.9	17.7	ν_{sym}(CNO)
404 (< 1)/243 (17)	349/349				9.3/5.5		3.1/1.8		δ(CNO)

[a] Computed harmonic frequencies (cm^{-1}) and IR intensities (km mol^{-1}) utilizing the 6-311+G(3df) basis set. A scaling factor of 0.966 was used for calibrating the wavenumbers of the fundamentals. [b] Computed harmonic frequencies (cm^{-1}) using the cc-pVQZ-F12 basis set.[32] [c] Observed band position for the most intense matrix site in different matrices. [d] Calculated isotope shifts at the UBP86/6-311+G(3df) level. [e] Observed isotope shifts in N_2-matrix. [f] Assignment based on the calculated vibrational displacement vectors for CNO• at the UBP86/6-311+G(3df) level.

Table S8. Vibrational fundamentals (cm^{-1}) and the corresponding IR intensities (km mol^{-1}, in parentheses) of different isomers of CNO•.

cyclic-OCN•			NOC•			NCO•		
B3LYP[a]	BP86[a]	M06-2X[a]	B3LYP[a]	BP86[a]	M06-2X[a]	B3LYP[a]	BP86[a]	M06-2X[a]
ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}	ν_{harm}
1479 (58)	1411 (49)	1547 (66)	1720 (22)	1527 (21)	1915 (2)	1994 (75)	1595 (56)	2063 (136)
952 (17)	926 (13)	1041 (20)	595 (45)	820 (44)	405 (30)	1298 (8)	1247 (10)	1334 (6)
573 (2)	567 (11)	639 (2)	402 (< 1)	427 (0)	389 (< 1)	597 (14)	568 (9)	623 (18)
			292 (2)	321 (2)	288 (2)	512 (37)	475 (32)	550 (38)

[a] Calculated with the 6-311+G(3df) basis set.

Table S9. Vibrational fundamentals of OCCNO• computed with different electronic-structure methods.

B3LYP		UCCSD(T)[a]		UCCSD(T)	B3LYP		B3LYP		B3LYP	
6-311+G(3df)		cc-pVDZ		cc-pVTZ	cc-pVTZ		Def2-TZVP		Def2-QZVP	
ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}
2208 (1212)	2161 (1026)	2201 (1042)	2154	2276 (1975)	2207 (1124)	2159 (947)	2204 (1160)	2156 (982)	2201 (1193)	2154 (1010)
1807 (636)	1769 (598)	1747 (929)	1709	1958 (521)	1808 (576)	1771 (543)	1805 (616)	1768 (579)	1802 (634)	1763 (604)
1504 (134)	1479 (120)	1459 (5)	1434	1568 (135)	1502 (121)	1477 (108)	1502 (126)	1477 (112)	1501 (132)	1475 (117)
908 (14)	868 (12)	930 (66)	890	924 (54)	906 (14)	864 (12)	909 (14)	870 (12)	908 (14)	868 (13)
595 (13)	586 (12)	611 (12)	602	597 (29)	592 (14)	584 (12)	594 (14)	585 (12)	593 (13)	591 (12)
517 (16)	507 (15)	576 (18)	566	570 (15)	517 (16)	507 (16)	519 (17)	509 (16)	518 (16)	512 (21)
493 (1)	473 (1)	513 (5)	493	552 (0)	489 (1)	468 (1)	492 (1)	472 (1)	492 (1)	474 (2)
170 (1)	172 (1)	190 (7)	192	168 (5)	171 (1)	173 (1)	171 (1)	173 (1)	171 (1)	175 (1)
163 (4)	167 (4)	144 (5)	148	155 (3)	163 (4)	167 (4)	162 (4)	167 (4)	162 (4)	157 (4)

[a] Calculated harmonic IR frequencies and corrected anharmonic contributions by B3LYP method with corresponding basis set.

Table S10. Vibrational fundamentals of OCCNO• computed with different DFT techniques.

BP86 6-311+G(3df)		UCCSD(T)[a] cc-pVDZ		BP86 cc-pVTZ		BP86 Def2-TZVP		BP86 Def2-QZVP	
ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}[a]	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}
2141 (944)	2088 (785)	2201 (1042)	2148	2137 (872)	2085 (726)	2135 (905)	2084 (757)	2132 (928)	2085 (778)
1750 (409)	1718 (389)	1747 (929)	1715	1748 (367)	1716 (340)	1748 (395)	1717 (383)	1745 (405)	1713 (412)
1445 (129)	1422 (112)	1459 (5)	1436	1442 (118)	1418 (110)	1443 (123)	1421 (108)	1442 (127)	1419 (115)
882 (10)	833 (9)	930 (66)	881	879 (10)	826 (9)	883 (10)	831 (9)	881 (10)	834 (9)
563 (9)	557 (8)	611 (12)	605	560 (10)	550 (9)	562 (10)	554 (9)	560 (9)	560 (9)
501 (9)	492 (9)	576 (18)	567	501 (10)	491 (9)	502 (10)	493 (9)	502 (9)	493 (11)
462 (3)	444 (3)	513 (5)	495	457 (3)	436 (2)	460 (3)	440 (2)	460 (3)	447 (2)
175 (1)	178 (1)	190 (7)	187	176 (1)	177 (1)	176 (1)	179 (1)	176 (1)	181 (1)
159 (3)	172 (3)	144 (5)	157	159 (3)	152 (3)	159 (3)	172 (3)	158 (3)	159 (3)

[a] Calculated harmonic IR frequencies and corrected anharmonic contributions by BP86 method with corresponding basis set.

Table S11. Vibrational fundamentals (cm^{-1}) and the corresponding IR intensities (km mol^{-1}, in parentheses) of OCCNO• obtained with different DFT techniques.[a]

M062X		B3PW91		B2PLYP		PBE1PBE		wb97xd		TPSs	
ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}	ν_{harm}	ν_{anharm}
2257 (1365)	2220 (1169)	2230 (1199)	2183 (1028)	2204 (1160)	2157 (984)	2247 (1244)	2202 (1073)	2247 (1320)	2198 (1135)	2145 (960)	2093 (792)
1852 (1137)	1822 (1053)	1846 (651)	1809 (616)	1805 (616)	1767 (584)	1868 (734)	1830 (694)	1842 (933)	1805 (872)	1743 (463)	1695 (342)
1554 (54)	1533 (42)	1523 (115)	1499 (103)	1502 (126)	1477 (112)	1541 (100)	1516 (88)	1536 (70)	1510 (60)	1449 (119)	1426 (101)
932 (21)	898 (18)	913 (13)	869 (12)	909 (14)	869 (12)	923 (14)	882 (12)	930 (20)	889 (16)	888 (11)	845 (10)
620 (16)	608 (14)	599 (13)	588 (11)	594 (14)	585 (12)	606 (13)	595 (12)	613 (15)	602 (13)	573 (9)	564 (8)
538 (19)	525 (19)	516 (16)	505 (15)	519 (17)	509 (16)	521 (17)	510 (16)	535 (19)	523 (18)	511 (9)	502 (10)
505 (4)	488 (2)	491 (1)	468 (1)	492 (1)	471 (1)	498 (< 1)	475 (1)	505 (1)	483 (<1)	474 (3)	454 (2)
169 (6)	187 (6)	170 (1)	171 (1)	171 (1)	172 (1)	169 (2)	170 (1)	166 (2)	167 (2)	177 (1)	178 (1)
157 (2)	161 (2)	164 (4)	167 (4)	162 (4)	165 (4)	166 (5)	171 (4)	167 (5)	172 (5)	164 (3)	167 (3)

[a] All calculation were performed with 6-311+G(3df) basis set.

Table S12. Calculated topological and energy properties of the critical points[a] in the OCC•••ON and ONC•••CO complexes (all values in a.u.).

Complex	ρ_{CP}	$\nabla^2\rho_{CP}$	G_{BCP}	V_{BCP}	$-G_{BCP}/V_{BCP}$	H_{BCP}
ONC•••CO	0.0040	0.0118	0.0022	-0.0015	1.4667	0.0007
OCC•••ON	0.0109	0.0408	0.0085	-0.0068	1.2500	0.0017

[a] The critical points in the noncovalent areas.

