SUPPORTING INFORMATION

Evidence of zinc superoxide formation in the gas phase: Comparisons in behaviour between ligated Zn(I/II) and Cu(I/II) with regard to the attachment of O_2 or H_2O.

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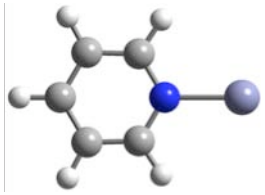
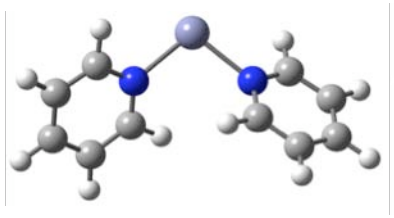
Complex	sym	state	E/au	ZPE /au	Metal-N / Å	N-Metal-N / º
$[Zn(pyridine)]^{+}$	C_{2v}	$^2A_1$	-2027.2962	0.0899	2.059	
$[Zn(pyridine)_2]^{+}$	C_2	^2A	-2275.6609	0.1802	2.127 (2)	101.2
	C_s	$^2A'$	-2275.6601	0.1801	2.125, 2.135	100.7
$[Zn(pyridine)_3]^{+}$	C_3	^2A	-2524.0114*	0.2690	2.160 (3)	98.0 (3)
$[Zn(pyridine)_4]^{+}$	D_{2d}	$^2B_2$	-2772.3672	0.3572	2.029 (4)	110.4 (4), 107.6 (2)
$[Zn(pyridine)]^{2+}$	C_{2v}	$^1A_1$	-2026.8227	0.0895	1.910	
	~η-py	^1A	-2026.7647	0.0889	2.279	
$[Zn(pyridine)_2]^{2+}$	D_{2d}	$^1A_1$	-2275.3190	0.1812	1.896 (2)	180.0
$[Zn(pyridine)_3]^{2+}$	C_3	^1A	-2523.7310*	0.2715	1.985 (3)	120.0 (3)
	C_s	$^1A'$	-2523.7279	0.2722	1.989 (2), 1.992	125.5, 117.0 (2)
$[Zn(pyridine)_4]^{2+}$	D_{2d}	$^1A_1$	-2772.1168	0.3628	2.048 (4)	110.9 (4), 106.6 (2)
$[Cu(pyridine)]^{+}$	C_{2v}	$^1A_1$	-1888.4856	0.0904	1.906	
	~ η-py	^1A	-1888.4505	0.0890	2.690	
$[Cu(pyridine)_2]^{+}$	D_{2d}	$^1A_1$	-2136.8930	0.1812	1.902 (2)	180.0
$[Cu(pyridine)_3]^{+}$	~C_2	^1A	-2385.2349*	0.2698	1.985 (2), 2.068	136.2, 111.9 (2)
$[Cu(pyridine)_4]^{+}$	D_{2d}	$^1A_1$	-2633.5750	0.3608	2.072 (4)	111.0 (4) 106.5 (2)

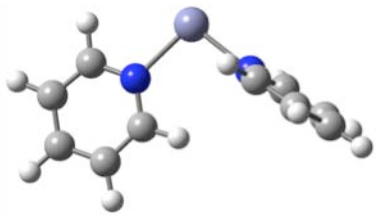
Figure S1



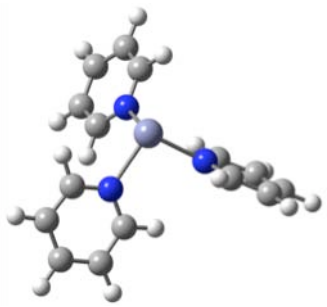
Zn(I)-1: C_{2v}



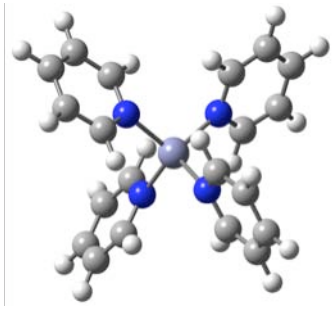
Zn(I)-2a:C_2



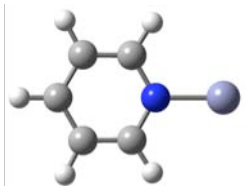
Zn(I)-2b:C_s



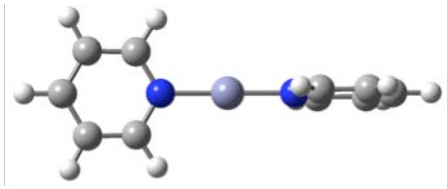
Zn(I)-3:C_3



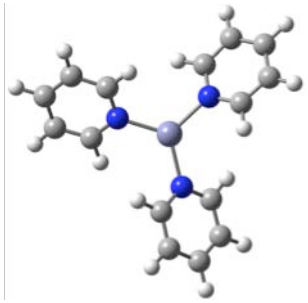
Zn(I)-4:D_{2d}



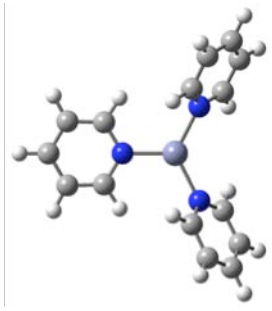
Zn(II)-1a:C_{2v}



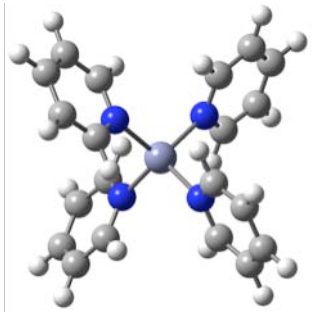
Zn(II)-2:D_{2d}



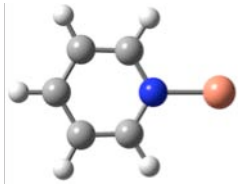
Zn(II)-3a:C_3



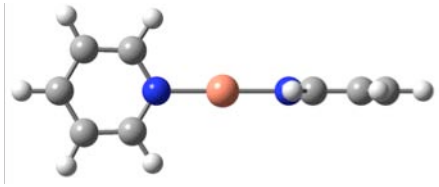
Zn(II)-3b:C_s



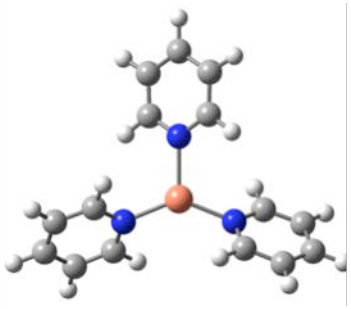
Zn(II)-4:D_{2d}

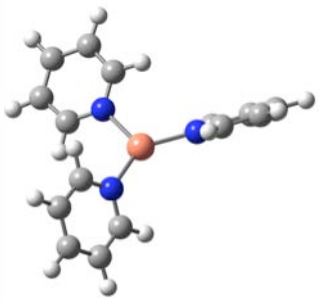


Cu(I)-1a:C_{2v}

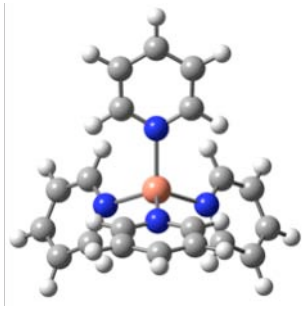


Cu(I)-2:D_{2d}

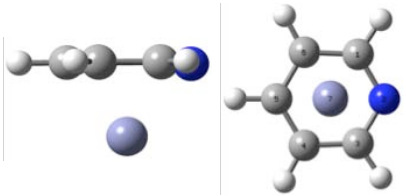




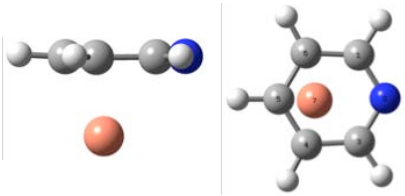
Cu(I)-3:~C_2 (2 views)



Cu(I)-4: D_{2d} (alternative view)



Zn(II)-1b:~□η-pyridine



Cu(I)-1b:~□η-pyridine

Table S2: Natural bond order analysis of charge transfer in the lower energy structural isomer of the $[Zn(pyridine)_n]^{+/2+}$ and $[Cu(pyridine)_n]^{+}$ complexes (see Table 2). The charge on N in an isolated pyridine molecule is –0.452e.

	Atomic Charge		Zn or Cu natural population			
Complex	Charge Metal	Charge N*	4s	3d	4p	4d
$[Zn(pyridine)]^{+}$	0.83	-0.64	1.12	9.98	0.07	
$[Zn(pyridine)_2]^{+}$	0.77	-0.62	1.06	9.98	0.19	
$[Zn(pyridine)_3]^{+}$	0.73	-0.59	0.92	9.98	0.36	0.01
$[Zn(pyridine)_4]^{+}$	1.30	-0.65	0.35	9.96	0.38	0.02
$[Zn(pyridine)]^{2+}$	1.63	-0.72	0.37	9.98	0.02	
$[Zn(pyridine)_2]^{2+}$	1.47	-0.71	0.50	9.94	0.08	
$[Zn(pyridine)_3]^{2+}$	1.40	-0.67	0.41	9.96	0.23	0.01
$[Zn(pyridine)_4]^{2+}$	1.31	-0.62	0.35	9.96	0.35	0.01
$[Cu(pyridine)]^{+}$	0.87	-0.64	0.25	9.87	0.01	
$[Cu(pyridine)_2]^{+}$	0.68	-0.58	0.52	9.75	0.05	
$[Cu(pyridine)_3]^{+}$	0.70	-0.57	0.33	9.78	0.18	0.01
$[Cu(pyridine)_4]^{+}$	0.67	-0.54	0.23	9.76	0.32	0.02

*Average N charge

Table S3: Selected geometric parameters and electronic data for $[Zn(pyridine)_nO_2]^{+/2+}$ complexes and $[Cu(pyridine)_nO_2]^{+}$ complexes. Bond length/bond angle degeneracy is given in parentheses. Approximate symmetries are indicated by ~. * indicates the calculation was run using Int=Ultrafine (value shown is using the standard grid), and + indicates that the calculation was performed using the 6-311++G(2df,p) basis set. The energy given in parenthesis is using the standard grid and basis set (to ensure consistency in the binding energy calculations).

