Electronic Supplementary Information

Noble Gas Hydrides in the Triplet State: $HNgCCO^+$ (Ng = He, Ne, Ar, Kr, and Xe)

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Table S1. Optimized Structural Parameters (Bond Length R in Å, Bond Angle θ in Degree) for Minima Structures of $^3HNgCCO^+$ (Ng = He, Ne, Ar, Kr, and Xe) Ions, Calculated using B3LYP and MP2 Methods with DEF2 and AVTZ Basis sets.

Geometrical Parameters	Methods	$^3HHeCCO^+$	$^3HNeCCO^+$	$^3HArCCO^+$	$^3HKrCCO^+$	$^3HXeCCO^+$
R(H–Ng)	B3LYP/DEF2	0.803	1.018	1.304	1.471	1.632
	B3LYP/AVTZ	0.803	1.021	1.307	1.453	1.636
	MP2/DEF2	0.764	0.990	1.283	1.429	1.611
	MP2/AVTZ	0.757	0.987	1.280	1.423	1.611
R(Ng–C)	B3LYP/DEF2	1.954	2.517	2.653	2.594	2.816
	B3LYP/AVTZ	1.951	2.510	2.671	2.693	2.810
	MP2/DEF2	2.038	2.574	2.688	2.745	2.825
	MP2/AVTZ	2.027	2.562	2.697	2.715	2.815
R(C–C)	B3LYP/DEF2	1.346	1.350	1.349	1.346	1.348
	B3LYP/AVTZ	1.342	1.346	1.345	1.344	1.344
	MP2/DEF2	1.357	1.360	1.359	1.358	1.358
	MP2/AVTZ	1.360	1.362	1.362	1.359	1.361
R(C–O)	B3LYP/DEF2	1.145	1.149	1.148	1.146	1.147
	B3LYP/AVTZ	1.147	1.151	1.151	1.149	1.149
	MP2/DEF2	1.151	1.154	1.153	1.153	1.152
	MP2/AVTZ	1.151	1.155	1.154	1.154	1.152
θ(H–Ng–C)	B3LYP/DEF2	180.0	180.0	180.0	180.0	180.0
	B3LYP/AVTZ	180.0	180.0	180.0	180.0	180.0
	MP2/DEF2	180.0	180.0	180.0	180.0	180.0
	MP2/AVTZ	180.0	180.0	180.0	180.0	180.0
θ(Ng–C–C)	B3LYP/DEF2	180.0	180.0	180.0	180.0	180.0
	B3LYP/AVTZ	180.0	180.0	180.0	180.0	180.0
	MP2/DEF2	180.0	180.0	180.0	180.0	180.0
	MP2/AVTZ	180.0	180.0	180.0	180.0	180.0
θ(C–C–O)	B3LYP/DEF2	180.0	180.0	180.0	180.0	180.0
	B3LYP/AVTZ	180.0	180.0	180.0	180.0	180.0
	MP2/DEF2	180.0	180.0	180.0	180.0	180.0
	MP2/AVTZ	180.0	180.0	180.0	180.0	180.0

Table S2. Optimized Structural Parameters (Bond Length R in Å, Bond Angle θ in Degree) for Transition State (TS) Structures of $^3HNgCCO^+$ (Ng = He, Ne, Ar, Kr, and Xe) Ions, Calculated using B3LYP and MP2 Methods with DEF2 and AVTZ Basis sets.