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Calculated atomic coordinates (in Angstroms) and Energies (in Hatrees) for all optimized structures

OCCCO

BP86/6-311+G(3df)

O	0.00000000	0.00000000	2.45110900
C	0.00000000	0.00000000	1.27948600
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	-1.27948600
O	0.00000000	0.00000000	-2.45110900

Zero-point correction= 0.020800

Thermal correction to Energy= 0.025756

Thermal correction to Enthalpy= 0.026700

Thermal correction to Gibbs Free Energy= -0.005660

Sum of electronic and zero-point Energies= -264.813064

Sum of electronic and thermal Energies= -264.808108

Sum of electronic and thermal Enthalpies= -264.807164

Sum of electronic and thermal Free Energies= -264.839524

$OC^{13}CCO$

BP86/6-311+G(3df)

O	0.00000000	0.00000000	2.42980900
C	0.00000000	0.00000000	1.27129500
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	-1.27129500
O	0.00000000	0.00000000	-2.42980900

Zero-point correction= 0.021380

Thermal correction to Energy= 0.026273

Thermal correction to Enthalpy= 0.027217

Thermal correction to Gibbs Free Energy= -0.005421

Sum of electronic and zero-point Energies= -264.801940

Sum of electronic and thermal Energies= -264.797047

Sum of electronic and thermal Enthalpies= -264.796103

Sum of electronic and thermal Free Energies= -264.828742

OCC_triplet

BP86/6-311+G(3df)

C	0.00000000	0.00000000	-1.42847100
C	0.00000000	0.00000000	-0.05788200
O	0.00000000	0.00000000	1.11476500

Zero-point correction= 0.008392
Thermal correction to Energy= 0.011556
Thermal correction to Enthalpy= 0.012501
Thermal correction to Gibbs Free Energy= -0.014251
Sum of electronic and zero-point Energies= -151.307363
Sum of electronic and thermal Energies= -151.304198
Sum of electronic and thermal Enthalpies= -151.303254
Sum of electronic and thermal Free Energies= -151.330005

$OC^{13}C$_triplet

BP86/6-311+G(3df)

C	0.00000000	0.00000000	-1.41230200
C	0.00000000	0.00000000	-0.05765400
O	0.00000000	0.00000000	1.10246700

Zero-point correction= 0.008850
Thermal correction to Energy= 0.011886
Thermal correction to Enthalpy= 0.012830
Thermal correction to Gibbs Free Energy= -0.013731
Sum of electronic and zero-point Energies= -151.306797
Sum of electronic and thermal Energies= -151.303762
Sum of electronic and thermal Enthalpies= -151.302817
Sum of electronic and thermal Free Energies= -151.329378

OCC_singlet

BP86/6-311+G(3df)

C	0.00000000	0.00000000	-1.43012300
C	0.00000000	0.00000000	-0.06103400
O	0.00000000	0.00000000	1.11836800

Zero-point correction= 0.008439
Thermal correction to Energy= 0.011621
Thermal correction to Enthalpy= 0.012566

Thermal correction to Gibbs Free Energy= -0.013255
Sum of electronic and zero-point Energies= -151.266243
Sum of electronic and thermal Energies= -151.263061
Sum of electronic and thermal Enthalpies= -151.262117
Sum of electronic and thermal Free Energies= -151.287938

$OC^{13}C$_singlet
BP86/6-311+G(3df)

C	0.00000000	0.00000000	-1.41484200
C	0.00000000	0.00000000	-0.05930400
O	0.00000000	0.00000000	1.10561000

Zero-point correction= 0.008948
Thermal correction to Energy= 0.011971
Thermal correction to Enthalpy= 0.012915
Thermal correction to Gibbs Free Energy= -0.012607
Sum of electronic and zero-point Energies= -151.266869
Sum of electronic and thermal Energies= -151.263846
Sum of electronic and thermal Enthalpies= -151.262902
Sum of electronic and thermal Free Energies= -151.288424

OCCNO•
BP86/6-311+G(3df)

O	-2.31937100	0.16990400	0.00000000
C	0.00000000	0.34448400	0.00000000
C	1.24074700	-0.08208200	0.00000000
O	2.40774800	-0.20144700	0.00000000
N	-1.16449900	-0.18886600	0.00000000

Zero-point correction= 0.018406
Thermal correction to Energy= 0.023192
Thermal correction to Enthalpy= 0.024137
Thermal correction to Gibbs Free Energy= -0.009243
Sum of electronic and zero-point Energies= -281.374157
Sum of electronic and thermal Energies= -281.369371
Sum of electronic and thermal Enthalpies= -281.368427
Sum of electronic and thermal Free Energies= -281.401807

$OCC^{15}NO$

BP86/6-311+G(3df)

O	-2.31952300	0.17035600	0.00000000
C	0.00000000	0.34386400	0.00000000
C	1.24074400	-0.08249900	0.00000000
O	2.40804800	-0.20109600	0.00000000
N	-1.16466700	-0.18889500	0.00000000

Zero-point correction= 0.018273

Thermal correction to Energy= 0.023069

Thermal correction to Enthalpy= 0.024014

Thermal correction to Gibbs Free Energy= -0.009420

Sum of electronic and zero-point Energies= -281.374290

Sum of electronic and thermal Energies= -281.369494

Sum of electronic and thermal Enthalpies= -281.368549

Sum of electronic and thermal Free Energies= -281.401983

$OC^{13}CNO•$

BP86/6-311+G(3df)

O	-2.31952300	0.17035600	0.00000000
C	0.00000000	0.34386400	0.00000000
C	1.24074400	-0.08249900	0.00000000
O	2.40804800	-0.20109600	0.00000000
N	-1.16466700	-0.18889500	0.00000000

Zero-point correction= 0.018247

Thermal correction to Energy= 0.023044

Thermal correction to Enthalpy= 0.023988

Thermal correction to Gibbs Free Energy= -0.009456

Sum of electronic and zero-point Energies= -281.374316

Sum of electronic and thermal Energies= -281.369519

Sum of electronic and thermal Enthalpies= -281.368575

Sum of electronic and thermal Free Energies= -281.402019

CNO•

BP86/6-311+G(3df)

O	0.00000000	0.00000000	1.10352900
C	0.00000000	0.00000000	-1.33827100

N	0.00000000	0.00000000	-0.11408700

Zero-point correction= 0.008422
Thermal correction to Energy= 0.011587
Thermal correction to Enthalpy= 0.012531
Thermal correction to Gibbs Free Energy= -0.013876
Sum of electronic and zero-point Energies= -167.966472
Sum of electronic and thermal Energies= -167.963308
Sum of electronic and thermal Enthalpies= -167.962364
Sum of electronic and thermal Free Energies= -167.988771

^{13}CNO•

BP86/6-311+G(3df)

O	0.00000000	0.00000000	1.10352900
C	0.00000000	0.00000000	-1.33827100
N	0.00000000	0.00000000	-0.11408700

Zero-point correction= 0.008318
Thermal correction to Energy= 0.011490
Thermal correction to Enthalpy= 0.012434
Thermal correction to Gibbs Free Energy= -0.014059
Sum of electronic and zero-point Energies= -167.966576
Sum of electronic and thermal Energies= -167.963405
Sum of electronic and thermal Enthalpies= -167.962461
Sum of electronic and thermal Free Energies= -167.988954

C^{15}NO•

BP86/6-311+G(3df)

O	0.00000000	0.00000000	1.10352900
C	0.00000000	0.00000000	-1.33827100
N	0.00000000	0.00000000	-0.11408700

Zero-point correction= 0.008296
Thermal correction to Energy= 0.011477
Thermal correction to Enthalpy= 0.012421
Thermal correction to Gibbs Free Energy= -0.014054
Sum of electronic and zero-point Energies= -167.966599
Sum of electronic and thermal Energies= -167.963418

Sum of electronic and thermal Enthalpies= -167.962474
Sum of electronic and thermal Free Energies= -167.988949

NCO
BP86/6-311+G(3df)

N	0.00000000	0.00000000	-1.27461300
C	0.00000000	0.00000000	-0.04123200
O	0.00000000	0.00000000	1.14621000

Zero-point correction= 0.009686
Thermal correction to Energy= 0.012482
Thermal correction to Enthalpy= 0.013426
Thermal correction to Gibbs Free Energy= -0.012354
Sum of electronic and zero-point Energies= -168.061421
Sum of electronic and thermal Energies= -168.058625
Sum of electronic and thermal Enthalpies= -168.057681
Sum of electronic and thermal Free Energies= -168.083460

NOC
BP86/6-311+G(3df)

C	0.00000000	0.00000000	1.29530400
O	0.00000000	0.00000000	0.09263700
N	0.00000000	0.00000000	-1.21613200

Zero-point correction= 0.007057
Thermal correction to Energy= 0.010171
Thermal correction to Enthalpy= 0.011115
Thermal correction to Gibbs Free Energy= -0.015126
Sum of electronic and zero-point Energies= -167.880320
Sum of electronic and thermal Energies= -167.877206
Sum of electronic and thermal Enthalpies= -167.876261
Sum of electronic and thermal Free Energies= -167.902503

cyclic_CNO
BP86/6-311+G(3df)