Complex	sym	state	E/au	ZPE /au	Metal-N / Å	N-Metal-N / º	Metal-O / Å	N-Metal-O / º (coordinating O)
$[ZnO_2]^+$	η^1-C_s	$^2A''$	-1929.2653	0.0045			2.209, 3.061	
$[Zn(pyridine)(O_2)]^+$	η^2-C_{2v}	$^2A_2$	-2177.6784	0.0953	1.910		1.934 (2)	159.2 (2)
$[Zn(pyridine)_2(O_2)]^+$	η^2-C_1	^2A	-2426.0727	0.1872	1.982 (2)	139.6	2.027 (2)	109.0 (4)
$[Zn(pyridine)_3(O_2)]^+$	η^1-C_1	^2A	-2674.4336	0.2767	2.074, 2.060, 2.057	106.0, 107.4, 111.5	1.950, 2.484	108.7, 109.1, 114.1
	η^1-C_1	^2A	-2674.4334	0.2767	2.072, 2.058, 2.048	106.9, 109.1, 112.9	1.952, 2.471	105.8, 108.9, 113.3
$[ZnO_2]^{2+}$	η^1-C_s	$^3A''$	-1928.6730	0.0047			2.058, 3.028	
$[Zn(pyridine)(O_2)]^{2+}$	η^1-C_s	$^3A''$	-2177.2189	0.0953	1.893		2.008, 3.002	176.4
$[Zn(pyridine)_2(O_2)]^{2+}$	η^1-C_1	^3A	-2425.6840 *	0.1858	1.911, 1.914	166.3	2.362, 3.317	95.9, 97.8
$[Zn(pyridine)_3(O_2)]^{2+}$	η^1-C_1	^3A	-2674.1376 + (-2674.0944)	0.2770	1.987, 1.984, 1.986	119.5 (2), 119.8	2.464, 3.328	93.9 (2), 91.6
$[CuO_2]^+$	η^1-C_s	$^3A''$	-1790.4469	0.0046	N/a		1.947, 2.903	n/a
$[Cu(pyridine)(O_2)]^+$	η^1-C_s	$^3A''$	-2038.8682 *	0.0955	1.908		1.863. 2.822	177.5
$[Cu(pyridine)_2(O_2)]^+$	η^1-C_1	^3A	-2287.2515 *	0.1855	1.924 (2)	169.9	2.293, 3.130	93.7, 96.5
$[Cu(pyridine)_3(O_2)]^+$	η^1-C_1	^3A	-2535.6407 + (-2535.5995)	0.2753	2.027, 2.044, 2.038	120.9, 119.9, 113.7	2.091, 2.857	93.9, 99.8, 100.5

Table S4: Selected geometric parameters and electronic data for $[Zn(pyridine)_nH_2O]^{+/2+}$ complexes and $[Cu(pyridine)_nH_2O]^{+}$ complexes. Bond length/bond angle degeneracy is given in parentheses. Approximate symmetries are indicated by ~ . * indicates the calculation was run

using Int=Ultrafine (value shown is using the standard grid), and + indicates that the calculation was performed using the 6-311++G(2df,p) basis set. The energy given in parenthesis is using the standard grid and basis set (to ensure consistency in the binding energy calculations).

Complex	sym	state	E/au	ZPE /au	Metal-N / Å	N-Metal-N / º	Metal-O / Å	N-Metal-O / º
$[Zn\ H_2O]^+$	C_{2v}	$^2A_1$	-1855.3911	0.0238			2.070	
$[Zn(pyridine)\ H_2O]^+$	C_1	^2A	-2103.7706	0.1145	2.086		2.217	95.3
$[Zn(pyridine)_2\ H_2O]^+$	C_1	^2A	-2352.1267	0.2047	2.138, 2.154	100.8	2.292	92.0, 88.6
$[Zn(pyridine)_3\ H_2O]^+$	C_1	^2A	-2600.4756	0.2928	1.991, 1.989, 1.983	118.0, 117.7, 116.4	2.202	105.9, 97.5, 94.8
$[Zn\ H_2O]^{2+}$	C_{2v}	$^1A_1$	-1854.8438	0.0239			1.876	
$[Zn(pyridine)\ H_2O]^{2+}$	C_{2v}	$^1A_1$	-2103.3795	0.1152	1.884		1.889	180.0
$[Zn(pyridine)_2\ H_2O]^{2+}$	C_1	^1A	-2351.8174	0.2068	1.944 (2)	144.4	2.052	107.8 (2)
$[Zn(pyridine)_3\ H_2O]^{2+}$	C_1	^1A	-2600.2531+ (-2600.2165)	0.2965	2.011, 2.012, 2.009	115.4, 114.3, 117.4	2.122	102.1, 99.2, 105.1
$[Cu\ H_2O]^+$	C_{2v}	$^1A_1$	-1716.5763	0.0241			1.945	
$[Cu(pyridine)\ H_2O]^+$	C_1	^1A	-1964.9911*	0.1153	1.891		1.916	178.6
$[Cu(pyridine)_2\ H_2O]^+$	C_1	^1A	-2213.3521*	0.2048	1.921 (2)	169.0	2.443	95.5 (2)
$[Cu(pyridine)_3\ H_2O]^+$	C_1	^1A	-2461.6922*	0.2935	1.996, 2.024, 2.053	111.9, 117.6, 127.6	2.434	92.4, 96.2, 97.8

Section 5: Cartesian coordinates and thermochemistry for all confirmed minima.

Geometries were confirmed as minima by frequency analysis, and identified by an absence of imaginary vibrational modes. To ensure global minima were located for each value of *n*, several starting structures were investigated that involved different relative orientations of the pyridine rings and binding modes of O_2. For example, for $[Zn(pyridine)_3]^{2+}$ the following geometric structures were investigated D_{3h}, C_{2v} (two rings in the plane), C_{2v} (one ring in the plane), a C_s geometry derived from the tetrahedral-like D_{2d} geometry with a pyridine removed, and planar C_3. Many of these structures had imaginary modes (with or without symmetry constraints). Low frequency vibrational modes involving pyridine made it necessary on occasion to tighten the convergence criteria to eliminate imaginary modes (opt=tight and Int=UltraFine). Only the confirmed minima are listed below.

* indicates that the calculation was performed with Int=Ultrafine.

+ indicates that M06L/6-311++G(2df,p) was used for the opt/freq calculation

When * and/or + was necessary, the energy used in the energy calculations presented in the main text was that of a single point energy (SPE) calculation performed using the standard integration grid and the 6-311++G(d,p) basis (for consistency).

Pyridine (singlet) – C_{2v}

Zero-point correction= 0.088144 (Hartree/Particle)
Thermal correction to Energy= 0.092471
Thermal correction to Enthalpy= 0.093415
Thermal correction to Gibbs Free Energy= 0.061374
Sum of electronic and zero-point Energies= -248.221825
Sum of electronic and thermal Energies= -248.217498
Sum of electronic and thermal Enthalpies= -248.216554
Sum of electronic and thermal Free Energies= -248.248595

N	0.00000000	0.00000000	1.41822800
C	0.00000000	1.13713600	0.71886900
C	0.00000000	1.19353400	-0.67079200
C	0.00000000	0.00000000	-1.38113800
C	0.00000000	-1.19353400	-0.67079200
C	0.00000000	-1.13713600	0.71886900
H	0.00000000	-2.05445100	1.30455600
H	0.00000000	-2.15162300	-1.18005800
H	0.00000000	0.00000000	-2.46669100
H	0.00000000	2.15162300	-1.18005800
H	0.00000000	2.05445100	1.30455600

O_2 (triplet) – C_{2v}

Zero-point correction= 0.003722 (Hartree/Particle)
Thermal correction to Energy= 0.006085
Thermal correction to Enthalpy= 0.007029
Thermal correction to Gibbs Free Energy= -0.016246
Sum of electronic and zero-point Energies= -150.347665
Sum of electronic and thermal Energies= -150.345302
Sum of electronic and thermal Enthalpies= -150.344358
Sum of electronic and thermal Free Energies= -150.367633

O	0.00000000	0.00000000	0.60374300
O	0.00000000	0.00000000	-0.60374300

H_2O (singlet) – C_{2v}

Zero-point correction= 0.021578 (Hartree/Particle)
Thermal correction to Energy= 0.024413
Thermal correction to Enthalpy= 0.025357
Thermal correction to Gibbs Free Energy= 0.003938
Sum of electronic and zero-point Energies= -76.419504
Sum of electronic and thermal Energies= -76.416669
Sum of electronic and thermal Enthalpies= -76.415725
Sum of electronic and thermal Free Energies= -76.437144

O	0.00000000	0.00000000	0.11819400
H	0.00000000	0.75616600	-0.47277500
H	0.00000000	-0.75616600	-0.47277500

Zn^+ COMPLEXES

$[Zn(pyridine)]^+$ (doublet) – C_{2v}

Zero-point correction= 0.089884 (Hartree/Particle)
Thermal correction to Energy= 0.096144
Thermal correction to Enthalpy= 0.097089
Thermal correction to Gibbs Free Energy= 0.058073
Sum of electronic and zero-point Energies= -2027.206291
Sum of electronic and thermal Energies= -2027.200030
Sum of electronic and thermal Enthalpies= -2027.199086
Sum of electronic and thermal Free Energies= -2027.238101

N	0.00000000	0.00000000	-0.04335400
C	0.00000000	1.16406200	-0.72296600
C	0.00000000	1.19934400	-2.10506000
C	0.00000000	0.00000000	-2.80848400
C	0.00000000	-1.19934400	-2.10506000
C	0.00000000	-1.16406200	-0.72296600
H	0.00000000	2.07532700	-0.13337300
H	0.00000000	2.15545200	-2.61444400
H	0.00000000	0.00000000	-3.89299100
H	0.00000000	-2.15545200	-2.61444400
H	0.00000000	-2.07532700	-0.13337300
Zn	0.00000000	0.00000000	2.01597700

$[Zn(pyridine)_2]^+$ (doublet) – C_2

Zero-point correction= 0.180232 (Hartree/Particle)

Thermal correction to Energy= 0.192519
Thermal correction to Enthalpy= 0.193464
Thermal correction to Gibbs Free Energy= 0.137530
Sum of electronic and zero-point Energies= -2275.480690
Sum of electronic and thermal Energies= -2275.468403
Sum of electronic and thermal Enthalpies= -2275.467459
Sum of electronic and thermal Free Energies= -2275.523393

Zn	0.00000000	0.00000000	1.58894500
N	0.00000000	1.64412400	0.23893400
C	0.72032800	1.64437700	-0.89710600
C	0.80681300	2.75462200	-1.71887300
C	0.12124500	3.90928000	-1.35775700
C	-0.62378300	3.91360300	-0.18470000
C	-0.65459800	2.76567500	0.58873200
H	-1.21290300	2.72350600	1.52021800
H	-1.17087900	4.79251000	0.13414400
H	0.17080600	4.79507000	-1.98148800
H	1.40325600	2.71176700	-2.62223000
H	1.23948400	0.72070000	-1.13913100
N	0.00000000	-1.64412400	0.23893400
C	0.65459800	-2.76567500	0.58873200
C	0.62378300	-3.91360300	-0.18470000
C	-0.12124500	-3.90928000	-1.35775700
C	-0.80681300	-2.75462200	-1.71887300
C	-0.72032800	-1.64437700	-0.89710600
H	-1.23948400	-0.72070000	-1.13913100
H	-1.40325600	-2.71176700	-2.62223000
H	-0.17080600	-4.79507000	-1.98148800
H	1.17087900	-4.79251000	0.13414400
H	1.21290300	-2.72350600	1.52021800

$[Zn(pyridine)_2]^+$ (doublet) – C_S

Zero-point correction= 0.180140 (Hartree/Particle)

Thermal correction to Energy= 0.192456
Thermal correction to Enthalpy= 0.193400
Thermal correction to Gibbs Free Energy= 0.137286
Sum of electronic and zero-point Energies= -2275.479951
Sum of electronic and thermal Energies= -2275.467635
Sum of electronic and thermal Enthalpies= -2275.466691
Sum of electronic and thermal Free Energies= -2275.522805