Geometrical Parameters	Methods	$^3HHeCCO^+$	$^3HNeCCO^+$	$^3HArCCO^+$	$^3HKrCCO^+$	$^3HXeCCO^+$
R(H–Ng)	B3LYP/DEF2	0.780	1.016	1.288	1.444	1.608
	B3LYP/AVTZ	0.774	1.009	1.289	1.429	1.611
	MP2/DEF2	0.760	0.990	1.278	1.429	1.596
	MP2/AVTZ	0.752	0.986	1.275	1.413	1.596
R(Ng–C)	B3LYP/DEF2	2.217	2.565	3.062	3.208	3.455
	B3LYP/AVTZ	2.212	2.562	3.067	3.231	3.453
	MP2/DEF2	2.227	2.589	3.025	2.745	3.394
	MP2/AVTZ	2.211	2.575	3.014	3.165	3.374
R(C–C)	B3LYP/DEF2	1.354	1.351	1.354	1.354	1.355
	B3LYP/AVTZ	1.354	1.350	1.354	1.354	1.355
	MP2/DEF2	1.362	1.363	1.364	1.358	1.365
	MP2/AVTZ	1.363	1.363	1.365	1.365	1.366
R(C–O)	B3LYP/DEF2	1.145	1.149	1.150	1.150	1.151
	B3LYP/AVTZ	1.146	1.150	1.151	1.151	1.152
	MP2/DEF2	1.151	1.154	1.154	1.153	1.155
	MP2/AVTZ	1.152	1.155	1.155	1.156	1.156
θ(H–Ng–C)	B3LYP/DEF2	110.7	141.0	106.6	100.0	97.8
	B3LYP/AVTZ	119.5	138.1	107.7	104.1	101.7
	MP2/DEF2	119.0	155.0	108.8	103.2	98.8
	MP2/AVTZ	118.4	138.1	107.7	104.1	101.7
θ(Ng–C–C)	B3LYP/DEF2	170.0	175.4	176.1	176.6	178.1
	B3LYP/AVTZ	172.6	174.4	176.6	176.8	178.0
	MP2/DEF2	172.4	177.6	176.6	177.1	108.8
	MP2/AVTZ	173.2	174.4	176.6	176.8	177.9
θ(C–C–O)	B3LYP/DEF2	179.9	180.0	180.0	180.0	180.0
	B3LYP/AVTZ	180.0	179.0	180.0	180.0	180.0
	MP2/DEF2	180.0	180.0	180.0	180.0	180.0
	MP2/AVTZ	179.0	179.0	180.0	180.0	180.0

Table S3. Energies (in kJ mol^{-1}) of the Various Dissociated Species Relative to the ^{3}HNgCCO$^+$ (Ng = He, Ne, Ar, Kr, and Xe) Ions, Calculated using B3LYP, MP2 and CCSD(T) Methods with DEF2 and AVTZ Basis sets.

Molecular Species	Methods	^{3}HHeCCO$^+$	^{3}HNeCCO$^+$	^{3}HArCCO$^+$	^{3}HKrCCO$^+$	^{3}HXeCCO$^+$
^{3}HNgCCO$^+$	All	0.0	0.0	0.0	0.0	0.0
Ng + ^{3}HCCO$^+$	B3LYP/DEF2	–477.0	–504.8	–321.2	–267.7	–197.6
	B3LYP/AVTZ	–465.5	–492.4	–313.8	–252.4	–187.6
	MP2/DEF2	–497.3	–510.0	–330.3	–277.1	–206.7
	MP2/AVTZ	–496.6	–507.7	–328.0	–269.8	–201.9
^{2}HNg + ^{2}CCO$^+$	B3LYP/DEF2	77.5	49.9	233.5	287.0	357.1
	B3LYP/AVTZ	93.7	66.7	245.4	306.8	371.5
	MP2/DEF2	32.2	19.5	199.1	252.3	322.6
	MP2/AVTZ	38.2	27.0	206.5	264.7	332.6
HNg$^+$ + ^{3}CCO	B3LYP/DEF2	117.5	65.3	75.3	77.8	80.4
	B3LYP/AVTZ	128.1	74.8	82.5	90.4	90.4
	MP2/DEF2	101.0	63.5	75.5	79.2	84.5
	MP2/AVTZ	102.4	63.9	75.2	82.9	86.1
H + ^{2}NgCCO$^+$	B3LYP/DEF2	75.3	43.7	160.8	168.8	170.2
	B3LYP/AVTZ	83.2	14.3	164.1	177.0	175.3
	MP2/DEF2	28.3	11.7	135.3	139.3	133.6
	MP2/AVTZ	50.9	51.3	145.6	149.2	141.2
H + Ng + ^{2}CCO$^+$	B3LYP/DEF2	77.7	49.9	233.5	287.0	357.1
	B3LYP/AVTZ	93.6	66.7	245.4	306.7	371.5
	MP2/DEF2	32.3	19.6	199.3	252.5	323.0
	MP2/AVTZ	38.2	27.1	206.8	265.0	332.9
H$^+$ + Ng + ^{3}CCO	B3LYP/DEF2	309.3	281.5	465.1	518.6	588.7
	B3LYP/AVTZ	321.0	294.1	472.7	534.1	598.9
	MP2/DEF2	292.2	279.5	459.2	512.4	582.8
	MP2/AVTZ	296.1	285.0	464.7	522.9	590.8
Barrier Height[a]	B3LYP/DEF2	24.3	1.5	26.4	34.0	42.1
	B3LYP/AVTZ	34.5	11.0	34.0	46.3	52.1
	MP2/DEF2	8.8	0.2	19.7	28.1	37.9
	MP2/AVTZ	8.8	0.2	19.2	30.8	39.2