O	0.00000000	0.78000700	0.00000000
C	0.72247100	-0.43764700	0.00000000

N -0.61926100 -0.51631000 0.00000000

Zero-point correction= 0.006617
Thermal correction to Energy= 0.009684
Thermal correction to Enthalpy= 0.010629
Thermal correction to Gibbs Free Energy= -0.017511
Sum of electronic and zero-point Energies= -167.938142
Sum of electronic and thermal Energies= -167.935074
Sum of electronic and thermal Enthalpies= -167.934130
Sum of electronic and thermal Free Energies= -167.962269

CO
BP86/6-311+G(3df)
O 0.00000000 0.00000000 0.48704000
C 0.00000000 0.00000000 -0.64938700

Zero-point correction= 0.004845
Thermal correction to Energy= 0.007206
Thermal correction to Enthalpy= 0.008150
Thermal correction to Gibbs Free Energy= -0.014291
Sum of electronic and zero-point Energies= -113.348566
Sum of electronic and thermal Energies= -113.346205
Sum of electronic and thermal Enthalpies= -113.345261
Sum of electronic and thermal Free Energies= -113.367702

NO•
BP86/6-311+G(3df)
O 0.00000000 0.00000000 0.54050400
N 0.00000000 0.00000000 -0.61771900

Zero-point correction= 0.004291
Thermal correction to Energy= 0.006653
Thermal correction to Enthalpy= 0.007597
Thermal correction to Gibbs Free Energy= -0.015714
Sum of electronic and zero-point Energies= -129.941037
Sum of electronic and thermal Energies= -129.938676
Sum of electronic and thermal Enthalpies= -129.937732
Sum of electronic and thermal Free Energies= -129.961042

OCNCO

BP86/6-311+G(3df)

O	-2.31075000	0.10845600	0.00000000
C	1.17832400	0.01341600	0.00000000
O	2.33007800	-0.19339800	0.00000000
N	0.00000000	0.36158800	0.00000000
C	-1.20409500	-0.32201300	0.00000000

Zero-point correction= 0.018937

Thermal correction to Energy= 0.023718

Thermal correction to Enthalpy= 0.024662

Thermal correction to Gibbs Free Energy= -0.009056

Sum of electronic and zero-point Energies= -281.451407

Sum of electronic and thermal Energies= -281.446627

Sum of electronic and thermal Enthalpies= -281.445682

Sum of electronic and thermal Free Energies= -281.479401

OCCON

BP86/6-311+G(3df)

C	1.16473700	-0.09549900	0.00000000
O	2.31100500	-0.34054800	0.00000000
N	-2.33213300	0.19175800	0.00000000
C	0.00000000	0.55138300	0.00000000
O	-1.14394100	-0.16915300	0.00000000

Zero-point correction= 0.016783

Thermal correction to Energy= 0.021536

Thermal correction to Enthalpy= 0.022480

Thermal correction to Gibbs Free Energy= -0.011034

Sum of electronic and zero-point Energies= -281.275604

Sum of electronic and thermal Energies= -281.270850

Sum of electronic and thermal Enthalpies= -281.269906

Sum of electronic and thermal Free Energies= -281.303420

OCONC

BP86/6-311+G(3df)

C	-0.99949300	-0.43379600	0.00000000

O	-2.14796300	-0.18123200	0.00000000
O	0.00000000	0.57070100	0.00000000
N	1.24962000	0.08443500	0.00000000
C	2.40555500	-0.18400500	0.00000000

Zero-point correction= 0.016354
Thermal correction to Energy= 0.021555
Thermal correction to Enthalpy= 0.022499
Thermal correction to Gibbs Free Energy= -0.012069
Sum of electronic and zero-point Energies= -281.303512
Sum of electronic and thermal Energies= -281.298312
Sum of electronic and thermal Enthalpies= -281.297368
Sum of electronic and thermal Free Energies= -281.331936

OCOCN
BP86/6-311+G(3df)

C	-1.05272600	-0.41095900	0.00000000
O	-2.19022900	-0.12496400	0.00000000
C	1.23021200	0.10110900	0.00000000
O	0.00000000	0.54988200	0.00000000
N	2.35098700	-0.22003500	0.00000000

Zero-point correction= 0.017792
Thermal correction to Energy= 0.022650
Thermal correction to Enthalpy= 0.023594
Thermal correction to Gibbs Free Energy= -0.010313
Sum of electronic and zero-point Energies= -281.390128
Sum of electronic and thermal Energies= -281.385271
Sum of electronic and thermal Enthalpies= -281.384327
Sum of electronic and thermal Free Energies= -281.418234

O_2CCN
BP86/6-311+G(3df)

O	-1.13621900	1.06737800	0.00000900
C	-0.46934300	-0.00004800	-0.00015800
C	0.98827600	-0.00008000	0.00006000
O	-1.13646300	-1.06724900	0.00001400
N	2.15255100	-0.00003800	0.00005800

Zero-point correction= 0.018187
Thermal correction to Energy= 0.022728
Thermal correction to Enthalpy= 0.023672
Thermal correction to Gibbs Free Energy= -0.009982
Sum of electronic and zero-point Energies= -281.408722
Sum of electronic and thermal Energies= -281.404181
Sum of electronic and thermal Enthalpies= -281.403237
Sum of electronic and thermal Free Energies= -281.436890

O_2CNC
BP86/6-311+G(3df)

O	-1.07216600	1.04296600	0.00002900
C	-0.41279900	-0.00003300	-0.00019000
O	-1.07224200	-1.04291300	0.00003400
C	2.14089600	-0.00000600	0.00005900
N	0.96952600	-0.00002600	0.00004000

Zero-point correction= 0.016929
Thermal correction to Energy= 0.021767
Thermal correction to Enthalpy= 0.022711
Thermal correction to Gibbs Free Energy= -0.011512
Sum of electronic and zero-point Energies= -281.259494
Sum of electronic and thermal Energies= -281.254656
Sum of electronic and thermal Enthalpies= -281.253712
Sum of electronic and thermal Free Energies= -281.287935

OCC(O)N
BP86/6-311+G(3df)

O	-2.18362400	-0.03159300	-0.02051900
C	0.33960200	0.07617100	-0.03246500
O	1.44117600	-0.82616700	0.00127400
N	1.40349800	0.90476700	0.00223000
C	-0.98708500	0.01194600	0.05552400

Zero-point correction= 0.015321
Thermal correction to Energy= 0.020620
Thermal correction to Enthalpy= 0.021564

Thermal correction to Gibbs Free Energy= -0.013612
Sum of electronic and zero-point Energies= -281.196878
Sum of electronic and thermal Energies= -281.191579
Sum of electronic and thermal Enthalpies= -281.190635
Sum of electronic and thermal Free Energies= -281.225811

O_2NCC
BP86/6-311+G(3df)

O	-1.24876300	-0.75939800	-0.10614400
C	1.09680500	-0.00099200	-0.00079700
C	2.38829100	0.00050500	-0.12450900
N	-0.13392300	-0.00031500	0.34970200
O	-1.24787600	0.76003900	-0.10586600

Zero-point correction= 0.014605
Thermal correction to Energy= 0.019688
Thermal correction to Enthalpy= 0.020632
Thermal correction to Gibbs Free Energy= -0.013954
Sum of electronic and zero-point Energies= -281.097777
Sum of electronic and thermal Energies= -281.092694
Sum of electronic and thermal Enthalpies= -281.091750
Sum of electronic and thermal Free Energies= -281.126337

TS1
BP86/6-311+G(3df)

O	2.28268400	-0.57870400	-0.00003600
C	-0.44391900	0.29531100	-0.00031500
C	-1.77707400	0.06723600	-0.00005300
O	-2.94290700	-0.12379600	0.00016500
N	2.65824800	0.49210200	0.00016800

Zero-point correction= 0.013642
Thermal correction to Energy= 0.019423
Thermal correction to Enthalpy= 0.020367
Thermal correction to Gibbs Free Energy= -0.017865
Sum of electronic and zero-point Energies= -281.253814
Sum of electronic and thermal Energies= -281.248032
Sum of electronic and thermal Enthalpies= -281.247088

Sum of electronic and thermal Free Energies= -281.285320

OCCCO

B3LYP/6-311+G(3df)