Zn	-1.29941200	-0.96828400	0.00000000
N	0.76286000	-1.48202700	0.00000000
C	1.74445800	-0.56311900	0.00000000
C	3.08419500	-0.91093200	0.00000000
C	3.42517600	-2.25884600	0.00000000
C	2.41354800	-3.21153900	0.00000000
C	1.09665000	-2.78515800	0.00000000
H	0.26950300	-3.49022700	0.00000000
H	2.63610700	-4.27167400	0.00000000
H	4.46625600	-2.56233500	0.00000000
H	3.84271300	-0.13718100	0.00000000
H	1.43108100	0.47663200	0.00000000
N	-1.17643700	1.16299900	0.00000000
C	-1.18066200	1.84919400	1.15624100
C	-1.18066200	3.23305900	1.19784700
C	-1.18173700	3.93866000	0.00000000
C	-1.18066200	3.23305900	-1.19784700
C	-1.18066200	1.84919400	-1.15624100
H	-1.18598300	1.25804400	-2.06814300
H	-1.18390800	3.74287400	-2.15396000
H	-1.18632500	5.02322200	0.00000000
H	-1.18390800	3.74287400	2.15396000
H	-1.18598300	1.25804400	2.06814300

$[Zn(pyridine)_3]^+$ (doublet)* - C_3

Zero-point correction= 0.269043 (Hartree/Particle)
Thermal correction to Energy= 0.287603

Thermal correction to Enthalpy= 0.288547
Thermal correction to Gibbs Free Energy= 0.213146
Sum of electronic and zero-point Energies= -2523.743094
Sum of electronic and thermal Energies= -2523.724534
Sum of electronic and thermal Enthalpies= -2523.723590
Sum of electronic and thermal Free Energies= -2523.798991

Zn	0.00000000	0.00000000	1.30494100
N	-0.37515900	1.84488400	0.24645000
C	-1.26827500	1.97453900	-0.74870200
C	-1.57654800	3.19812600	-1.32175000
C	-0.93109100	4.33742500	-0.85541700
C	0.00000000	4.20941700	0.16980200
C	0.24162600	2.95162600	0.69616400
H	0.94648600	2.80156600	1.51125400
H	0.52723100	5.06990900	0.56385800
H	-1.15124100	5.30983300	-1.28210000
H	-2.30724700	3.25181800	-2.11998200
H	-1.74288800	1.05815500	-1.08817100
N	-1.41013700	-1.24733900	0.24645000
C	-1.07586400	-2.08562800	-0.74870200
C	-1.98138500	-2.96439400	-1.32175000
C	-3.29077500	-2.97506100	-0.85541700
C	-3.64546200	-2.10470800	0.16980200
C	-2.67699600	-1.26655900	0.69616400
H	-2.89947100	-0.58110300	1.51125400
H	-4.65428600	-2.07835900	0.56385800
H	-4.02283000	-3.65192100	-1.28210000
H	-1.66253300	-3.62404400	-2.11998200
H	-0.04494500	-2.03846300	-1.08817100
N	1.78529600	-0.59754500	0.24645000
C	2.34413900	0.11108900	-0.74870200
C	3.55793300	-0.23373200	-1.32175000
C	4.22186600	-1.36236400	-0.85541700
C	3.64546200	-2.10470800	0.16980200
C	2.43537000	-1.68506700	0.69616400

H	1.95298500	-2.22046400	1.51125400
H	4.12705500	-2.99155000	0.56385800
H	5.17407100	-1.65791300	-1.28210000
H	3.96978100	0.37222600	-2.11998200
H	1.78783300	0.98030800	-1.08817100

$[Zn(pyridine)_4]^+$ (doublet) – D_{2d}

Zero-point correction= 0.357217 (Hartree/Particle)
Thermal correction to Energy= 0.381147
Thermal correction to Enthalpy= 0.382091
Thermal correction to Gibbs Free Energy= 0.299344
Sum of electronic and zero-point Energies= -2772.009992
Sum of electronic and thermal Energies= -2771.986062
Sum of electronic and thermal Enthalpies= -2771.985118
Sum of electronic and thermal Free Energies= -2772.067866

Zn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.63666500	1.19888400
C	-1.16093200	2.12247700	1.71088500
C	-1.19815200	3.08645700	2.69581000
C	0.00000000	3.59063700	3.20541700
C	1.19815200	3.08645700	2.69581000
C	1.16093200	2.12247700	1.71088500
H	2.07519800	1.70544000	1.29712500
H	2.15588500	3.43883300	3.06000900
H	0.00000000	4.34846800	3.97994200
H	-2.15588500	3.43883300	3.06000900
H	-2.07519800	1.70544000	1.29712500
N	-1.63666500	0.00000000	-1.19888400
C	-2.12247700	-1.16093200	-1.71088500
C	-3.08645700	-1.19815200	-2.69581000
C	-3.59063700	0.00000000	-3.20541700
C	-3.08645700	1.19815200	-2.69581000
C	-2.12247700	1.16093200	-1.71088500

H	-1.70544000	2.07519800	-1.29712500
H	-3.43883300	2.15588500	-3.06000900
H	-4.34846800	0.00000000	-3.97994200
H	-3.43883300	-2.15588500	-3.06000900
H	-1.70544000	-2.07519800	-1.29712500
N	0.00000000	-1.63666500	1.19888400
C	1.16093200	-2.12247700	1.71088500
C	1.19815200	-3.08645700	2.69581000
C	0.00000000	-3.59063700	3.20541700
C	-1.19815200	-3.08645700	2.69581000
C	-1.16093200	-2.12247700	1.71088500
H	-2.07519800	-1.70544000	1.29712500
H	-2.15588500	-3.43883300	3.06000900
H	0.00000000	-4.34846800	3.97994200
H	2.15588500	-3.43883300	3.06000900
H	2.07519800	-1.70544000	1.29712500
N	1.63666500	0.00000000	-1.19888400
C	2.12247700	1.16093200	-1.71088500
C	3.08645700	1.19815200	-2.69581000
C	3.59063700	0.00000000	-3.20541700
C	3.08645700	-1.19815200	-2.69581000
C	2.12247700	-1.16093200	-1.71088500
H	1.70544000	-2.07519800	-1.29712500
H	3.43883300	-2.15588500	-3.06000900
H	4.34846800	0.00000000	-3.97994200
H	3.43883300	2.15588500	-3.06000900
H	1.70544000	2.07519800	-1.29712500

$[Zn(O_2)]^+$ (doublet) – C_S

Zero-point correction= 0.004519 (Hartree/Particle)
Thermal correction to Energy= 0.008421
Thermal correction to Enthalpy= 0.009365
Thermal correction to Gibbs Free Energy= -0.023113
Sum of electronic and zero-point Energies= -1929.260754
Sum of electronic and thermal Energies= -1929.256852

Sum of electronic and thermal Enthalpies= -1929.255907
Sum of electronic and thermal Free Energies= -1929.288386

Zn	0.00000000	0.90448300	0.00000000
O	0.42189000	-1.26412800	0.00000000
O	-0.42189000	-2.12768300	0.00000000

[Zn(pyridine)(O_2)]$^+$ (doublet) – C_{2v}

Zero-point correction= 0.095316 (Hartree/Particle)
Thermal correction to Energy= 0.104489
Thermal correction to Enthalpy= 0.105433
Thermal correction to Gibbs Free Energy= 0.058039
Sum of electronic and zero-point Energies= -2177.583045
Sum of electronic and thermal Energies= -2177.573872
Sum of electronic and thermal Enthalpies= -2177.572927
Sum of electronic and thermal Free Energies= -2177.620322

Zn	0.00000000	0.00000000	1.25085100
O	0.00000000	0.68593700	3.05957600
O	0.00000000	-0.68593700	3.05957600
N	0.00000000	0.00000000	-0.65871600
C	0.00000000	1.16964400	-1.34409000
C	0.00000000	1.19968600	-2.72377600
C	0.00000000	0.00000000	-3.42722100
C	0.00000000	-1.19968600	-2.72377600
C	0.00000000	-1.16964400	-1.34409000
H	0.00000000	-2.08097400	-0.75660900
H	0.00000000	-2.15587700	-3.23253900
H	0.00000000	0.00000000	-4.51174000
H	0.00000000	2.15587700	-3.23253900
H	0.00000000	2.08097400	-0.75660900

[Zn(pyridine)$_2$(O_2)]$^+$ (doublet) – C_1

Zero-point correction= 0.187175 (Hartree/Particle)
Thermal correction to Energy= 0.201678
Thermal correction to Enthalpy= 0.202622
Thermal correction to Gibbs Free Energy= 0.142529
Sum of electronic and zero-point Energies= -2425.885515
Sum of electronic and thermal Energies= -2425.871013
Sum of electronic and thermal Enthalpies= -2425.870068
Sum of electronic and thermal Free Energies= -2425.930162

Zn	-0.00000100	0.44148300	0.00024600
N	-1.85987500	-0.24370200	0.00000200
C	-2.22379400	-1.54218500	0.00040300
C	-3.54847700	-1.93550500	0.00025700
C	-4.53949000	-0.96033600	-0.00033200
C	-4.16859900	0.37861700	-0.00073300
C	-2.82446300	0.70316700	-0.00054500
H	-2.48493200	1.73384300	-0.00083600
H	-4.90699700	1.17105000	-0.00119000
H	-5.58662200	-1.24172100	-0.00046800
H	-3.79360600	-2.99029800	0.00059200
H	-1.42257600	-2.27310600	0.00085300
N	1.85987300	-0.24370300	0.00001600
C	2.82446200	0.70316500	-0.00029800
C	4.16859800	0.37861500	-0.00049600
C	4.53948900	-0.96033800	-0.00036600
C	3.54847600	-1.93550700	-0.00003400
C	2.22379200	-1.54218600	0.00014400
H	1.42257500	-2.27310700	0.00040100
H	3.79360400	-2.99030000	0.00008400
H	5.58662100	-1.24172300	-0.00051200
H	4.90699600	1.17104900	-0.00075100
H	2.48493200	1.73384100	-0.00038400
O	-0.00001000	2.35258000	0.67651700
O	0.00002100	2.35276600	-0.67567800

$[Zn(pyridine)_3(O_2)]^+$ (doublet) – C_1

Zero-point correction= 0.276658 (Hartree/Particle)
Thermal correction to Energy= 0.297423
Thermal correction to Enthalpy= 0.298367
Thermal correction to Gibbs Free Energy= 0.222174
Sum of electronic and zero-point Energies= -2674.156980
Sum of electronic and thermal Energies= -2674.136215
Sum of electronic and thermal Enthalpies= -2674.135271
Sum of electronic and thermal Free Energies= -2674.211464