[a]Barrier Height corresponding to TS (Transition State), ($HNgCCO^+ \rightarrow HCCO^+ + Ng$).

Table S4. Harmonic Vibrational Frequencies (in cm^{-1}) Calculated Using MP2 Method using DEF2 and AVTZ Basis Sets for the Minima Structures of $^3HNgCCO^+$ (Ng = He, Ne, Ar, Kr, and Xe) Compounds. Corresponding IR Values are Given within the Parentheses (in km mol^{-1}).

Normal Modes	Methods	$^3HHeCCO^+$	$^3HNeCCO^+$	$^3HArCCO^+$	$^3HKrCCO^+$	$^3HXeCCO^+$
H–Ng Str.	**DEF2**	3436.1 (214.9)	2981.4 (760.1)	2731.7 (248.0)	2514.2 (93.4)	2294.7 (13.4)
	AVTZ	3437.1 (215.0)	3018.4 (751.4)	2745.5 (247.2)	2517.4 (77.3)	2300.2 (11.5)
Ng–C Str.	**DEF2**	407.6 (345.8)	176.0 (46.4)	159.4 (35.8)	140.5 (22.2)	134.9 (20.2)
	AVTZ	414.9 (345.1)	178.9 (42.7)	159.9 (34.7)	146.2 (22.9)	137.5 (20.4)
C–C Str.	**DEF2**	1144.1 (33.0)	1120.4 (2.3)	1127.4 (8.7)	1128.7 (12.0)	1130.6 (16.8)
	AVTZ	1134.9 (35.5)	1111.5 (2.6)	1116.3 (8.5)	1126.6 (13.1)	1120.8 (18.1)
C–O Str.	**DEF2**	2085.0 (167.5)	2070.6 (165.8)	2075.3 (177.0)	2076.8 (4.4)	2078.2 (194.4)
	AVTZ	2083.7 (170.1)	2069.0 (168.5)	2073.3 (180.2)	2074.7 (185.4)	2077.5 (199.7)
H–Ng–C Bend[a]	**DEF2**	473.6 (187.0)	115.0 (331.0)	388.7 (121.3)	400.8 (83.7)	402.5 (38.9)
	AVTZ	481.8 (169.9)	114.7 (328.2)	378.7 (119.9)	414.9 (82.3)	406.9 (47.9)
Ng–C–C Bend[a]	**DEF2**	124.3 (82.9)	83.5 (0.4)	85.7 (10.2)	81.4 (5.8)	82.0 (2.8)
	AVTZ	124.1 (85.2)	83.9 (1.2)	85.1 (10.4)	82.6 (5.3)	81.4 (2.6)
C–C–O Bend[a]	**DEF2**	487.1 (18.4)	469.4 (0.8)	479.5 (13.7)	481.4 (9.3)	484.3 (11.3)
	AVTZ	492.9 (32.1)	469.0 (31.0)	477.1 (13.4)	482.4 (6.7)	484.8 (9.6)

[a]It is doubly degenerate mode for minima energy structure.

Table S5. Harmonic Vibrational Frequencies (in cm^{-1}) Calculated Using B3LYP Method using DEF2 and AVTZ Basis Sets for the Minima Structures of $^3HNgCCO^+$ (Ng = He, Ne, Ar, Kr, and Xe) Compounds. Corresponding IR Intensity and Raman Intensity Values are Given within the Parentheses (in km mol^{-1}) and in Square Brackets (in $Å^4$ amu^{-1}), respectively.