O	0.00000000	0.00000000	2.42980900
C	0.00000000	0.00000000	1.27129500
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	-1.27129500
O	0.00000000	0.00000000	-2.42980900

Zero-point correction= 0.021549

Thermal correction to Energy= 0.026432

Thermal correction to Enthalpy= 0.027377

Thermal correction to Gibbs Free Energy= -0.005186

Sum of electronic and zero-point Energies= -264.801771

Sum of electronic and thermal Energies= -264.796888

Sum of electronic and thermal Enthalpies= -264.795944

Sum of electronic and thermal Free Energies= -264.828506

OC^{13}CCO

B3LYP/6-311+G(3df)

O	0.00000000	0.00000000	2.42980900
C	0.00000000	0.00000000	1.27129500
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	-1.27129500
O	0.00000000	0.00000000	-2.42980900

Zero-point correction= 0.021380

Thermal correction to Energy= 0.026273

Thermal correction to Enthalpy= 0.027217

Thermal correction to Gibbs Free Energy= -0.005421

Sum of electronic and zero-point Energies= -264.801940

Sum of electronic and thermal Energies= -264.797047

Sum of electronic and thermal Enthalpies= -264.796103

Sum of electronic and thermal Free Energies= -264.828742

OCC_triplet

B3LYP/6-311+G(3df)

C	0.00000000	0.00000000	-1.41230200
C	0.00000000	0.00000000	-0.05765400
O	0.00000000	0.00000000	1.10246700

Zero-point correction= 0.008931
Thermal correction to Energy= 0.011960
Thermal correction to Enthalpy= 0.012904
Thermal correction to Gibbs Free Energy= -0.013568
Sum of electronic and zero-point Energies= -151.306716
Sum of electronic and thermal Energies= -151.303688
Sum of electronic and thermal Enthalpies= -151.302743
Sum of electronic and thermal Free Energies= -151.329216

OCC_singlet
B3LYP/6-311+G(3df)

C	0.00000000	0.00000000	-1.41484200
C	0.00000000	0.00000000	-0.05930400
O	0.00000000	0.00000000	1.10561000

Zero-point correction= 0.009031
Thermal correction to Energy= 0.012046
Thermal correction to Enthalpy= 0.012990
Thermal correction to Gibbs Free Energy= -0.012444
Sum of electronic and zero-point Energies= -151.266786
Sum of electronic and thermal Energies= -151.263770
Sum of electronic and thermal Enthalpies= -151.262826
Sum of electronic and thermal Free Energies= -151.288260

$OC^{13}C$_triplet
B3LYP/6-311+G(3df)

C	0.00000000	0.00000000	-1.41230200
C	0.00000000	0.00000000	-0.05765400
O	0.00000000	0.00000000	1.10246700

Zero-point correction= 0.008850
Thermal correction to Energy= 0.011886
Thermal correction to Enthalpy= 0.012830
Thermal correction to Gibbs Free Energy= -0.013731

Sum of electronic and zero-point Energies= -151.306797
Sum of electronic and thermal Energies= -151.303762
Sum of electronic and thermal Enthalpies= -151.302817
Sum of electronic and thermal Free Energies= -151.329378

$OC^{13}C$_singlet
B3LYP/6-311+G(3df)

C	0.00000000	0.00000000	-1.41484200
C	0.00000000	0.00000000	-0.05930400
O	0.00000000	0.00000000	1.10561000

Zero-point correction= 0.008948
Thermal correction to Energy= 0.011971
Thermal correction to Enthalpy= 0.012915
Thermal correction to Gibbs Free Energy= -0.012607
Sum of electronic and zero-point Energies= -151.266869
Sum of electronic and thermal Energies= -151.263846
Sum of electronic and thermal Enthalpies= -151.262902
Sum of electronic and thermal Free Energies= -151.288424

OCCNO•
B3LYP/6-311+G(3df)

O	-2.31937100	0.16990400	0.00000000
C	0.00000000	0.34448400	0.00000000
C	1.24074700	-0.08208200	0.00000000
O	2.40774800	-0.20144700	0.00000000
N	-1.16449900	-0.18886600	0.00000000

Zero-point correction= 0.018406
Thermal correction to Energy= 0.023192
Thermal correction to Enthalpy= 0.024137
Thermal correction to Gibbs Free Energy= -0.009243
Sum of electronic and zero-point Energies= -281.374157
Sum of electronic and thermal Energies= -281.369371
Sum of electronic and thermal Enthalpies= -281.368427
Sum of electronic and thermal Free Energies= -281.401807

$OC^{13}CNO$•

B3LYP/6-311+G(3df)

O	-2.29939500	0.15648300	0.00000000
C	0.00000000	0.35281800	0.00000000
C	1.23286400	-0.07298500	0.00000000
O	2.38335200	-0.20884800	0.00000000
N	-1.15269100	-0.18001200	0.00000000

Zero-point correction= 0.018896
Thermal correction to Energy= 0.023634
Thermal correction to Enthalpy= 0.024578
Thermal correction to Gibbs Free Energy= -0.008768
Sum of electronic and zero-point Energies= -281.348048
Sum of electronic and thermal Energies= -281.343310
Sum of electronic and thermal Enthalpies= -281.342366
Sum of electronic and thermal Free Energies= -281.375712

$OCC^{15}NO\bullet$

B3LYP/6-311+G(3df)

O	-2.29939500	0.15648300	0.00000000
C	0.00000000	0.35281800	0.00000000
C	1.23286400	-0.07298500	0.00000000
O	2.38335200	-0.20884800	0.00000000
N	-1.15269100	-0.18001200	0.00000000

Zero-point correction= 0.018920
Thermal correction to Energy= 0.023658
Thermal correction to Enthalpy= 0.024602
Thermal correction to Gibbs Free Energy= -0.008733
Sum of electronic and zero-point Energies= -281.348024
Sum of electronic and thermal Energies= -281.343286
Sum of electronic and thermal Enthalpies= -281.342341
Sum of electronic and thermal Free Energies= -281.375677

CNO•

B3LYP/6-311+G(3df)

O	0.00000000	0.00000000	1.10352900
C	0.00000000	0.00000000	-1.33827100
N	0.00000000	0.00000000	-0.11408700

Zero-point correction= 0.008422
Thermal correction to Energy= 0.011587
Thermal correction to Enthalpy= 0.012531
Thermal correction to Gibbs Free Energy= -0.013876
Sum of electronic and zero-point Energies= -167.966472
Sum of electronic and thermal Energies= -167.963308
Sum of electronic and thermal Enthalpies= -167.962364
Sum of electronic and thermal Free Energies= -167.988771

^{13}CNO•

B3LYP/6-311+G(3df)

O	0.00000000	0.00000000	1.09545500
C	0.00000000	0.00000000	-1.32174400
N	0.00000000	0.00000000	-0.11902500

Zero-point correction= 0.008764
Thermal correction to Energy= 0.011820
Thermal correction to Enthalpy= 0.012764
Thermal correction to Gibbs Free Energy= -0.013459
Sum of electronic and zero-point Energies= -167.957243
Sum of electronic and thermal Energies= -167.954187
Sum of electronic and thermal Enthalpies= -167.953242
Sum of electronic and thermal Free Energies= -167.979466

C^{15}NO•

B3LYP/6-311+G(3df)

O	0.00000000	0.00000000	1.09545500
C	0.00000000	0.00000000	-1.32174400
N	0.00000000	0.00000000	-0.11902500

Zero-point correction= 0.008743
Thermal correction to Energy= 0.011809
Thermal correction to Enthalpy= 0.012753
Thermal correction to Gibbs Free Energy= -0.013451
Sum of electronic and zero-point Energies= -167.957264
Sum of electronic and thermal Energies= -167.954197
Sum of electronic and thermal Enthalpies= -167.953253

Sum of electronic and thermal Free Energies= -167.979458

NOC

B3LYP/6-311+G(3df)

C	0.00000000	0.00000000	1.28474100
O	0.00000000	0.00000000	0.11565500
N	0.00000000	0.00000000	-1.23338400

Zero-point correction= 0.006860

Thermal correction to Energy= 0.010121

Thermal correction to Enthalpy= 0.011065

Thermal correction to Gibbs Free Energy= -0.015425

Sum of electronic and zero-point Energies= -167.868278

Sum of electronic and thermal Energies= -167.865016

Sum of electronic and thermal Enthalpies= -167.864072

Sum of electronic and thermal Free Energies= -167.890562

NCO

B3LYP /6-311+G(3df)