Zn	-0.01751200	-0.02849800	0.63201200
N	-1.86758000	-0.44928800	-0.16252600
C	-2.16837000	-0.21994900	-1.45433400
C	-3.40573500	-0.51874700	-1.99591700
C	-4.37630500	-1.07872300	-1.17202000
C	-4.07084000	-1.31744800	0.16164800
C	-2.80915100	-0.99275600	0.63254500
H	-2.51274200	-1.17628200	1.66029500
H	-4.79587700	-1.75448600	0.83728300
H	-5.35584600	-1.32665600	-1.56680700
H	-3.59991200	-0.31779400	-3.04251700
H	-1.37959500	0.21614200	-2.06247400
N	1.43990200	-1.24677800	-0.16473400
C	2.00966600	-1.02394700	-1.36394400
C	2.98511400	-1.85204900	-1.89039800
C	3.39223500	-2.95755600	-1.15134600
C	2.80860600	-3.19082000	0.08673400
C	1.83694800	-2.31810300	0.54932600
H	1.33822600	-2.45706700	1.50400000
H	3.09632400	-4.03947000	0.69512700
H	4.15398200	-3.62619500	-1.53772700
H	3.41311100	-1.63222500	-2.86113200
H	1.66413800	-0.14769000	-1.90674800
N	0.47819400	1.90324800	0.06437900
C	-0.46876900	2.83597500	-0.14907400
C	-0.17105600	4.17919500	-0.30122900
C	1.15639300	4.58373600	-0.22827900

C	2.13959300	3.62668600	-0.00621700
C	1.76176700	2.30357800	0.13759700
H	2.49675500	1.52637200	0.32688300
H	3.18594400	3.89826800	0.06314800
H	1.42053800	5.63003400	-0.33736300
H	-0.96978200	4.89180500	-0.46742500
H	-1.49373400	2.47822200	-0.18834700
O	-0.08981100	-0.29822700	2.56206600
O	-0.43648300	-1.59086600	2.51706700

$[Zn(H_2O)]^+$ (doublet) – C_{2V}

Zero-point correction= 0.023754 (Hartree/Particle)
Thermal correction to Energy= 0.027668
Thermal correction to Enthalpy= 0.028612
Thermal correction to Gibbs Free Energy= -0.001273
Sum of electronic and zero-point Energies= -1855.367382
Sum of electronic and thermal Energies= -1855.363468
Sum of electronic and thermal Enthalpies= -1855.362524
Sum of electronic and thermal Free Energies= -1855.392409

Zn	0.00000000	0.00000000	0.54617300
O	0.00000000	0.00000000	-1.52433900
H	0.00000000	0.78139800	-2.09523400
H	0.00000000	-0.78139800	-2.09523400

$[Zn(pyridine)(H_2O)]^+$ (doublet) – C_1

Zero-point correction= 0.114535 (Hartree/Particle)
Thermal correction to Energy= 0.124137
Thermal correction to Enthalpy= 0.125082
Thermal correction to Gibbs Free Energy= 0.077323
Sum of electronic and zero-point Energies= -2103.656090
Sum of electronic and thermal Energies= -2103.646487

Sum of electronic and thermal Enthalpies= -2103.645543
Sum of electronic and thermal Free Energies= -2103.693301

Zn	1.65460200	-0.60679900	-0.16272100
N	-0.38041700	-0.16872100	-0.02247000
C	-0.85509100	1.06979900	-0.25420200
C	-2.20970300	1.35196600	-0.23587100
C	-3.10653900	0.32358900	0.03119800
C	-2.61736600	-0.95558700	0.26941000
C	-1.25045000	-1.16458000	0.23047700
H	-0.82207600	-2.14754500	0.40335000
H	-3.28112500	-1.78527500	0.48009800
H	-4.17369400	0.51638400	0.05117300
H	-2.54992000	2.36213100	-0.42962700
H	-0.11589800	1.83798300	-0.45788600
O	2.34223500	1.41958900	0.41753000
H	3.18890100	1.74079200	0.08452100
H	2.27568200	1.75270000	1.32097700

$[Zn(pyridine)_2(H_2O)]^+$ (doublet) – C_1

Zero-point correction= 0.204657 (Hartree/Particle)
Thermal correction to Energy= 0.220123
Thermal correction to Enthalpy= 0.221067
Thermal correction to Gibbs Free Energy= 0.158776
Sum of electronic and zero-point Energies= -2351.922008
Sum of electronic and thermal Energies= -2351.906542
Sum of electronic and thermal Enthalpies= -2351.905598
Sum of electronic and thermal Free Energies= -2351.967888

C	-1.47092500	1.33224200	0.08310700
N	-1.64021700	0.02127800	-0.15507100
C	-2.89423900	-0.45156900	-0.26363200
C	-4.01162500	0.35407700	-0.12726200
C	-3.82973000	1.71016400	0.11864300
C	-2.53598000	2.20729000	0.22417900

Zn	-0.04625400	-1.36679400	-0.56766000
N	1.66127700	-0.14164700	-0.17422800
C	2.43268700	0.21637500	-1.21486800
C	3.58937500	0.96211600	-1.06225000
C	3.97113700	1.34744700	0.21732000
C	3.17832500	0.97652300	1.29782000
C	2.03333800	0.23380500	1.06172500
H	1.38301900	-0.08676600	1.87041200
H	3.44164400	1.25486100	2.31134000
H	4.87542200	1.92659600	0.37089900
H	4.17884300	1.22710900	-1.93154800
H	2.09789600	-0.12074200	-2.19303900
H	-0.44362900	1.67804400	0.15759200
H	-2.34973100	3.25800500	0.41221800
H	-4.68366900	2.37097800	0.22178500
H	-5.00203000	-0.07494900	-0.22081100
H	-2.98262600	-1.51490500	-0.47776000
O	-0.15584800	-2.05657900	1.61505200
H	-1.01136000	-2.02658800	2.05831400
H	0.20904200	-2.92343900	1.82640700

$[Zn(pyridine)_3(H_2O)]^+$ (doublet) – C_1

Zero-point correction= 0.292789 (Hartree/Particle)
Thermal correction to Energy= 0.313822
Thermal correction to Enthalpy= 0.314766
Thermal correction to Gibbs Free Energy= 0.239281
Sum of electronic and zero-point Energies= -2600.182781
Sum of electronic and thermal Energies= -2600.161748
Sum of electronic and thermal Enthalpies= -2600.160804
Sum of electronic and thermal Free Energies= -2600.236289

H	-0.18225000	-0.91305900	2.96132400
O	-0.25548000	-0.06804800	2.50462700
H	0.14498400	0.58387400	3.08964300
Zn	0.04819300	-0.00634500	0.32466200

N	2.01195100	-0.00884400	0.05042900
C	2.72656000	-1.17351300	0.04997000
C	4.09566300	-1.20904300	-0.08384800
C	4.80904700	-0.01440700	-0.22121200
C	4.08784500	1.18389800	-0.20592500
C	2.71916500	1.15377800	-0.06939000
H	2.15057200	-2.08623300	0.17032100
H	4.60152500	-2.16763500	-0.07853700
H	5.88653600	-0.01665400	-0.33009700
H	4.58749600	2.14108000	-0.29879100
H	2.13696300	2.06980800	-0.04372400
N	-0.93821700	-1.69756100	-0.02830400
C	-2.15569900	-1.92175900	0.55121400
C	-2.95319900	-2.99400100	0.21713200
C	-2.51978500	-3.90275600	-0.75025100
C	-1.27987100	-3.67478200	-1.35732300
C	-0.53159800	-2.58241100	-0.98451500
H	-2.46801700	-1.19981200	1.29976000
H	-3.90806300	-3.11721600	0.71480100
H	-3.12713400	-4.75604200	-1.02566900
H	-0.89698500	-4.34223900	-2.12022700
H	0.42509400	-2.37268100	-1.45331100
N	-0.89290100	1.71458800	-0.01989900
C	-2.00060100	2.06494400	0.69553300
C	-2.77499900	3.16000500	0.37783400
C	-2.42868300	3.95664200	-0.71380800
C	-1.29738300	3.60165800	-1.45576000
C	-0.56900500	2.49250600	-1.09152900
H	-2.23741500	1.43431300	1.54605200
H	-3.64211600	3.38851700	0.98625900
H	-3.02035600	4.82354500	-0.98109700
H	-0.98492200	4.18113800	-2.31620500
H	0.30155900	2.18220000	-1.66168800

Zn^{2+} COMPLEXES

[Zn(pyridine)]$^{2+}$ (singlet) – C_{2v}

Zero-point correction= 0.089532 (Hartree/Particle)
Thermal correction to Energy= 0.095609
Thermal correction to Enthalpy= 0.096554
Thermal correction to Gibbs Free Energy= 0.059005
Sum of electronic and zero-point Energies= -2026.733135
Sum of electronic and thermal Energies= -2026.727058
Sum of electronic and thermal Enthalpies= -2026.726114
Sum of electronic and thermal Free Energies= -2026.763663

N	0.00000000	0.00000000	0.01348500
C	0.00000000	1.18841100	-0.65647800
C	0.00000000	1.20260900	-2.03578800
C	0.00000000	0.00000000	-2.73796900
C	0.00000000	-1.20260900	-2.03578800
C	0.00000000	-1.18841100	-0.65647800
H	0.00000000	2.10506500	-0.07772900
H	0.00000000	2.16373700	-2.53997000
H	0.00000000	0.00000000	-3.82385500
H	0.00000000	-2.16373700	-2.53997000
H	0.00000000	-2.10506500	-0.07772900
Zn	0.00000000	0.00000000	1.92332900

[Zn(pyridine)]$^{2+}$ (singlet) – ~η^6

Zero-point correction= 0.088880 (Hartree/Particle)
Thermal correction to Energy= 0.094910
Thermal correction to Enthalpy= 0.095854
Thermal correction to Gibbs Free Energy= 0.058381
Sum of electronic and zero-point Energies= -2026.675796
Sum of electronic and thermal Energies= -2026.669765
Sum of electronic and thermal Enthalpies= -2026.668821
Sum of electronic and thermal Free Energies= -2026.706294

C	-0.86599322	-1.17139002	-0.62062690
N	-0.92959581	0.00009083	-1.30903823
C	-0.86569752	1.17156424	-0.62065055
C	-0.63446829	1.22585311	0.77967341
C	-0.50875441	0.00006577	1.49228889
C	-0.63472889	-1.22570534	0.77968749
Zn	1.03102457	-0.00011157	-0.14739617
H	-0.96676259	-2.07903735	-1.21379612
H	-0.55591830	-2.18127970	1.29317457
H	-0.32129137	0.00005847	2.56421915
H	-0.55555269	2.18141676	1.29316567
H	-0.96618755	2.07922647	-1.21384460

$[Zn(pyridine)_2]^{2+}$ (singlet) – D_{2d}

Zero-point correction= 0.181212 (Hartree/Particle)
Thermal correction to Energy= 0.192953
Thermal correction to Enthalpy= 0.193897
Thermal correction to Gibbs Free Energy= 0.141452
Sum of electronic and zero-point Energies= -2275.137829
Sum of electronic and thermal Energies= -2275.126088
Sum of electronic and thermal Enthalpies= -2275.125144
Sum of electronic and thermal Free Energies= -2275.177588

C	0.00000000	1.17494616	2.58417891
N	0.00000000	0.00000000	1.89608561
C	0.00000000	-1.17494616	2.58417891
C	0.00000000	-1.20203633	3.96132530
C	0.00000000	0.00000000	4.66571697
C	-0.00000000	1.20203633	3.96132530
Zn	0.00000000	-0.00000000	0.00000000
H	0.00000000	2.09073055	2.00276190
H	0.00000000	2.15671944	4.47249363
H	0.00000000	0.00000000	5.75060713
H	0.00000000	-2.15671944	4.47249363