Normal Modes	Methods	$^3HHeCCO^+$	$^3HNeCCO^+$	$^3HArCCO^+$	$^3HKrCCO^+$	$^3HXeCCO^+$
H–Ng Str.	DEF2	2849.5 (125.3) [3054.5]	2512.5 (42.0) […][b]	2508.1 (6.4) [2652.0]	2322.0 (0.02) [1988.6]	2149.7 (2.0) [1373.2]
	AVTZ	2700.8 (398.0) [6348.9]	2363.8 (544.3) […][b]	2477.0 (0.1) [3979.9]	2291.3 (4.4) [2437.8]	2133.6 (6.7) [1664.5]
Ng–C Str.	DEF2	459.2 (348.1) [24.5]	185.1 (57.3) […][b]	165.4 (41.1) [0.3]	144.0 (23.5) [0.2]	135.6 (18.8) [0.3]
	AVTZ	460.8 (335.6) [53.0]	186.9 (57.6) […][b]	162.9 (40.2) [0.3]	148.3 (24.1) [0.3]	136.9 (19.0) [0.2]
C–C Str.	DEF2	1183.8 (11.8) [10.6]	1148.5 (1.9) […][b]	1157.4 (0.4) [32.7]	1159.4 (0.8) [41.0]	1161.0 (1.5) [56.0]
	AVTZ	1189.3 (7.8) [2.3]	1155.4 (5.8) […][b]	1161.6 (0.01) [27.1]	1167.7 (0.4) [36.7]	1167.3 (0.8) [49.8]
C–O Str.	DEF2	2113.8 (204.1) [14.5]	2093.1 (2.8) […][b]	2098.7 (219.0) [8.3]	2100.4 (226.5) [8.1]	2102.1 (241.0) [5.9]
	AVTZ	2077.8 (170.4) [7.8]	2062.4 (210.5) [...][b]	2065.5 (169.7) [9.2]	2068.6 (174.6) [11.8]	2068.9 (185.8) [10.1]
H–Ng–C Bend[a]	DEF2	639.8 (141.2) [2.5]	196.4 (281.0) […][b]	430.8 (121.5) [0.01]	422.8 (80.7) [0.002]	408.2 (37.0) [0.01]
	AVTZ	482.6 (35.4) [0.7]	211.6 (271.8) […][b]	419.4 (122.0) [0.0]	435.2 (82.2) [0.03]	412.8 (39.4) [0.03]
Ng–C–C Bend[a]	DEF2	117.2 (64.3) [0.2]	81.4 (13.5) […][b]	83.9 (6.8) [0.4]	88.5 (3.2) [0.3]	78.2 (1.4) [0.3]
	AVTZ	122.6 (63.5) [0.0]	84.8 (14.0) […][b]	83.7 (7.1) [0.3]	82.4 (3.0) [0.2]	79.2 (1.4) [0.3]
C–C–O Bend[a]	DEF2	480.1 (28.6) [0.04]	468.0 (523.5) […][b]	478.5 (4.5) [0.5]	479.3 (6.4) [0.5]	480.2 (10.4) [0.6]
	AVTZ	655.4 (138.2) [2.7]	465.9 (29.5) […][b]	474.3 (4.7) [0.9]	482.0 (0.8) [0.8]	479.8 (7.5) [0.8]

[a]It is doubly degenerate mode for minima energy structure.

[b] It has not been possible to calculate the Raman intensity for $^3HNeCCO^+$ ion by using B3LYP method with both DEF2 and AVTZ basis sets due to convergence problem.

Table S6. Harmonic Vibrational Frequencies (in cm^{-1}) Calculated Using B3LYP and MP2 Methods using DEF2 and AVTZ Basis Sets for the Transition State (TS) Structures of $^3HNgCCO^+$ (Ng = He, Ne, Ar, Kr, and Xe) Compounds. Corresponding IR Intensity Values are Given within the Parentheses (in km mol^{-1}).