N	0.00000000	0.00000000	-1.26172700
C	0.00000000	0.00000000	-0.04015700
O	0.00000000	0.00000000	1.13413000

Zero-point correction= 0.010032

Thermal correction to Energy= 0.012780

Thermal correction to Enthalpy= 0.013724

Thermal correction to Gibbs Free Energy= -0.011962

Sum of electronic and zero-point Energies= -168.056530

Sum of electronic and thermal Energies= -168.053781

Sum of electronic and thermal Enthalpies= -168.052837

Sum of electronic and thermal Free Energies= -168.078524

cyclic_CNO

B3LYP /6-311+G(3df)

O	0.00000000	0.76873900	0.00000000
C	0.71443000	-0.42675600	0.00000000
N	-0.61236900	-0.51276800	0.00000000

Zero-point correction= 0.006846
Thermal correction to Energy= 0.009904
Thermal correction to Enthalpy= 0.010848
Thermal correction to Gibbs Free Energy= -0.017241
Sum of electronic and zero-point Energies= -167.927123
Sum of electronic and thermal Energies= -167.924066
Sum of electronic and thermal Enthalpies= -167.923122
Sum of electronic and thermal Free Energies= -167.951211

CO
B3LYP/6-311+G(3df)

C	0.00000000	0.00000000	-0.64253800
O	0.00000000	0.00000000	0.48190400

Zero-point correction= 0.005051
Thermal correction to Energy= 0.007411
Thermal correction to Enthalpy= 0.008355
Thermal correction to Gibbs Free Energy= -0.014065
Sum of electronic and zero-point Energies= -113.351742
Sum of electronic and thermal Energies= -113.349382
Sum of electronic and thermal Enthalpies= -113.348437
Sum of electronic and thermal Free Energies= -113.370858

NO•
B3LYP/6-311+G(3df)

O	0.00000000	0.00000000	0.53416400
N	0.00000000	0.00000000	-0.61047300

Zero-point correction= 0.004509
Thermal correction to Energy= 0.006870
Thermal correction to Enthalpy= 0.007814
Thermal correction to Gibbs Free Energy= -0.015473
Sum of electronic and zero-point Energies= -129.935394
Sum of electronic and thermal Energies= -129.933032
Sum of electronic and thermal Enthalpies= -129.932088
Sum of electronic and thermal Free Energies= -129.955376

OCNCO

B3LYP /6-311+G(3df)

O	-2.29094500	0.08472000	0.00000000
C	1.16924300	0.02675000	0.00000000
O	2.30761700	-0.17800100	0.00000000
N	0.00000000	0.36644800	0.00000000
C	-1.19147400	-0.32989800	0.00000000

Zero-point correction= 0.019700
Thermal correction to Energy= 0.024408
Thermal correction to Enthalpy= 0.025352
Thermal correction to Gibbs Free Energy= -0.008248
Sum of electronic and zero-point Energies= -281.438372
Sum of electronic and thermal Energies= -281.433664
Sum of electronic and thermal Enthalpies= -281.432720
Sum of electronic and thermal Free Energies= -281.466320

OCCON

B3LYP /6-311+G(3df)

C	1.15972900	-0.12936300	0.00000000
O	2.28677100	-0.39774300	0.00000000
N	-2.29897400	0.33606100	0.00000000
C	0.00000000	0.50980100	0.00000000
O	-1.14496500	-0.18163900	0.00000000

Zero-point correction= 0.016905
Thermal correction to Energy= 0.021681
Thermal correction to Enthalpy= 0.022625
Thermal correction to Gibbs Free Energy= -0.010954
Sum of electronic and zero-point Energies= -281.253162
Sum of electronic and thermal Energies= -281.248386
Sum of electronic and thermal Enthalpies= -281.247441
Sum of electronic and thermal Free Energies= -281.281021

OCONC

B3LYP /6-311+G(3df)

C	-0.98851300	-0.42481000	0.00000000
O	-2.12730900	-0.18462900	0.00000000
O	0.00000000	0.56316400	0.00000000

N	1.23810600	0.08154700	0.00000000
C	2.38046800	-0.17504200	0.00000000

Zero-point correction= 0.017272
Thermal correction to Energy= 0.022384
Thermal correction to Enthalpy= 0.023329
Thermal correction to Gibbs Free Energy= -0.011051
Sum of electronic and zero-point Energies= -281.290848
Sum of electronic and thermal Energies= -281.285735
Sum of electronic and thermal Enthalpies= -281.284791
Sum of electronic and thermal Free Energies= -281.319170

OCOCN
B3LYP /6-311+G(3df)

C	-1.04144200	-0.39198600	0.00000000
O	-2.16968300	-0.11516300	0.00000000
C	1.22250500	0.09473100	0.00000000
O	0.00000000	0.54569200	0.00000000
N	2.32444100	-0.23724400	0.00000000

Zero-point correction= 0.018740
Thermal correction to Energy= 0.023478
Thermal correction to Enthalpy= 0.024422
Thermal correction to Gibbs Free Energy= -0.009230
Sum of electronic and zero-point Energies= -281.380058
Sum of electronic and thermal Energies= -281.375320
Sum of electronic and thermal Enthalpies= -281.374376
Sum of electronic and thermal Free Energies= -281.408028

O_2CCN
B3LYP /6-311+G(3df)

O	1.13315000	1.05132800	0.00001300
C	0.46467600	-0.00014300	0.00011200
C	-0.99078300	-0.00046600	-0.00011500
O	1.13423100	-1.05077300	0.00000800
N	-2.14034300	-0.00011200	-0.00002100

Zero-point correction= 0.018300

Thermal correction to Energy= 0.022769
Thermal correction to Enthalpy= 0.023713
Thermal correction to Gibbs Free Energy= -0.009759
Sum of electronic and zero-point Energies= -281.392825
Sum of electronic and thermal Energies= -281.388357
Sum of electronic and thermal Enthalpies= -281.387413
Sum of electronic and thermal Free Energies= -281.420885

O_2CNC
B3LYP /6-311+G(3df)

O	1.06696400	1.05760000	0.00004100
C	0.41694000	-0.00003500	0.00001500
O	1.06706900	-1.05753000	0.00003600
C	-2.13825300	-0.00000700	0.00000700
N	-0.96348400	-0.00004300	-0.00010700

Zero-point correction= 0.017653
Thermal correction to Energy= 0.022359
Thermal correction to Enthalpy= 0.023303
Thermal correction to Gibbs Free Energy= -0.010759
Sum of electronic and zero-point Energies= -281.373168
Sum of electronic and thermal Energies= -281.368462
Sum of electronic and thermal Enthalpies= -281.367518
Sum of electronic and thermal Free Energies= -281.401581

OCC(O)N
B3LYP /6-311+G(3df)

O	2.15880700	-0.02993100	0.00066000
C	-0.31257600	0.07514800	0.01723200
O	-1.43474900	-0.73541900	-0.00292500
N	-1.41512700	0.79587700	-0.00428900
C	0.99814700	0.01679600	-0.00920800

Zero-point correction= 0.016675
Thermal correction to Energy= 0.021776
Thermal correction to Enthalpy= 0.022721
Thermal correction to Gibbs Free Energy= -0.011925
Sum of electronic and zero-point Energies= -281.288007

Sum of electronic and thermal Energies= -281.282906

Sum of electronic and thermal Enthalpies= -281.281961

Sum of electronic and thermal Free Energies= -281.316607

O_2NCC

B3LYP /6-311+G(3df)

O	1.22965700	0.74727200	-0.10884600
C	-1.08373600	0.00007800	-0.00299500
C	-2.36019200	0.00002800	-0.12476500
N	0.14157000	-0.00003300	0.35831000
O	1.22941500	-0.74732300	-0.10885600

Zero-point correction= 0.015581

Thermal correction to Energy= 0.020448

Thermal correction to Enthalpy= 0.021392

Thermal correction to Gibbs Free Energy= -0.012668

Sum of electronic and zero-point Energies= -281.068106

Sum of electronic and thermal Energies= -281.063239

Sum of electronic and thermal Enthalpies= -281.062295

Sum of electronic and thermal Free Energies= -281.096355

TS1

B3LYP/6-311+G(3df)

O	1.93418100	-0.18790700	-0.53728500
C	-0.78966000	1.33385600	0.00214900
C	-1.50388400	0.18577500	0.01238000
O	-2.11855900	-0.79966300	0.02125600
N	2.17661300	-0.17389000	0.57729300