H	0.00000000	-2.09073055	2.00276190
N	-0.00000000	-0.00000000	-1.89608561
C	1.17494616	-0.00000000	-2.58417891
C	1.20203633	-0.00000000	-3.96132530
C	-0.00000000	-0.00000000	-4.66571697
C	-1.20203633	-0.00000000	-3.96132530
C	-1.17494616	-0.00000000	-2.58417891
H	-2.09073055	0.00000000	-2.00276190
H	-2.15671944	-0.00000000	-4.47249363
H	-0.00000000	-0.00000000	-5.75060713
H	2.15671944	-0.00000000	-4.47249363
H	2.09073055	-0.00000000	-2.00276190

$[Zn(pyridine)_3]^{2+}$ (singlet)* - C_3

Zero-point correction= 0.271481 (Hartree/Particle)
Thermal correction to Energy= 0.289128
Thermal correction to Enthalpy= 0.290072
Thermal correction to Gibbs Free Energy= 0.222483
Sum of electronic and zero-point Energies= -2523.459965
Sum of electronic and thermal Energies= -2523.442318
Sum of electronic and thermal Enthalpies= -2523.441374
Sum of electronic and thermal Free Energies= -2523.508964

Zn	0.00000000	0.00000000	0.01507200
N	0.00000000	1.98518600	0.00745900
C	-0.95756300	2.67041700	-0.66097500
C	-0.98557000	4.05121200	-0.69435000
C	-0.00154600	4.76208600	-0.01451500
C	0.98299800	4.06303700	0.67669100
C	0.95668300	2.68180300	0.66528300
H	1.70682000	2.10057300	1.19266800
H	1.76543900	4.57793700	1.22054900
H	-0.00188400	5.84661400	-0.02321600
H	-1.76851000	4.55667200	-1.24625600
H	-1.70691500	2.08023400	-1.17948200

N	-1.71922200	-0.99259300	0.00745900
C	-1.83386800	-2.16448300	-0.66097500
C	-3.01566800	-2.87913400	-0.69435000
C	-4.12331500	-2.38238200	-0.01451500
C	-4.01019200	-1.18021700	0.67669100
C	-2.80085100	-0.51238900	0.66528300
H	-2.67256000	0.42786400	1.19266800
H	-4.84733000	-0.76005400	1.22054900
H	-5.06237400	-2.92493800	-0.02321600
H	-3.06193900	-3.80991000	-1.24625600
H	-0.94807800	-2.51834800	-1.17948200
N	1.71922200	-0.99259300	0.00745900
C	2.79143100	-0.50593500	-0.66097500
C	4.00123700	-1.17207800	-0.69435000
C	4.12486100	-2.37970400	-0.01451500
C	3.02719400	-2.88282000	0.67669100
C	1.84416700	-2.16941300	0.66528300
H	0.96573900	-2.52843600	1.19266800
H	3.08189100	-3.81788400	1.22054900
H	5.06425800	-2.92167600	-0.02321600
H	4.83044800	-0.74676200	-1.24625600
H	2.65499300	0.43811500	-1.17948200

$[Zn(pyridine)_3]^{2+}$ (singlet) - C_S

Zero-point correction= 0.272172 (Hartree/Particle)
Thermal correction to Energy= 0.289716
Thermal correction to Enthalpy= 0.290660
Thermal correction to Gibbs Free Energy= 0.222477
Sum of electronic and zero-point Energies= -2523.455713
Sum of electronic and thermal Energies= -2523.438169
Sum of electronic and thermal Enthalpies= -2523.437224
Sum of electronic and thermal Free Energies= -2523.505408

Zn	0.09824600	-0.15846500	0.00000000
N	1.00001600	-0.02825000	1.76853500

C	1.88403900	-0.94337100	2.22683800
C	2.50280000	-0.81513600	3.45647700
C	2.21313500	0.29183300	4.24709200
C	1.30779800	1.23851700	3.77865700
C	0.72213300	1.04778600	2.54239900
H	2.08601400	-1.79502200	1.58515200
H	3.20153900	-1.57576400	3.78313700
H	2.68675000	0.41495300	5.21496200
H	1.05619900	2.11690600	4.36022500
H	0.01230900	1.76702800	2.14367700
N	-1.89355200	-0.16135400	0.00000000
C	-2.58491600	-0.16154700	-1.16362200
C	-3.96572000	-0.15164400	-1.19913800
C	-4.67097800	-0.14379100	0.00000000
C	-3.96572000	-0.15164400	1.19913800
C	-2.58491600	-0.16154700	1.16362200
H	-1.99800900	-0.17623100	-2.07660900
H	-4.47606000	-0.15234100	-2.15477100
H	-5.75557800	-0.13462700	0.00000000
H	-4.47606000	-0.15234100	2.15477100
H	-1.99800900	-0.17623100	2.07660900
N	1.00001600	-0.02825000	-1.76853500
C	1.88403900	-0.94337100	-2.22683800
C	2.50280000	-0.81513600	-3.45647700
C	2.21313500	0.29183300	-4.24709200
C	1.30779800	1.23851700	-3.77865700
C	0.72213300	1.04778600	-2.54239900
H	2.08601400	-1.79502200	-1.58515200
H	3.20153900	-1.57576400	-3.78313700
H	2.68675000	0.41495300	-5.21496200
H	1.05619900	2.11690600	-4.36022500
H	0.01230900	1.76702800	-2.14367700

$[Zn(pyridine)_4]^{2+}$ (singlet)

Zero-point correction= 0.362817 (Hartree/Particle)
Thermal correction to Energy= 0.386213
Thermal correction to Enthalpy= 0.387157
Thermal correction to Gibbs Free Energy= 0.306561
Sum of electronic and zero-point Energies= -2771.753976
Sum of electronic and thermal Energies= -2771.730580
Sum of electronic and thermal Enthalpies= -2771.729635
Sum of electronic and thermal Free Energies= -2771.810232

Zn	0.00000000	0.00000000	0.00000000
N	0.00000000	1.64140200	1.22394800
C	-1.15780000	2.15034800	1.69314100
C	-1.19813700	3.17521600	2.62149100
C	0.00000000	3.69904100	3.09466700
C	1.19813700	3.17521600	2.62149100
C	1.15780000	2.15034800	1.69314100
H	2.07204500	1.70869500	1.30559100
H	2.15343900	3.55077400	2.96735200
H	0.00000000	4.50227400	3.82358300
H	-2.15343900	3.55077400	2.96735200
H	-2.07204500	1.70869500	1.30559100
N	-1.64140200	0.00000000	-1.22394800
C	-2.15034800	-1.15780000	-1.69314100
C	-3.17521600	-1.19813700	-2.62149100
C	-3.69904100	0.00000000	-3.09466700
C	-3.17521600	1.19813700	-2.62149100
C	-2.15034800	1.15780000	-1.69314100
H	-1.70869500	2.07204500	-1.30559100
H	-3.55077400	2.15343900	-2.96735200
H	-4.50227400	0.00000000	-3.82358300
H	-3.55077400	-2.15343900	-2.96735200
H	-1.70869500	-2.07204500	-1.30559100
N	0.00000000	-1.64140200	1.22394800
C	1.15780000	-2.15034800	1.69314100
C	1.19813700	-3.17521600	2.62149100
C	0.00000000	-3.69904100	3.09466700

C	-1.19813700	-3.17521600	2.62149100
C	-1.15780000	-2.15034800	1.69314100
H	-2.07204500	-1.70869500	1.30559100
H	-2.15343900	-3.55077400	2.96735200
H	0.00000000	-4.50227400	3.82358300
H	2.15343900	-3.55077400	2.96735200
H	2.07204500	-1.70869500	1.30559100
N	1.64140200	0.00000000	-1.22394800
C	2.15034800	1.15780000	-1.69314100
C	3.17521600	1.19813700	-2.62149100
C	3.69904100	0.00000000	-3.09466700
C	3.17521600	-1.19813700	-2.62149100
C	2.15034800	-1.15780000	-1.69314100
H	1.70869500	-2.07204500	-1.30559100
H	3.55077400	-2.15343900	-2.96735200
H	4.50227400	0.00000000	-3.82358300
H	3.55077400	2.15343900	-2.96735200
H	1.70869500	2.07204500	-1.30559100

$[Zn(O_2)]^{2+}$ (triplet) – C_S

Zero-point correction= 0.004668 (Hartree/Particle)
Thermal correction to Energy= 0.008447
Thermal correction to Enthalpy= 0.009392
Thermal correction to Gibbs Free Energy= -0.022865
Sum of electronic and zero-point Energies= -1928.668314
Sum of electronic and thermal Energies= -1928.664535
Sum of electronic and thermal Enthalpies= -1928.663591
Sum of electronic and thermal Free Energies= -1928.695848

Zn	0.00000000	0.87612108	0.00000000
O	0.34531355	-1.15293493	0.00000000
O	-0.34531355	-2.13251911	0.00000000

$[Zn(pyridine)(O_2)]^{2+}$ (triplet) – C_S

Zero-point correction= 0.095265 (Hartree/Particle)
Thermal correction to Energy= 0.104708
Thermal correction to Enthalpy= 0.105652
Thermal correction to Gibbs Free Energy= 0.057424
Sum of electronic and zero-point Energies= -2177.123619
Sum of electronic and thermal Energies= -2177.114176
Sum of electronic and thermal Enthalpies= -2177.113231
Sum of electronic and thermal Free Energies= -2177.161460

Zn	-0.11545500	-1.11522700	0.00000000
O	0.35294100	-4.08002500	0.00000000
O	-0.36454000	-3.10805400	0.00000000
N	0.00000000	0.77389900	0.00000000
C	1.22260100	1.37985100	0.00000000
C	1.32559200	2.75394500	0.00000000
C	0.16768500	3.52867800	0.00000000
C	-1.07571300	2.90031400	0.00000000
C	-1.14025500	1.52357000	0.00000000
H	-2.09011300	0.99986700	0.00000000
H	-2.00095800	3.46560000	0.00000000
H	0.23349100	4.61199200	0.00000000
H	2.31267300	3.20302900	0.00000000
H	2.10187000	0.74552200	0.00000000

$[Zn(pyridine)_2(O_2)]^{2+}$ (triplet)* - C_1

Zero-point correction= 0.185833 (Hartree/Particle)
Thermal correction to Energy= 0.201308
Thermal correction to Enthalpy= 0.202253
Thermal correction to Gibbs Free Energy= 0.137217
Sum of electronic and zero-point Energies= -2425.498429
Sum of electronic and thermal Energies= -2425.482954
Sum of electronic and thermal Enthalpies= -2425.482010
Sum of electronic and thermal Free Energies= -2425.547045