Normal Modes	Methods	$^3HHeCCO^+$	$^3HNeCCO^+$	$^3HArCCO^+$	$^3HKrCCO^+$	$^3HXeCCO^+$
H–Ng Str.	**B3LYP/DEF2**	3093.0 (456.5)	2613.4 (172.6)	2269.0 (473.3)	2472.8 (343.0)	2269.8 (193.3)
	B3LYP/AVTZ	3121.1 (411.6)	2644.3 (162.2)	2664.1 (465.1)	2459.9 (341.7)	2260.0 (197.7)
	MP2/DEF2	3506.0 (748.3)	2986.0 (794.6)	2772.1 (543.0)	2574.6 (383.2)	2364.2 (214.0)
	MP2/AVTZ	3519.2 (739.0)	3024.7 (14.0)	2789.8 (528.1)	2581.5 (374.1)	2366.1 (213.0)
Ng–C Str.	**B3LYP/DEF2**	385.5 (280.2)	181.9 (63.0)	119.2 (24.7)	94.0 (10.8)	79.2 (6.4)
	B3LYP/AVTZ	388.1 (282.5)	184.1 (64.9)	119.1 (24.5)	94.8 (10.9)	79.6 (6.4)
	MP2/DEF2	376.6 (287.1)	175.9 (56.8)	125.3 (24.6)	101.0 (10.7)	88.0 (6.3)
	MP2/AVTZ	384.0 (289.1)	179.4 (0.7)	128.0 (24.3)	103.9 (10.7)	89.0 (6.4)
C–C Str.	**B3LYP/DEF2**	1134.3 (33.1)	1144.2 (1.7)	1127.6 (0.6)	1124.0 (0.9)	1120.3 (1.3)
	B3LYP/AVTZ	1133.3 (29.5)	1142.6 (1.6)	1125.5 (0.7)	1122.1 (0.9)	1118.2 (1.3)
	MP2/DEF2	1119.4 (22.0)	1112.1 (2.6)	1100.8 (1.8)	1097.2 (1.3)	1094.1 (1.0)
	MP2/AVTZ	1116.6 (23.1)	1110.0 (2.6)	1097.5 (1.8)	1094.1 (1.4)	1090.5 (1.0)
C–O Str.	**B3LYP/DEF2**	2095.7 (377.1)	2091.6 (212.8)	2082.4 (208.5)	2079.7 (210.7)	2076.9 (216.7)
	B3LYP/AVTZ	2092.0 (352.9)	2086.9 (210.1)	2077.1 (206.1)	2075.4 (209.3)	2072.3 (215.4)
	MP2/DEF2	2081.2 (172.7)	2072.2 (168.4)	2066.9 (169.7)	2064.8 (172.6)	2062.8 (177.7)
	MP2/AVTZ	2077.9 (173.1)	2068.8 (168.0)	2063.4 (170.0)	2061.5 (173.2)	2059.3 (178.7)
H–Ng–C Bend	**B3LYP/DEF2**	–929.4 (100.8)	–268.6 (232.8)	–294.9 (88.6)	–255.6 (63.1)	–222.6 (31.6)
	B3LYP/AVTZ	–921.3 (95.7)	–245.3 (230.4)	–290.4 (92.0)	–257.9 (60.0)	–222.3 (31.8)
	MP2/DEF2	–613.6 (107.7)	–148.8 (278.6)	–281.2 (101.2)	–256.1 (70.4)	–231.1 (34.1)
	MP2/AVTZ	–618.8 (105.7)	–144.1 (277.6)	–285.8 (94.9)	–261.5 (67.1)	–229.6 (33.2)
Ng–C–C Bend	**B3LYP/DEF2**	126.5 (63.7)	82.5 (19.4)	75.8 (5.7)	71.0 (3.0)	66.3 (1.8)
	B3LYP/AVTZ	124.6 (63.9)	83.1 (21.7)	74.9 (5.7)	70.8 (2.7)	65.6 (1.7)
	MP2/DEF2	121.8 (80.0)	87.9 (36.4)	79.4 (7.9)	74.5 (4.3)	69.3 (2.8)
	MP2/AVTZ	121.9 (79.2)	85.9 (35.2)	75.9 (7.6)	71.3 (4.1)	66.3 (2.7)
C–C–O Bend	**B3LYP/DEF2**	484.2 (37.7)	467.9 (31.7)	461.7 (30.3)	457.6 (29.5)	452.8 (28.5)
	B3LYP/AVTZ	483.0 (37.0)	467.4 (31.8)	460.6 (30.3)	457.2 (29.3)	452.2 (28.5)
	MP2/DEF2	486.2 (38.4)	470.5 (33.8)	464.5 (30.1)	460.0 (28.8)	455.7 (27.7)
	MP2/AVTZ	484.8 (38.1)	469.2 (31.7)	462.8 (29.6)	459.4 (28.2)	455.1 (27.6)
H–Ng–C–C Tors.	**B3LYP/DEF2**	137.0 (165.1)	75.7 (88.6)	77.2 (14.5)	71.5 (6.7)	65.8 (2.5)
	B3LYP/AVTZ	135.8 (164.6)	91.4 (87.9)	76.0 (15.8)	71.1 (6.8)	65.3 (2.6)
	MP2/DEF2	127.8 (160.7)	89.8 (78.1)	78.7 (15.4)	73.3 (8.1)	68.2 (3.6)
	MP2/AVTZ	128.5 (159.5)	87.8 (77.5)	76.5 (16.9)	72.2 (7.9)	66.7 (3.3)