Zero-point correction= 0.013604

Thermal correction to Energy= 0.019661

Thermal correction to Enthalpy= 0.020605

Thermal correction to Gibbs Free Energy= -0.019784

Sum of electronic and zero-point Energies= -281.242405

Sum of electronic and thermal Energies= -281.236347

Sum of electronic and thermal Enthalpies= -281.235403

Sum of electronic and thermal Free Energies= -281.275793

TS2

B3LYP/6-311+G(3df)

C	0.29751900	0.85167700	0.00000200
C	-1.50036800	-0.41902700	0.00000400
O	-2.56537300	-0.05074600	-0.00000300
N	1.28603500	0.16293400	-0.00000100
O	2.34222900	-0.41630900	-0.00000100

Zero-point correction= 0.015352

Thermal correction to Energy= 0.020711

Thermal correction to Enthalpy= 0.021656

Thermal correction to Gibbs Free Energy= -0.014431

Sum of electronic and zero-point Energies= -281.304176

Sum of electronic and thermal Energies= -281.298816

Sum of electronic and thermal Enthalpies= -281.297872

Sum of electronic and thermal Free Energies= -281.333959

OCCCO

M06-2X/6-311+G(3df)

O	0.00000000	0.00000000	2.42296500
C	0.00000000	0.00000000	1.27252900
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	-1.27252900
O	0.00000000	0.00000000	-2.42296500

Zero-point correction= 0.021998

Thermal correction to Energy= 0.025069

Thermal correction to Enthalpy= 0.026014

Thermal correction to Gibbs Free Energy= -0.001032

Sum of electronic and zero-point Energies= -264.693948

Sum of electronic and thermal Energies= -264.690877

Sum of electronic and thermal Enthalpies= -264.689933

Sum of electronic and thermal Free Energies= -264.716978

OCC_triplet

M06-2X/6-311+G(3df)

C	0.00000000	0.00000000	-1.40916900
C	0.00000000	0.00000000	-0.05512400

O	0.00000000	0.00000000	1.09821900

Zero-point correction= 0.009464
Thermal correction to Energy= 0.012362
Thermal correction to Enthalpy= 0.013306
Thermal correction to Gibbs Free Energy= -0.012933
Sum of electronic and zero-point Energies= -151.246049
Sum of electronic and thermal Energies= -151.243152
Sum of electronic and thermal Enthalpies= -151.242208
Sum of electronic and thermal Free Energies= -151.268447

OCC_singlet
M06-2X/6-311+G(3df)

C	0.00000000	0.00000000	-1.41322300
C	0.00000000	0.00000000	-0.05548100
O	0.00000000	0.00000000	1.10152800

Zero-point correction= 0.009428
Thermal correction to Energy= 0.012361
Thermal correction to Enthalpy= 0.013306
Thermal correction to Gibbs Free Energy= -0.011974
Sum of electronic and zero-point Energies= -151.204547
Sum of electronic and thermal Energies= -151.201613
Sum of electronic and thermal Enthalpies= -151.200669
Sum of electronic and thermal Free Energies= -151.225948

OCCNO•
M06-2X/6-311+G(3df)

O	-2.28236700	0.12780900	0.00000000
C	0.00000000	0.40256600	0.00000000
C	1.22389900	-0.06387000	0.00000000
O	2.35936700	-0.23901800	0.00000000
N	-1.13705600	-0.16321400	0.00000000

Zero-point correction= 0.019583
Thermal correction to Energy= 0.024253
Thermal correction to Enthalpy= 0.025197
Thermal correction to Gibbs Free Energy= -0.008033

Sum of electronic and zero-point Energies= -281.225317
Sum of electronic and thermal Energies= -281.220647
Sum of electronic and thermal Enthalpies= -281.219703
Sum of electronic and thermal Free Energies= -281.252934

CNO•
M06-2X/6-311+G(3df)

O	0.00000000	0.00000000	1.09117900
C	0.00000000	0.00000000	-1.31548600
N	0.00000000	0.00000000	-0.11950200

Zero-point correction= 0.009325
Thermal correction to Energy= 0.012269
Thermal correction to Enthalpy= 0.013213
Thermal correction to Gibbs Free Energy= -0.012727
Sum of electronic and zero-point Energies= -167.888633
Sum of electronic and thermal Energies= -167.885689
Sum of electronic and thermal Enthalpies= -167.884744
Sum of electronic and thermal Free Energies= -167.910684

NCO
M06-2X/6-311+G(3df)

N	0.00000000	0.00000000	-1.25866000
C	0.00000000	0.00000000	-0.03690500
O	0.00000000	0.00000000	1.12900600

Zero-point correction= 0.010415
Thermal correction to Energy= 0.013123
Thermal correction to Enthalpy= 0.014067
Thermal correction to Gibbs Free Energy= -0.011551
Sum of electronic and zero-point Energies= -167.986420
Sum of electronic and thermal Energies= -167.983712
Sum of electronic and thermal Enthalpies= -167.982768
Sum of electronic and thermal Free Energies= -168.008385

NOC
M06-2X/6-311+G(3df)

C	0.00000000	0.00000000	1.28535300

O 0.00000000 0.00000000 0.13725300
N 0.00000000 0.00000000 -1.25859100

Zero-point correction= 0.006830
Thermal correction to Energy= 0.010250
Thermal correction to Enthalpy= 0.011194
Thermal correction to Gibbs Free Energy= -0.015582
Sum of electronic and zero-point Energies= -167.796792
Sum of electronic and thermal Energies= -167.793371
Sum of electronic and thermal Enthalpies= -167.792427
Sum of electronic and thermal Free Energies= -167.819203

cyclic_CNO
M06-2X/6-311+G(3df)
O 0.00000000 0.75549200 0.00000000
C 0.71249200 -0.42994800 0.00000000
N -0.61070700 -0.49489200 0.00000000

Zero-point correction= 0.007354
Thermal correction to Energy= 0.010362
Thermal correction to Enthalpy= 0.011306
Thermal correction to Gibbs Free Energy= -0.016683
Sum of electronic and zero-point Energies= -167.865084
Sum of electronic and thermal Energies= -167.862076
Sum of electronic and thermal Enthalpies= -167.861132
Sum of electronic and thermal Free Energies= -167.889121

OCNCO
M06-2X/6-311+G(3df)
O -2.27746900 0.06335200 0.00000000
C 1.16260000 0.03680100 0.00000000
O 2.28978100 -0.18772700 0.00000000
N 0.00000000 0.39581300 0.00000000
C -1.17901600 -0.33275000 0.00000000

Zero-point correction= 0.020203
Thermal correction to Energy= 0.024887
Thermal correction to Enthalpy= 0.025831

Thermal correction to Gibbs Free Energy= -0.007792
Sum of electronic and zero-point Energies= -281.327149
Sum of electronic and thermal Energies= -281.322464
Sum of electronic and thermal Enthalpies= -281.321520
Sum of electronic and thermal Free Energies= -281.355143

OCCON
M06-2X/6-311+G(3df)

C	1.15180400	-0.16384300	0.00000000
O	2.26267200	-0.46373800	0.00000000
N	-2.26570300	0.44173900	0.00000000
C	0.00000000	0.49959900	0.00000000
O	-1.14403600	-0.17460200	0.00000000

Zero-point correction= 0.017370
Thermal correction to Energy= 0.022120
Thermal correction to Enthalpy= 0.023064
Thermal correction to Gibbs Free Energy= -0.010492
Sum of electronic and zero-point Energies= -281.136249
Sum of electronic and thermal Energies= -281.131500
Sum of electronic and thermal Enthalpies= -281.130555
Sum of electronic and thermal Free Energies= -281.164111

OCONC
M06-2X/6-311+G(3df)

C	-0.96973000	-0.40719400	0.00000000
O	-2.10631600	-0.18639300	0.00000000
O	0.00000000	0.58160100	0.00000000
N	1.22860200	0.09877300	0.00000000
C	2.34478100	-0.23498600	0.00000000

Zero-point correction= 0.018371
Thermal correction to Energy= 0.023265
Thermal correction to Enthalpy= 0.024209
Thermal correction to Gibbs Free Energy= -0.009684
Sum of electronic and zero-point Energies= -281.186504
Sum of electronic and thermal Energies= -281.181610
Sum of electronic and thermal Enthalpies= -281.180666

Sum of electronic and thermal Free Energies= -281.214559

OCOCN

M06-2X/6-311+G(3df)

C	-1.02669300	-0.37074500	0.00000000
O	-2.15188600	-0.10497700	0.00000000
C	1.21387300	0.08715800	0.00000000
O	0.00000000	0.56216800	0.00000000
N	2.29885900	-0.27943000	0.00000000