Zn	0.04994500	-0.08001000	-0.00571500

N	1.95159800	-0.26431300	0.01279000
C	2.75145500	0.66957300	-0.56591900
C	4.12512800	0.54291100	-0.56695400
C	4.70592900	-0.56653900	0.04101400
C	3.88704400	-1.52326600	0.63441000
C	2.51915600	-1.34948000	0.60448000
H	1.84962900	-2.07383400	1.05599700
H	4.29849600	-2.40051400	1.11870600
H	5.78423500	-0.68411500	0.05261900
H	4.72648300	1.30917300	-1.04082200
H	2.26327800	1.52007900	-1.02827800
N	-1.84447400	-0.35155000	-0.01217800
C	-2.42399700	-1.15838100	-0.93984800
C	-3.78693800	-1.37266700	-0.96012700
C	-4.58654200	-0.75033800	-0.00585900
C	-3.99271700	0.07400900	0.94660800
C	-2.62579600	0.25584500	0.91963200
H	-2.12668600	0.88869600	1.64649300
H	-4.57894700	0.57424200	1.70791400
H	-5.66008500	-0.90593300	-0.00363100
H	-4.20922300	-2.02135800	-1.71798400
H	-1.76925700	-1.62679900	-1.66692200
O	0.03581700	2.28120500	0.04239400
O	-0.81862600	3.11900800	-0.11758800

$[Zn(pyridine)_3(O_2)]^{2+}$ (triplet)*+ – C_1

Zero-point correction= 0.277045 (Hartree/Particle)
Thermal correction to Energy= 0.298342
Thermal correction to Enthalpy= 0.299286
Thermal correction to Gibbs Free Energy= 0.220456
Sum of electronic and zero-point Energies= -2673.860529
Sum of electronic and thermal Energies= -2673.839232
Sum of electronic and thermal Enthalpies= -2673.838288
Sum of electronic and thermal Free Energies= -2673.917118

Zn	0.04354800	0.00297700	-0.13355200
N	-0.38147700	1.93894800	-0.25686600
C	-1.49043400	2.42874200	0.33674200
C	-1.82051400	3.76577000	0.28610300
C	-0.98605800	4.63765700	-0.39999800
C	0.15429300	4.13890400	-1.01354100
C	0.42728200	2.79059200	-0.92122600
H	-2.11726200	1.71395600	0.86185200
H	-2.71939700	4.11459700	0.77872700
H	0.83002600	4.78495000	-1.55974500
H	1.30827900	2.36128700	-1.38744900
N	1.93370700	-0.59832500	-0.18645700
C	2.30228000	-1.67783700	-0.90770000
C	3.60912900	-2.11362700	-0.95896000
C	4.57667000	-1.42291200	-0.24301300
C	4.20226600	-0.31301700	0.50181100
C	2.87866900	0.07107200	0.50723900
H	1.51630000	-2.19025400	-1.45321400
H	3.85975500	-2.98343300	-1.55302700
H	4.92585800	0.25245200	1.07539300
H	2.54451900	0.93210200	1.07805900
N	-1.42139200	-1.33123300	-0.28168100
C	-1.33562400	-2.50673400	0.37706900
C	-2.32313000	-3.46490900	0.29914200
C	-3.44133600	-3.21491900	-0.48468100
C	-3.53319100	-2.00928300	-1.16559300
C	-2.51088400	-1.09257100	-1.04151100
H	-0.44456300	-2.66287600	0.97791900
H	-2.21315700	-4.39267100	0.84648100
H	-4.38744600	-1.77639600	-1.78877700
H	-2.54411400	-0.13898100	-1.55872200
H	-1.22263300	5.69425400	-0.45599000
H	5.61141200	-1.74590700	-0.26506800
H	-4.23214900	-3.95236300	-0.56421200
O	0.03621900	-0.01242500	2.33055300
O	-0.93549900	-0.02099000	3.04670700

$[Zn(H_2O)]^{2+}$ (singlet) – C_{2v}

Zero-point correction= 0.023946 (Hartree/Particle)
Thermal correction to Energy= 0.027500
Thermal correction to Enthalpy= 0.028445
Thermal correction to Gibbs Free Energy= 0.000022
Sum of electronic and zero-point Energies= -1854.819810
Sum of electronic and thermal Energies= -1854.816255
Sum of electronic and thermal Enthalpies= -1854.815311
Sum of electronic and thermal Free Energies= -1854.843734

Zn	0.00000000	0.00000000	0.49749500
O	0.00000000	0.00000000	-1.37886400
H	0.00000000	0.79801100	-1.94696800
H	0.00000000	-0.79801100	-1.94696800

$[Zn(pyridine)(H_2O)]^{2+}$ (singlet)* – C_{2v}

Zero-point correction= 0.115233 (Hartree/Particle)
Thermal correction to Energy= 0.124268
Thermal correction to Enthalpy= 0.125212
Thermal correction to Gibbs Free Energy= 0.080411
Sum of electronic and zero-point Energies= -2103.264511
Sum of electronic and thermal Energies= -2103.255476
Sum of electronic and thermal Enthalpies= -2103.254532
Sum of electronic and thermal Free Energies= -2103.299332

Zn	0.00000000	0.00000000	1.43727500
N	0.00000000	0.00000000	-0.44718200
C	0.00000000	1.18035000	-1.13117500
C	0.00000000	1.20265000	-2.50906000
C	0.00000000	0.00000000	-3.21234600
C	0.00000000	-1.20265000	-2.50906000
C	0.00000000	-1.18035000	-1.13117500
H	0.00000000	-2.09631900	-0.55049600

H	0.00000000	-2.15921600	-3.01834200
H	0.00000000	0.00000000	-4.29741600
H	0.00000000	2.15921600	-3.01834200
H	0.00000000	2.09631900	-0.55049600
O	0.00000000	0.00000000	3.32645900
H	0.78768500	0.00000000	3.89616200
H	-0.78768500	0.00000000	3.89616200

$[Zn(pyridine)_2(H_2O)]^{2+}$ (singlet) – C_1

Zero-point correction= 0.206769 (Hartree/Particle)
Thermal correction to Energy= 0.221427
Thermal correction to Enthalpy= 0.222371
Thermal correction to Gibbs Free Energy= 0.162645
Sum of electronic and zero-point Energies= -2351.610645
Sum of electronic and thermal Energies= -2351.595987
Sum of electronic and thermal Enthalpies= -2351.595043
Sum of electronic and thermal Free Energies= -2351.654769

C	2.22110500	-1.13918200	0.79207500
N	1.85113100	-0.07157100	0.04068900
C	2.79284900	0.56689000	-0.69918800
C	4.11253200	0.16270200	-0.70623100
C	4.48978800	-0.92922500	0.07006600
C	3.52654400	-1.58671100	0.82894700
Zn	-0.00003400	0.52234600	0.00005400
N	-1.85107900	-0.07191500	-0.04035500
C	-2.22033900	-1.14098000	-0.79002600
C	-3.52574800	-1.58855100	-0.82733100
C	-4.48972900	-0.92954200	-0.07070000
C	-4.11319800	0.16386700	0.70386400
C	-2.79349900	0.56802100	0.69733100
H	-2.46030500	1.41223800	1.29245000
H	-4.83156800	0.70237000	1.31026900
H	-5.52140000	-1.26408900	-0.08325400
H	-3.77652600	-2.44393000	-1.44272800

H	-1.44137600	-1.63076300	-1.36511200
H	1.44270400	-1.62777200	1.36894700
H	3.77790100	-2.44091200	1.44574700
H	5.52145500	-1.26379300	0.08224300
H	4.83031400	0.70001100	-1.31439100
H	2.45910900	1.41000700	-1.29557800
O	-0.00029800	2.57454800	0.00057900
H	0.67599400	3.14978700	0.38171900
H	-0.67509500	3.15074200	-0.38175700

$[Zn(pyridine)_3(H_2O)]^{2+}$ (singlet)*+ - C_1

Zero-point correction= 0.296502 (Hartree/Particle)
Thermal correction to Energy= 0.317488
Thermal correction to Enthalpy= 0.318433
Thermal correction to Gibbs Free Energy= 0.242019
Sum of electronic and zero-point Energies= -2599.956613
Sum of electronic and thermal Energies= -2599.935627
Sum of electronic and thermal Enthalpies= -2599.934682
Sum of electronic and thermal Free Energies= -2600.011096

Zn	-0.00297116	-0.02148000	0.41340613
N	0.08922700	1.94663327	0.00568880
C	1.04692010	2.71569384	0.56049724
C	1.14850481	4.06729373	0.30766809
C	0.23330921	4.65832485	-0.55240197
C	-0.75270120	3.87212535	-1.13015577
C	-0.79505173	2.52630900	-0.82929401
H	-1.54937238	1.87732071	-1.26293347
H	-1.48391296	4.29276135	-1.80891399
H	0.28954561	5.71882165	-0.77047584
H	1.93480638	4.64411361	0.77817834
H	1.74900999	2.21538372	1.22145041
N	1.67903208	-1.03456640	-0.01179895
C	1.94074111	-2.21509964	0.58446158
C	3.07409525	-2.94824532	0.30163563

C	3.97738717	-2.45483151	-0.62947151
C	3.71290445	-1.24106284	-1.24720234
C	2.55950453	-0.56102418	-0.91557648
H	2.31574576	0.39070342	-1.37714157
H	4.39081537	-0.82136563	-1.97972411
H	4.87665517	-3.01030650	-0.87067307
H	3.24259312	-3.89122530	0.80641991
H	1.21001234	-2.56374850	1.30767207
N	-1.75402668	-0.91007323	-0.01953928
C	-2.91117035	-0.39323118	0.44275240
C	-4.13631607	-0.96260580	0.16659190
C	-4.18182319	-2.10699105	-0.61794492
C	-2.99569715	-2.64168283	-1.09892051
C	-1.80529071	-2.02058741	-0.78080703
H	-0.85631716	-2.40686241	-1.13883874
H	-2.98740260	-3.53166040	-1.71553279
H	-5.13119244	-2.57519798	-0.85228472
H	-5.03876799	-0.51214618	0.56053309
H	-2.83266435	0.50670247	1.04654038
O	-0.07414990	-0.14391371	2.53114158
H	-0.79570487	-0.52477063	3.04383004
H	0.55696104	0.20692084	3.16912970

$[Zn(pyridine)_2(H_2O)_2]^{2+}$ (singlet)* – C_1

Zero-point correction= 0.230457 (Hartree/Particle)
Thermal correction to Energy= 0.248659
Thermal correction to Enthalpy= 0.249603
Thermal correction to Gibbs Free Energy= 0.181332
Sum of electronic and zero-point Energies= -2428.079360
Sum of electronic and thermal Energies= -2428.061157
Sum of electronic and thermal Enthalpies= -2428.060213
Sum of electronic and thermal Free Energies= -2428.128484

H	-0.74510100	2.12523300	2.33045100
O	0.03456300	1.84732900	1.83414900

H	0.79203700	1.98390600	2.41625300
Zn	0.01715800	0.73512900	0.07611900
N	-1.79219300	-0.08179600	-0.01670000
C	-2.64370800	0.18240300	-1.03373100
C	-3.89263800	-0.40402400	-1.11857400
C	-4.28898900	-1.29502500	-0.12697300
C	-3.41702500	-1.57089400	0.92197400
C	-2.18278400	-0.95066400	0.94581900
H	-2.29871500	0.88362600	-1.78605000
H	-4.54071300	-0.16142500	-1.95183200
H	-5.26373600	-1.76856800	-0.17043900
H	-3.68604500	-2.25796000	1.71493800
H	-1.47478000	-1.13974300	1.74790300
N	1.76467100	-0.19995800	-0.06025300
C	2.92631300	0.49100800	0.00781900
C	4.15851600	-0.12942500	-0.06784200
C	4.20778800	-1.51175400	-0.22144900
C	3.01713100	-2.22693700	-0.29425000
C	1.81873000	-1.54338400	-0.21030400
H	2.84511200	1.56851600	0.11950500
H	5.06205000	0.46506200	-0.00910900
H	5.16172600	-2.02384900	-0.28481800
H	3.01121100	-3.30313400	-0.41608000
H	0.86859000	-2.06543400	-0.26692900
O	0.13211700	2.36601800	-1.20074500
H	-0.12654700	3.27053900	-0.98671500
H	0.51939700	2.38703100	-2.08415500