Table S7. Harmonic Vibrational Frequencies (in cm^{-1}) and Intrinsic Force Constants in the Parentheses (in N m^{-1}) Corresponding to Individual Internal Coordinates in the $^3HNgCCO^+$ (Ng = He, Ne, Ar, Kr, and Xe) Ions, Calculated using B3LYP and MP2 Methods with DEF2 and AVTZ Basis Sets.

Int Coord	Methods	$^3HHeCCO^+$	$^3HNeCCO^+$	$^3HArCCO^+$	$^3HKrCCO^+$	$^3HXeCCO^+$
H–Ng Str.	**B3LYP/DEF2**	2848.9 (385.0)	2513.9 (357.3)	2508.9 (364.6)	2322.4 (316.5)	2149.9 (272.5)
	B3LYP/AVTZ	2699.7 (345.8)	2365 (316.2)	2477.8 (355.6)	2291.9 (308.3)	2133.8 (268.3)
	MP2/DEF2	3433.0 (559.1)	2981.4 (502.4)	2732.2 (371.0)	2514.5 (371.0)	2294.9 (310.3)
	MP2/AVTZ	3434.1 (559.4)	3018.4 (515.0)	2745.9 (436.7)	2517.8 (372.0)	2300.4 (311.8)
Ng–C Str.	**B3LYP/DEF2**	531.2 (50.0)	239.6 (25.4)	243.1 (32.1)	235.5 (34.2)	233.4 (35.3)
	B3LYP/AVTZ	534.7 (50.6)	242.5 (26.0)	239.3 (31.1)	243.2 (36.6)	235.6 (36.0)
	MP2/DEF2	487.4 (42.0)	235.9 (24.6)	230.6 (30.8)	223.5 (30.8)	226.3 (33.2)
	MP2/AVTZ	494.4 (43.3)	239.8 (25.4)	230.7 (29.0)	232.2 (33.3)	229.7 (34.2)
C–C Str.	**B3LYP/DEF2**	1342.4 (637.1)	1323.3 (619.0)	1329.4 (624.8)	1331.1 (626.3)	1332.2 (627.4)
	B3LYP/AVTZ	1342.0 (636.6)	1326.7 (622.1)	1329.8 (625.3)	1334.2 (629.3)	1333.7 (628.8)
	MP2/DEF2	1308.8 (605.5)	1297.9 (595.5)	1302.0 (599.6)	1302.3 (599.1)	1302.6 (599.9)
	MP2/AVTZ	1295.8 (593.6)	1285.8 (584.5)	1287.8 (586.2)	1299.0 (596.4)	1289.3 (587.7)
C–O Str.	**B3LYP/DEF2**	1999.9 (1615.8)	1979.7 (1583.1)	1985.2 (1591.9)	1968.8 (1594.6)	1988.8 (1597.7)
	B3LYP/AVTZ	1965.4 (1560.5)	1949.1 (1534.6)	1952.4 (1539.9)	1955.3 (1544.5)	1956.2 (1545.7)
	MP2/DEF2	1973.1 (605.5)	1958.0 (1548.7)	1962.8 (1559.1)	1964.5 (1559.1)	1966.3 (1561.9)
	MP2/AVTZ	1974.6 (1575.1)	1959.0 (1550.2)	1963.8 (1557.8)	1962.6 (1556.0)	1968.5 (1565.3)
H–Ng–C Bend[a]	**B3LYP/DEF2**	642.0	196.7	434.5	427.4	413.8
	B3LYP/AVTZ	655.6	211.9	423.6	444.8	421.0
	MP2/DEF2	475.4	114.0	390.6	404.8	408.1
	MP2/AVTZ	488.1	114.1	380.6	419.8	413.6
Ng–C–C Bend[a]	**B3LYP/DEF2**	147.5	131.6	141.4	137.3	135.8
	B3LYP/AVTZ	172.1	141.3	146.2	145.1	142.5
	MP2/DEF2	175.0	140.8	147.9	143.7	146.7
	MP2/AVTZ	180.8	144.4	151.6	143.4	150.5
C–C–O Bend[a]	**B3LYP/DEF2**	468.7	456.3	461.3	462.0	462.3
	B3LYP/AVTZ	467.0	451.8	455.0	457.8	457.5
	MP2/DEF2	469.5	455.8	462.6	462.9	464.3
	MP2/AVTZ	468.6	454.3	458.7	463.4	462.1