Zero-point correction= 0.019616

Thermal correction to Energy= 0.024248

Thermal correction to Enthalpy= 0.025193

Thermal correction to Gibbs Free Energy= -0.008263

Sum of electronic and zero-point Energies= -281.275417

Sum of electronic and thermal Energies= -281.270785

Sum of electronic and thermal Enthalpies= -281.269840

Sum of electronic and thermal Free Energies= -281.303296

O_2CCN

M06-2X/6-311+G(3df)

O	-1.13923100	1.03633600	-0.00000800
C	-0.46285500	-0.00010500	-0.00011200
C	1.00003400	-0.00009500	0.00007200
O	-1.13947600	-1.03617200	-0.00000300
N	2.14379800	-0.00001700	0.00004700

Zero-point correction= 0.017239

Thermal correction to Energy= 0.021997

Thermal correction to Enthalpy= 0.022942

Thermal correction to Gibbs Free Energy= -0.011048

Sum of electronic and zero-point Energies= -281.275803

Sum of electronic and thermal Energies= -281.271044

Sum of electronic and thermal Enthalpies= -281.270100

Sum of electronic and thermal Free Energies= -281.304090

O_2CNC

M06-2X/6-311+G(3df)

O	-1.07216600	1.04296600	0.00002900

C	-0.41279900	-0.00003300	-0.00019000
O	-1.07224200	-1.04291300	0.00003400
C	2.14089600	-0.00000600	0.00005900
N	0.96952600	-0.00002600	0.00004000

Zero-point correction= 0.016929
Thermal correction to Energy= 0.021767
Thermal correction to Enthalpy= 0.022711
Thermal correction to Gibbs Free Energy= -0.011512
Sum of electronic and zero-point Energies= -281.259494
Sum of electronic and thermal Energies= -281.254656
Sum of electronic and thermal Enthalpies= -281.253712
Sum of electronic and thermal Free Energies= -281.287935

OCC(O)N
M06-2X/6-311+G(3df)

O	2.15878000	-0.02728600	-0.00085800
C	-0.30145600	0.07270300	0.01403200
O	-1.43839400	-0.70907400	-0.00248100
N	-1.42651800	0.76605000	-0.00368700
C	1.00521200	0.01538600	-0.00527800

Zero-point correction= 0.017286
Thermal correction to Energy= 0.022261
Thermal correction to Enthalpy= 0.023205
Thermal correction to Gibbs Free Energy= -0.011184
Sum of electronic and zero-point Energies= -281.176676
Sum of electronic and thermal Energies= -281.171701
Sum of electronic and thermal Enthalpies= -281.170757
Sum of electronic and thermal Free Energies= -281.205146

O_2NCC
M06-2X/6-311+G(3df)

O	-1.21430600	-0.72752700	-0.11565400
C	1.07476000	0.00032300	-0.00445300
C	2.34727100	-0.00016900	-0.12804800
N	-0.15728800	0.00011500	0.37804600
O	-1.21459100	0.72731200	-0.11576100

Zero-point correction= 0.016847
Thermal correction to Energy= 0.021514
Thermal correction to Enthalpy= 0.022458
Thermal correction to Gibbs Free Energy= -0.011170
Sum of electronic and zero-point Energies= -280.953700
Sum of electronic and thermal Energies= -280.949034
Sum of electronic and thermal Enthalpies= -280.948090
Sum of electronic and thermal Free Energies= -280.981718

OCCCO
MP2/6-311+G(3df)

O	0.00000000	0.00000000	2.44403800
C	0.00000000	0.00000000	1.27585200
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	-1.27585200
O	0.00000000	0.00000000	-2.44403800

Zero-point correction= 0.021369
Thermal correction to Energy= 0.026265
Thermal correction to Enthalpy= 0.027209
Thermal correction to Gibbs Free Energy= -0.005043
Sum of electronic and zero-point Energies= -264.258265
Sum of electronic and thermal Energies= -264.253369
Sum of electronic and thermal Enthalpies= -264.252425
Sum of electronic and thermal Free Energies= -264.284678

OCC_triplet
MP2/6-311+G(3df)

C	0.00000000	0.00000000	-1.42242000
C	0.00000000	0.00000000	-0.05174500
O	0.00000000	0.00000000	1.10562400

Zero-point correction= 0.009211
Thermal correction to Energy= 0.012159
Thermal correction to Enthalpy= 0.013103
Thermal correction to Gibbs Free Energy= -0.013235
Sum of electronic and zero-point Energies= -150.970159

Sum of electronic and thermal Energies= -150.967211
Sum of electronic and thermal Enthalpies= -150.966267
Sum of electronic and thermal Free Energies= -150.992605

OCC_singlet
MP2/6-311+G(3df)

C	0.00000000	0.00000000	-1.42452100
C	0.00000000	0.00000000	-0.06009600
O	0.00000000	0.00000000	1.11346200

Zero-point correction= 0.008895
Thermal correction to Energy= 0.011910
Thermal correction to Enthalpy= 0.012854
Thermal correction to Gibbs Free Energy= -0.012588
Sum of electronic and zero-point Energies= -150.936190
Sum of electronic and thermal Energies= -150.933175
Sum of electronic and thermal Enthalpies= -150.932231
Sum of electronic and thermal Free Energies= -150.957673

OCCNO•
MP2/6-311+G(3df)

O	-2.28071100	-0.03357400	0.00000000
C	0.00000000	0.54139600	0.00000000
C	1.21175600	0.05804000	0.00000000
O	2.33314500	-0.24394100	0.00000000
N	-1.09857300	-0.19664200	0.00000000

Zero-point correction= 0.022742
Thermal correction to Energy= 0.027234
Thermal correction to Enthalpy= 0.028178
Thermal correction to Gibbs Free Energy= -0.004979
Sum of electronic and zero-point Energies= -280.766007
Sum of electronic and thermal Energies= -280.761514
Sum of electronic and thermal Enthalpies= -280.760570
Sum of electronic and thermal Free Energies= -280.793727

CNO•
MP2/6-311+G(3df)

O	0.00000000	0.00000000	1.08805500
C	0.00000000	0.00000000	-1.31937200
N	0.00000000	0.00000000	-0.11260200

Zero-point correction= 0.009353
Thermal correction to Energy= 0.012300
Thermal correction to Enthalpy= 0.013244
Thermal correction to Gibbs Free Energy= -0.012705
Sum of electronic and zero-point Energies= -167.597173
Sum of electronic and thermal Energies= -167.594226
Sum of electronic and thermal Enthalpies= -167.593282
Sum of electronic and thermal Free Energies= -167.619231

OCCNO•
B2PLYP/6-311+G(3df)

O	-2.29253400	0.13719600	0.00000000
C	0.00000000	0.39790600	0.00000000
C	1.22462100	-0.06364100	0.00000000
O	2.37033600	-0.24126100	0.00000000
N	-1.13859300	-0.16758100	0.00000000

Zero-point correction= 0.019428
Thermal correction to Energy= 0.024127
Thermal correction to Enthalpy= 0.025072
Thermal correction to Gibbs Free Energy= -0.008283
Sum of electronic and zero-point Energies= -281.154222
Sum of electronic and thermal Energies= -281.149522
Sum of electronic and thermal Enthalpies= -281.148578
Sum of electronic and thermal Free Energies= -281.181933

OCCNO•
B3Pw91/6-311+G(3df)

O	-2.29570700	0.15624900	0.00000000
C	0.00000000	0.35374000	0.00000000
C	1.23152800	-0.07420900	0.00000000
O	2.38065000	-0.21360500	0.00000000
N	-1.15267300	-0.17404800	0.00000000

Zero-point correction= 0.019254
Thermal correction to Energy= 0.023977
Thermal correction to Enthalpy= 0.024921
Thermal correction to Gibbs Free Energy= -0.008340
Sum of electronic and zero-point Energies= -281.229942
Sum of electronic and thermal Energies= -281.225219
Sum of electronic and thermal Enthalpies= -281.224275
Sum of electronic and thermal Free Energies= -281.257535

OCCNO•
wb97xd/6-311+G(3df)

O	-2.28307300	0.13638500	0.00000000
C	0.00000000	0.39816300	0.00000000
C	1.22286600	-0.06691200	0.00000000
O	2.36120400	-0.23798300	0.00000000
N	-1.13746200	-0.16781800	0.00000000

Zero-point correction= 0.019460
Thermal correction to Energy= 0.024148
Thermal correction to Enthalpy= 0.025092
Thermal correction to Gibbs Free Energy= -0.008178
Sum of electronic and zero-point Energies= -281.234812
Sum of electronic and thermal Energies= -281.230124
Sum of electronic and thermal Enthalpies= -281.229180
Sum of electronic and thermal Free Energies= -281.262450