CU^{+} COMPLEXES

[Cu(pyridine)]$^{+}$ (singlet) – C_{2v}

Zero-point correction= 0.090399 (Hartree/Particle)
Thermal correction to Energy= 0.096436
Thermal correction to Enthalpy= 0.097381
Thermal correction to Gibbs Free Energy= 0.059807
Sum of electronic and zero-point Energies= -1888.395196
Sum of electronic and thermal Energies= -1888.389159
Sum of electronic and thermal Enthalpies= -1888.388215
Sum of electronic and thermal Free Energies= -1888.425788

N	0.00000000	0.00000000	0.05353700
C	0.00000000	1.16185800	-0.63684700
C	0.00000000	1.19659100	-2.01891000
C	0.00000000	0.00000000	-2.72526300
C	0.00000000	-1.19659100	-2.01891000
C	0.00000000	-1.16185800	-0.63684700
H	0.00000000	2.07583500	-0.05379200
H	0.00000000	2.15387100	-2.52587600
H	0.00000000	0.00000000	-3.80962400
H	0.00000000	-2.15387100	-2.52587600
H	0.00000000	-2.07583500	-0.05379200
Cu	0.00000000	0.00000000	1.95913300

[Cu(pyridine)]$^{+}$ (singlet) – ~□ɳ

Zero-point correction= 0.089044 (Hartree/Particle)
Thermal correction to Energy= 0.095427
Thermal correction to Enthalpy= 0.096371
Thermal correction to Gibbs Free Energy= 0.056933
Sum of electronic and zero-point Energies= -1888.361501
Sum of electronic and thermal Energies= -1888.355118
Sum of electronic and thermal Enthalpies= -1888.354174
Sum of electronic and thermal Free Energies= -1888.393612

C	1.18652586	1.14859413	-0.22526589
N	1.63743791	0.00003605	-0.74923653
C	1.18656738	-1.14855557	-0.22530378
C	0.27393707	-1.21387108	0.84368045
C	-0.18128474	-0.00003265	1.41238010
C	0.27389578	1.21384185	0.84372351
Cu	-1.03945444	-0.00000229	-0.48599568
H	1.57268933	2.06252850	-0.66949380
H	-0.03337152	2.17058607	1.25161722
H	-0.83451915	-0.00005932	2.27914185
H	-0.03329915	-2.17064002	1.25153978
H	1.57276560	-2.06246121	-0.66956096

$[Cu(pyridine)_2]^+$ (singlet) – D_{2d}

Zero-point correction= 0.181160 (Hartree/Particle)
Thermal correction to Energy= 0.192857
Thermal correction to Enthalpy= 0.193801
Thermal correction to Gibbs Free Energy= 0.141845
Sum of electronic and zero-point Energies= -2136.711822
Sum of electronic and thermal Energies= -2136.700125
Sum of electronic and thermal Enthalpies= -2136.699181
Sum of electronic and thermal Free Energies= -2136.751136

C	0.00000000	1.15831405	2.59629569
N	0.00000000	0.00000000	1.90198632
C	-0.00000000	-1.15831405	2.59629569
C	-0.00000000	-1.19595795	3.97875514
C	0.00000000	0.00000000	4.68608146
C	0.00000000	1.19595795	3.97875514
Cu	0.00000000	0.00000000	-0.00000000
H	0.00000000	2.07034172	2.00964069
H	0.00000000	2.15318007	4.48595437
H	0.00000000	0.00000000	5.77052544
H	-0.00000000	-2.15318007	4.48595437

H	-0.00000000	-2.07034172	2.00964069
N	0.00000000	0.00000000	-1.90198632
C	1.15831405	-0.00000000	-2.59629569
C	1.19595795	-0.00000000	-3.97875514
C	0.00000000	0.00000000	-4.68608146
C	-1.19595795	0.00000000	-3.97875514
C	-1.15831405	0.00000000	-2.59629569
H	-2.07034172	0.00000000	-2.00964069
H	-2.15318007	0.00000000	-4.48595437
H	0.00000000	0.00000000	-5.77052544
H	2.15318007	-0.00000000	-4.48595437
H	2.07034172	-0.00000000	-2.00964069

$[Cu(pyridine)_3]^+$ (singlet)* – C_1

Zero-point correction= 0.269774 (Hartree/Particle)
Thermal correction to Energy= 0.288009
Thermal correction to Enthalpy= 0.288954
Thermal correction to Gibbs Free Energy= 0.216934
Sum of electronic and zero-point Energies= -2384.965589
Sum of electronic and thermal Energies= -2384.947354
Sum of electronic and thermal Enthalpies= -2384.946410
Sum of electronic and thermal Free Energies= -2385.018429

Cu	0.00000000	0.27277900	0.00000000
N	-1.84122700	1.01385300	-0.00709600
C	-2.74502300	0.58887300	-0.91367000
C	-4.04841500	1.05426200	-0.95415200
C	-4.45635400	1.99485900	-0.01572600
C	-3.53630200	2.43486000	0.92791200
C	-2.24778500	1.92859500	0.89632100
H	-1.50037500	2.25911100	1.61041600
H	-3.80536100	3.16739400	1.67936400
H	-5.47090900	2.37747900	-0.02053400
H	-4.72810100	0.68015800	-1.71035500
H	-2.39298000	-0.15164500	-1.62613000

N	-0.00023100	-1.79553500	0.00000000
C	1.02726400	-2.49232200	-0.51839900
C	1.06541500	-3.87728700	-0.54137900
C	-0.00067200	-4.58540700	0.00000000
C	-1.06653500	-3.87694400	0.54140000
C	-1.02794600	-2.49199200	0.51840400
H	-1.84398000	-1.90289600	0.92836600
H	-1.91914400	-4.38553100	0.97535800
H	-0.00084300	-5.66988100	0.00000000
H	1.91786400	-4.38614800	-0.97533100
H	1.84348400	-1.90348900	-0.92836700
N	1.84152600	1.01347600	0.00709200
C	2.24826300	1.92814400	-0.89632100
C	3.53687600	2.43416200	-0.92790900
C	4.45684300	1.99397900	0.01572900
C	4.04872100	1.05345800	0.95415100
C	2.74524100	0.58831900	0.91366600
H	2.39305500	-0.15213500	1.62612200
H	4.72833400	0.67922100	1.71035400
H	5.47147100	2.37640400	0.02054100
H	3.80607700	3.16664600	-1.67935700
H	1.50091800	2.25880600	-1.61041700

$[Cu(pyridine)_4]^+$ (singlet) – D_{2d}

Zero-point correction= 0.360776 (Hartree/Particle)
Thermal correction to Energy= 0.384601
Thermal correction to Enthalpy= 0.385545
Thermal correction to Gibbs Free Energy= 0.304089
Sum of electronic and zero-point Energies= -2633.214186
Sum of electronic and thermal Energies= -2633.190361
Sum of electronic and thermal Enthalpies= -2633.189417
Sum of electronic and thermal Free Energies= -2633.270872

Cu	0.00000000	0.00000000	0.00000000
N	0.00000000	1.66087700	1.23924500

C	-1.14926900	2.16412900	1.72421500
C	-1.19506100	3.16412700	2.68293700
C	0.00000000	3.67658100	3.17354600
C	1.19506100	3.16412700	2.68293700
C	1.14926900	2.16412900	1.72421500
H	2.06279500	1.73248800	1.32188300
H	2.15189100	3.52949300	3.03709800
H	0.00000000	4.45864300	3.92518500
H	-2.15189100	3.52949300	3.03709800
H	-2.06279500	1.73248800	1.32188300
N	-1.66087700	0.00000000	-1.23924500
C	-2.16412900	-1.14926900	-1.72421500
C	-3.16412700	-1.19506100	-2.68293700
C	-3.67658100	0.00000000	-3.17354600
C	-3.16412700	1.19506100	-2.68293700
C	-2.16412900	1.14926900	-1.72421500
H	-1.73248800	2.06279500	-1.32188300
H	-3.52949300	2.15189100	-3.03709800
H	-4.45864300	0.00000000	-3.92518500
H	-3.52949300	-2.15189100	-3.03709800
H	-1.73248800	-2.06279500	-1.32188300
N	0.00000000	-1.66087700	1.23924500
C	1.14926900	-2.16412900	1.72421500
C	1.19506100	-3.16412700	2.68293700
C	0.00000000	-3.67658100	3.17354600
C	-1.19506100	-3.16412700	2.68293700
C	-1.14926900	-2.16412900	1.72421500
H	-2.06279500	-1.73248800	1.32188300
H	-2.15189100	-3.52949300	3.03709800
H	0.00000000	-4.45864300	3.92518500
H	2.15189100	-3.52949300	3.03709800
H	2.06279500	-1.73248800	1.32188300
N	1.66087700	0.00000000	-1.23924500
C	2.16412900	1.14926900	-1.72421500
C	3.16412700	1.19506100	-2.68293700
C	3.67658100	0.00000000	-3.17354600

C	3.16412700	-1.19506100	-2.68293700
C	2.16412900	-1.14926900	-1.72421500
H	1.73248800	-2.06279500	-1.32188300
H	3.52949300	-2.15189100	-3.03709800
H	4.45864300	0.00000000	-3.92518500
H	3.52949300	2.15189100	-3.03709800
H	1.73248800	2.06279500	-1.32188300

$[Cu(O_2)]^+$ (triplet) - C_S

Zero-point correction= 0.004585 (Hartree/Particle)
Thermal correction to Energy= 0.008463
Thermal correction to Enthalpy= 0.009407
Thermal correction to Gibbs Free Energy= -0.023089
Sum of electronic and zero-point Energies= -1790.442322
Sum of electronic and thermal Energies= -1790.438444
Sum of electronic and thermal Enthalpies= -1790.437500
Sum of electronic and thermal Free Energies= -1790.469997

1 3

Cu	-0.00000000	0.85183323	0.00000000
O	0.36742604	-1.06000733	-0.00000000
O	-0.36742604	-2.02788813	-0.00000000

$[Cu(pyridine)(O_2)]^+$ (triplet)* - C_S

Zero-point correction= 0.095528 (Hartree/Particle)
Thermal correction to Energy= 0.104968
Thermal correction to Enthalpy= 0.105912
Thermal correction to Gibbs Free Energy= 0.056943
Sum of electronic and zero-point Energies= -2038.773057
Sum of electronic and thermal Energies= -2038.763617
Sum of electronic and thermal Enthalpies= -2038.762673
Sum of electronic and thermal Free Energies= -2038.811642