[a] It is doubly degenerate mode for minima energy structure.

Table S8. B3LYP and MP2 Calculated Values of the Mulliken Atomic Charges (in au) in the Minima and Transition State Structures of ^{3}HNgCCO$^+$ (Ng = He, Ne, Ar, Kr, and Xe) Ions using DEF2 (AVTZ) Basis Sets.

Species	Methods	*q*(H)		*q*(Ng)		*q*(C)[a]		*q*(C)[b]		*q*(O)	
		Min	TS	Min	TS	Min	TS	Min	TS	Min	TS
^{3}HHeCCO$^+$	B3LYP	0.593 (0.527)	0.685 (0.575)	0.206 (0.262)	0.267 (0.357)	0.534 (-0.073)	-0.456 (-0.254)	0.815 (0.294)	0.580 (0.381)	-0.080 (-0.009)	-0.077 (-0.059)
	MP2	0.652 (0.611)	0.731 (0.632)	0.202 (0.237)	0.255 (0.326)	-0.606 (-0.177)	-0.496 (-0.331)	0.795 (0.293)	0.558 (0.360)	-0.044 (0.037)	-0.048 (0.012)
^{3}HNeCCO$^+$	B3LYP	0.603 (0.595)	0.625 (0.652)	0.341 (0.354)	0.329 (0.308)	-0.459 (-0.310)	-0.451 (-0.262)	0.637 (0.435)	0.602 (0.361)	-0.116 (-0.074)	-0.105 (-0.058)
	MP2	0.671 (0.648)	0.661 (0.682)	0.309 (0.361)	0.330 (0.315)	-0.489 (-0.407)	-0.456 (-0.352)	0.587 (0.414)	0.555 (0.343)	-0.078 (-0.016)	-0.089 (0.013)
^{3}HArCCO$^+$	B3LYP	0.341 (0.266)	0.490 (0.346)	0.171 (0.617)	0.459 (0.625)	-0.005 (-0.154)	-0.307 (-0.191)	0.639 (0.306)	0.471 (0.281)	-0.147 (-0.035)	-0.114 (-0.062)
	MP2	0.542 (0.314)	0.534 (0.383)	0.315 (0.613)	0.419 (0.595)	-0.502 (-0.236)	-0.289 (-0.238)	0.707 (0.286)	0.416 (0.251)	-0.061 (0.023)	-0.081 (0.009)
^{3}HKrCCO$^+$	B3LYP	0.462 (0.146)	0.453 (0.259)	0.433 (0.734)	0.486 (0.714)	-0.268 (-0.121)	-0.276 (-0.181)	0.476 (0.281)	0.442 (0.278)	-0.103 (-0.039)	-0.105 (-0.069)
	MP2	0.504 (0.161)	0.476 (0.274)	0.351 (0.791)	0.478 (0.699)	-0.282 (-0.224)	-0.247 (-0.228)	0.483 (0.254)	0.379 (0.251)	-0.056 (0.018)	-0.086 (0.004)
^{3}HXeCCO$^+$	B3LYP	0.221 (0.025)	0.330 (0.091)	0.655 (0.948)	0.628 (0.900)	-0.354 (-0.246)	-0.306 (-0.174)	0.622 (0.349)	0.458 (0.252)	-0.144 (-0.076)	-0.110 (-0.069)
	MP2	0.331 (-0.011)	0.363 (0.069)	0.661 (1.033)	0.607 (0.900)	-0.399 (-0.353)	-0.266 (-0.201)	0.456 (0.357)	0.380 (0.226)	-0.049 (-0.026)	-0.084 (0.006)

[a]This C atom is attached to Ng atom; [b]This C atom is connected to O atom.