OCCNO•
PBE1PBE/6-311+G(3df)

O	-2.29030200	0.15296100	0.00000000
C	0.00000000	0.36305800	0.00000000
C	1.22885500	-0.07354100	0.00000000
O	2.37449700	-0.22148800	0.00000000
N	-1.14952800	-0.16984000	0.00000000

Zero-point correction= 0.019450
Thermal correction to Energy= 0.024158

Thermal correction to Enthalpy= 0.025102
Thermal correction to Gibbs Free Energy= -0.008142
Sum of electronic and zero-point Energies= -281.035222
Sum of electronic and thermal Energies= -281.030515
Sum of electronic and thermal Enthalpies= -281.029571
Sum of electronic and thermal Free Energies= -281.062815

OCCNO•
TPSSTPSS/6-311+G(3df)

O	-2.31242900	0.15320200	0.00000000
C	0.00000000	0.36568100	0.00000000
C	1.23432900	-0.07965300	0.00000000
O	2.39751900	-0.20134300	0.00000000
N	-1.15524200	-0.19014900	0.00000000

Zero-point correction= 0.018505
Thermal correction to Energy= 0.023254
Thermal correction to Enthalpy= 0.024199
Thermal correction to Gibbs Free Energy= -0.009127
Sum of electronic and zero-point Energies= -281.402942
Sum of electronic and thermal Energies= -281.398192
Sum of electronic and thermal Enthalpies= -281.397248
Sum of electronic and thermal Free Energies= -281.430574

OCCNO•
B3LYP/cc-pVTZ

O	-2.30142900	0.15629800	0.00000000
C	0.00000000	0.34972200	0.00000000
C	1.23348200	-0.07496800	0.00000000
O	2.38682300	-0.20342500	0.00000000
N	-1.15486300	-0.18164400	0.00000000

Zero-point correction= 0.019032
Thermal correction to Energy= 0.023762
Thermal correction to Enthalpy= 0.024706
Thermal correction to Gibbs Free Energy= -0.008567
Sum of electronic and zero-point Energies= -281.349284

Sum of electronic and thermal Energies= -281.344554

Sum of electronic and thermal Enthalpies= -281.343610

Sum of electronic and thermal Free Energies= -281.376883

OCCNO•

B3LYP/def2-TZVP

O	-2.29991800	0.15630600	0.00000000
C	0.00000000	0.35525600	0.00000000
C	1.23294300	-0.07423400	0.00000000
O	2.38416500	-0.21052700	0.00000000
N	-1.15309100	-0.17891000	0.00000000

Zero-point correction= 0.019042

Thermal correction to Energy= 0.023767

Thermal correction to Enthalpy= 0.024712

Thermal correction to Gibbs Free Energy= -0.008563

Sum of electronic and zero-point Energies= -281.361981

Sum of electronic and thermal Energies= -281.357256

Sum of electronic and thermal Enthalpies= -281.356312

Sum of electronic and thermal Free Energies= -281.389586

OCCNO•

B3LYP/ def2-QZVP

O	-2.29885600	0.15712000	0.00000000
C	0.00000000	0.35290700	0.00000000
C	1.23258100	-0.07403100	0.00000000
O	2.38291800	-0.20912200	0.00000000
N	-1.15256900	-0.17960500	0.00000000

Zero-point correction= 0.019016

Thermal correction to Energy= 0.023743

Thermal correction to Enthalpy= 0.024687

Thermal correction to Gibbs Free Energy= -0.008588

Sum of electronic and zero-point Energies= -281.377754

Sum of electronic and thermal Energies= -281.373027

Sum of electronic and thermal Enthalpies= -281.372082

Sum of electronic and thermal Free Energies= -281.405358

OCCNO•

BP86/cc-pVTZ

O	-2.32121700	0.16717500	0.00000000
C	0.00000000	0.34352800	0.00000000
C	1.24084700	-0.08454900	0.00000000
O	2.41072400	-0.19433600	0.00000000
N	-1.16587700	-0.19094100	0.00000000

Zero-point correction= 0.018364

Thermal correction to Energy= 0.023154

Thermal correction to Enthalpy= 0.024099

Thermal correction to Gibbs Free Energy= -0.009285

Sum of electronic and zero-point Energies= -281.375252

Sum of electronic and thermal Energies= -281.370462

Sum of electronic and thermal Enthalpies= -281.369518

Sum of electronic and thermal Free Energies= -281.402901

OCCNO•

BP86/def2-TZVP

O	-2.31991900	0.16796700	0.00000000
C	0.00000000	0.34817400	0.00000000
C	1.24053100	-0.08401300	0.00000000
O	2.40853100	-0.20148500	0.00000000
N	-1.16458300	-0.18811800	0.00000000

Zero-point correction= 0.018381

Thermal correction to Energy= 0.023167

Thermal correction to Enthalpy= 0.024111

Thermal correction to Gibbs Free Energy= -0.009273

Sum of electronic and zero-point Energies= -281.388409

Sum of electronic and thermal Energies= -281.383623

Sum of electronic and thermal Enthalpies= -281.382678

Sum of electronic and thermal Free Energies= -281.416062

OCCNO•

BP86/ def2-QZVP

O	-2.31883100	0.16851300	0.00000000
C	0.00000000	0.34614700	0.00000000

C	1.24012400	-0.08372300	0.00000000
O	2.40723300	-0.19992500	0.00000000
N	-1.16399400	-0.18903500	0.00000000

Zero-point correction= 0.018353
Thermal correction to Energy= 0.023142
Thermal correction to Enthalpy= 0.024087
Thermal correction to Gibbs Free Energy= -0.009300
Sum of electronic and zero-point Energies= -281.404757
Sum of electronic and thermal Energies= -281.399968
Sum of electronic and thermal Enthalpies= -281.399023
Sum of electronic and thermal Free Energies= -281.432410

CCO_singlet
CCSD(T)/cc-pVTZ

C	-0.18818484802779	0.17915308464111	0.00000000534815
O	0.98779040998352	0.17915309267948	-0.00000000267409
C	-1.55601466195572	0.17915309267941	-0.00000000267406

E(CCSD) -150.959391704
E(CCSD(T)) -150.986307607

CCO_triplet
CCSD(T)/cc-pVTZ

C	-0.18305776899088	0.17915310511625	-0.00000001515384
O	0.98130861379581	0.17915308246466	0.00000000755413
C	-1.55465994480493	0.17915308241909	0.00000000759971

E(CCSD) -150.993331043
E(CCSD(T)) -151.017326165

OCCNO•
CCSD(T)/cc-pVDZ

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.35226862
N	1.09724364	0.00000000	-0.71318631
O	-0.29643806	0.00000000	2.47910834
O	1.35232194	-0.00000000	-1.88801496

E(CCSD) = -280.528632738890

E(CCSD(T)) = -280.567041474695

OCCNO•

CCSD(T)/cc-pVTZ

O	-2.28490559562533	0.09791074601201	0.00000000325304
C	-0.00287645542526	0.46250852112012	0.00000000095358
C	1.21514361503465	-0.06982907641258	-0.00000000056595
O	2.35653523746690	-0.26635952720361	0.00000000122658
N	-1.11973980145096	-0.17630866351593	-0.00000000486725

E(CCSD) -280.771420267

E(CCSD(T)) -280.826828391

CNO•

CCSD(T)/cc-pVTZ

C	1.33176469100241	-0.00009427595382	0.00371606000130
N	0.11794449305416	0.00013897154686	0.00032923230337
O	-1.10441418405657	-0.00005069559304	-0.00308229230466

E(CCSD) -167.622823054

E(CCSD(T)) -167.651097293

OCCNO•

UCCSD(T)/aug-cc-pVQZ

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.32782475
N	1.03649610	0.00000000	-0.75638281
O	-0.26616284	0.00000000	2.45096547
O	1.26073287	-0.00000000	-1.93023975

E(CCSD) = -280.856728029671

E(CCSD(T)) = -280.917519185909

OCCNO•

ROCCSD(T)/aug-cc-pVQZ

C	0.00000000	0.00000000	0.00000000

C	0.00000000	0.00000000	1.32177219
N	1.00338632	0.00000000	-0.80838722
O	-0.27001409	0.00000000	2.44983840
O	1.18380915	-0.00000000	-1.99057619

E(CCSD) = -280.857146194499

E(CCSD(T)) = -280.921782902109