C	-0.99965700	2.90635100	0.00000000
C	0.25807100	3.49794100	0.00000000
C	1.38473400	2.68394500	0.00000000
C	1.22094700	1.31172200	0.00000000
N	0.00000000	0.73080100	0.00000000
C	-1.09269700	1.52744200	0.00000000
Cu	-0.17544100	-1.16945800	0.00000000
O	-0.42729400	-3.01528800	0.00000000
O	0.37746800	-3.93726100	0.00000000
H	2.07665400	0.64550800	0.00000000
H	2.38420800	3.10062300	0.00000000
H	0.35867800	4.57753500	0.00000000
H	-1.90499400	3.50047400	0.00000000
H	-2.05653900	1.03052300	0.00000000

$[Cu(pyridine)_2(O_2)]^+$ (triplet)* – C_1

Zero-point correction= 0.185480 (Hartree/Particle)
Thermal correction to Energy= 0.201026
Thermal correction to Enthalpy= 0.201970
Thermal correction to Gibbs Free Energy= 0.136484
Sum of electronic and zero-point Energies= -2287.066523
Sum of electronic and thermal Energies= -2287.050977
Sum of electronic and thermal Enthalpies= -2287.050032
Sum of electronic and thermal Free Energies= -2287.115518

Cu	-0.05977500	-0.12730800	0.00880900
N	-1.98022600	-0.24412000	0.01969600
C	-2.75369800	0.73116700	-0.50018600
C	-4.13521500	0.65545500	-0.51381100
C	-4.75492400	-0.46296900	0.02944700
C	-3.96479600	-1.47134600	0.56784100
C	-2.58916600	-1.32930300	0.54414400
H	-1.93994100	-2.09542800	0.95409300
H	-4.40200000	-2.36140300	1.00316700
H	-5.83597000	-0.54757300	0.03374600

H	-4.70907100	1.46647400	-0.94483800
H	-2.23457400	1.59024500	-0.90982600
N	1.85110900	-0.34951600	0.00752500
C	2.45594800	-1.14666900	-0.89801300
C	3.82763700	-1.32335400	-0.93385600
C	4.61648300	-0.66019000	-0.00204000
C	4.00029900	0.15992700	0.93544800
C	2.62364800	0.29156800	0.90893800
H	2.10770500	0.92636200	1.62162900
H	4.57341900	0.69595000	1.68179000
H	5.69414300	-0.78020800	-0.00632000
H	4.26273900	-1.97184500	-1.68418100
H	1.80737800	-1.64773400	-1.60846400
O	0.97243100	2.82345200	-0.13719700
O	-0.05290900	2.16490000	-0.03958800

$[Cu(pyridine)_3(O_2)]^+$ (triplet) – C_1

Zero-point correction= 0.275280 (Hartree/Particle)
Thermal correction to Energy= 0.296920
Thermal correction to Enthalpy= 0.297864
Thermal correction to Gibbs Free Energy= 0.216789
Sum of electronic and zero-point Energies= -2535.365398
Sum of electronic and thermal Energies= -2535.343757
Sum of electronic and thermal Enthalpies= -2535.342813
Sum of electronic and thermal Free Energies= -2535.423889

Cu	-0.09504200	-0.01337900	0.10679800
N	1.01001700	-1.69974400	-0.19121000
C	2.19583000	-1.84854200	0.42054800
C	2.97293100	-2.98255400	0.27876700
C	2.51443400	-4.01093500	-0.52961800
C	1.29150500	-3.86567400	-1.16606300
C	0.57264800	-2.70188400	-0.97047000
H	2.51678300	-1.02203600	1.04838800

H	3.92107200	-3.05272100	0.79727400
H	0.89246200	-4.64350200	-1.80524200
H	-0.39162000	-2.55222900	-1.44717800
N	-2.10809100	-0.03361200	-0.12895300
C	-2.72737500	0.82802900	-0.95189800
C	-4.09849900	0.84637900	-1.12190500
C	-4.87250000	-0.05870100	-0.41247900
C	-4.24237100	-0.95048200	0.44149800
C	-2.86590900	-0.90677900	0.55438400
H	-2.08718100	1.52418600	-1.48565300
H	-4.54691500	1.56327000	-1.79847800
H	-4.80601600	-1.67415400	1.01712000
H	-2.33507100	-1.58574400	1.21508400
N	0.94512200	1.71753400	-0.21091300
C	0.62566700	2.83183700	0.46755900
C	1.31431000	4.02083500	0.32152400
C	2.38002200	4.07223300	-0.56346200
C	2.71654700	2.92799300	-1.26979300
C	1.97940000	1.77725700	-1.06456600
H	-0.21378800	2.75102500	1.15202900
H	1.01567100	4.88915500	0.89564200
H	3.54156300	2.92073000	-1.97132300
H	2.21454000	0.85960300	-1.59579400
H	3.10084800	-4.91325000	-0.66071900
H	-5.95091700	-0.06795100	-0.52246800
H	2.94022300	4.99018700	-0.70036800
O	-0.19597400	-0.01920800	2.19521200
O	0.88039600	0.09897000	2.78952700

$[Cu(H_2O)]^+$ (singlet) – C_{2v}

Zero-point correction= 0.024053 (Hartree/Particle)
Thermal correction to Energy= 0.027979
Thermal correction to Enthalpy= 0.028924
Thermal correction to Gibbs Free Energy= -0.000292
Sum of electronic and zero-point Energies= -1716.552227

Sum of electronic and thermal Energies= -1716.548301
Sum of electronic and thermal Enthalpies= -1716.547356
Sum of electronic and thermal Free Energies= -1716.576572

H	0.00000000	-0.77683876	1.98739600
O	0.00000000	-0.00000000	1.41696800
H	-0.00000000	0.77683876	1.98739600
Cu	0.00000000	0.00000000	-0.52790400

[Cu(pyridine)$(H_2O)]^+$ (singlet) – C_1

Zero-point correction= 0.115290 (Hartree/Particle)
Thermal correction to Energy= 0.124598
Thermal correction to Enthalpy= 0.125543
Thermal correction to Gibbs Free Energy= 0.079345
Sum of electronic and zero-point Energies= -1964.876210
Sum of electronic and thermal Energies= -1964.866901
Sum of electronic and thermal Enthalpies= -1964.865957
Sum of electronic and thermal Free Energies= -1964.912155

Cu	-1.46111700	-0.00396100	-0.00001100
N	0.43008500	-0.00425300	-0.00000300
C	1.12682400	-1.16198900	-0.00000200
C	2.50922700	-1.19381100	0.00000400
C	3.21217200	0.00487100	0.00000700
C	2.50151400	1.19896000	0.00000500
C	1.11932300	1.15811400	0.00000000
H	0.53075500	2.06869300	-0.00000100
H	3.00554800	2.15746000	0.00000800
H	4.29645900	0.00838500	0.00001100
H	3.01959200	-2.14895900	0.00000500
H	0.54424900	-2.07632000	-0.00000400
O	-3.37675800	0.04482500	0.00002300
H	-3.91757100	-0.13002000	-0.77740900
H	-3.91754200	-0.13007400	0.77746200

$[Cu(pyridine)_2(H_2O)]^+$ (singlet) – C_1

Zero-point correction= 0.204779 (Hartree/Particle)
Thermal correction to Energy= 0.220214
Thermal correction to Enthalpy= 0.221158
Thermal correction to Gibbs Free Energy= 0.159042
Sum of electronic and zero-point Energies= -2213.147736
Sum of electronic and thermal Energies= -2213.132301
Sum of electronic and thermal Enthalpies= -2213.131356
Sum of electronic and thermal Free Energies= -2213.193473

C	-2.51651800	-1.16794400	-0.70601800
N	-1.91186800	-0.17086100	-0.02676300
C	-2.69106200	0.68815100	0.66311100
C	-4.07047900	0.58109000	0.69781300
C	-4.68508600	-0.44668200	-0.00704900
C	-3.89038000	-1.33411700	-0.72202700
Cu	0.00000900	0.01269000	-0.00017600
N	1.91187700	-0.17088200	0.02667100
C	2.51640300	-1.16809200	0.70584600
C	3.89026400	-1.33427000	0.72206700
C	4.68509700	-0.44670300	0.00739400
C	4.07061700	0.58120100	-0.69738500
C	2.69119400	0.68825600	-0.66290700
H	2.16987800	1.47795300	-1.19266900
H	4.64814600	1.29606400	-1.27077800
H	5.76402200	-0.55481200	-0.00103600
H	4.32261400	-2.15134800	1.28647500
H	1.86344800	-1.84362100	1.24737500
H	-1.86365900	-1.84337500	-1.24778500
H	-4.32283200	-2.15108900	-1.28651200
H	-5.76401000	-0.55478900	0.00155000
H	-4.64790500	1.29584700	1.27144100
H	-2.16965200	1.47775100	1.19292300
O	-0.00006700	2.45575400	-0.00002000

H	-0.49444900	3.04206100	-0.58159500
H	0.49431000	3.04217900	0.58144100

$[Cu(pyridine)_3(H_2O)]^+$ (singlet) – C_1

Zero-point correction= 0.293467 (Hartree/Particle)
Thermal correction to Energy= 0.315339
Thermal correction to Enthalpy= 0.316283
Thermal correction to Gibbs Free Energy= 0.237257
Sum of electronic and zero-point Energies= -2461.399220
Sum of electronic and thermal Energies= -2461.377348
Sum of electronic and thermal Enthalpies= -2461.376404
Sum of electronic and thermal Free Energies= -2461.455430

H	-0.15095900	0.91784300	3.01903000
O	0.06616200	0.11137100	2.54128100
H	-0.18084400	-0.60239400	3.13741200
Cu	0.06994600	-0.14196400	0.12100500
N	-1.60646200	-1.27186900	0.01786000
C	-2.72627300	-0.90249200	0.66830900
C	-3.91342200	-1.61339000	0.59570200
C	-3.96113800	-2.76118800	-0.18658600
C	-2.81287400	-3.15199000	-0.86459500
C	-1.66501300	-2.38696900	-0.73433900
H	-2.64835000	0.00223800	1.26533000
H	-4.78259800	-1.26815000	1.14307400
H	-4.87494300	-3.33961500	-0.26593500
H	-2.79943600	-4.04031200	-1.48479200
H	-0.74638500	-2.66742100	-1.24159900
N	-0.32969300	1.84951000	-0.17541200
C	0.50346800	2.78471000	0.31673500
C	0.30371100	4.14469700	0.14099200
C	-0.80296900	4.57070800	-0.58415000
C	-1.66784300	3.61454700	-1.10225600
C	-1.39734300	2.27423600	-0.87419300
H	1.36566000	2.41122200	0.86419200

H	1.00924600	4.85238500	0.56005200
H	-0.98581100	5.62748500	-0.74479500
H	-2.54184900	3.89781700	-1.67672200
H	-2.05118400	1.49751400	-1.26184200
N	1.96096900	-0.74588600	-0.08457800
C	2.81750600	-0.74644200	0.95717900
C	4.14695200	-1.11752900	0.84026500
C	4.63265800	-1.50978300	-0.40126400
C	3.76019900	-1.51132600	-1.48294200
C	2.44496800	-1.12585600	-1.28455600
H	2.39690100	-0.43457700	1.90794900
H	4.78740300	-1.09745000	1.71418200
H	5.66832000	-1.80659800	-0.52376400
H	4.08884100	-1.80696000	-2.47221200
H	1.73904600	-1.11093800	-2.10984800