Supporting information for:

How the nature and charge of metal cations affect vibrations in acetone solvent molecules

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Experimental and calculated vibrational spectra of low-lying isomers of $Ni^{2+}(Ace)_4$ in triplet and singlet states (Fig. S1); Mass spectrum (Fig. S2); Mass-gated mass spectrum (top) and difference mass spectrum (bottom) of $Cu^+(Ace)(N_2)_2$ losing N_2 (Fig. S3); Correlation of red shift in C=O stretch frequency of $M^+(Ace)$ with ionic radius (Fig. S4); Correlation of red shift in C=O stretch frequency with change in populations in antibonding orbitals $\Delta\sigma^*(CO)$ (top) and $\Delta\pi^*(CO)$ (bottom) (Fig. S5); Correlation of red shift in C=O stretch frequency with hardness for closed-shell ions (Fig. S6); Experimental vibrational spectra highlighting the region below the carbonyl stretch and simulated spectra of low-lying isomers of $Cu^+(Ace)(N_2)_2$ and $Cu^+(Ace)_4$ (Fig. S7); Energies, geometries, vibrational frequencies and intensities of $Cu^+(Ace)(N_2)_k$ (k = 0-2), $Cu^+(Ace)_4$ and $M^{2+}(Ace)_4$ (M = Co, Ni, Cu, and Zn) at the B3LYP+D3/6-311+G(d,p) level of theory (Table S1) and ωB97X-D/6-311+G(d,p) (Table S2); Calculated bond lengths and angles of $M^{2+}(Ace)_4$, M = Co, Ni, Cu, and Zn, $Cu^+(Ace)_4$, $Cu^+(Ace)(N_2)_k$ (k = 0–2) and $Al^+(Ace)(N_2)$ (Table S3, page 103); Properties of the metal cations and of the complexes calculated at the B3LYP+D3/6-311+G(d, p) (for $Z < 37$) and B3LYP+D3/Def2-TZVP (for $Z \geq 37$) level of theory (Table S4, page 104).

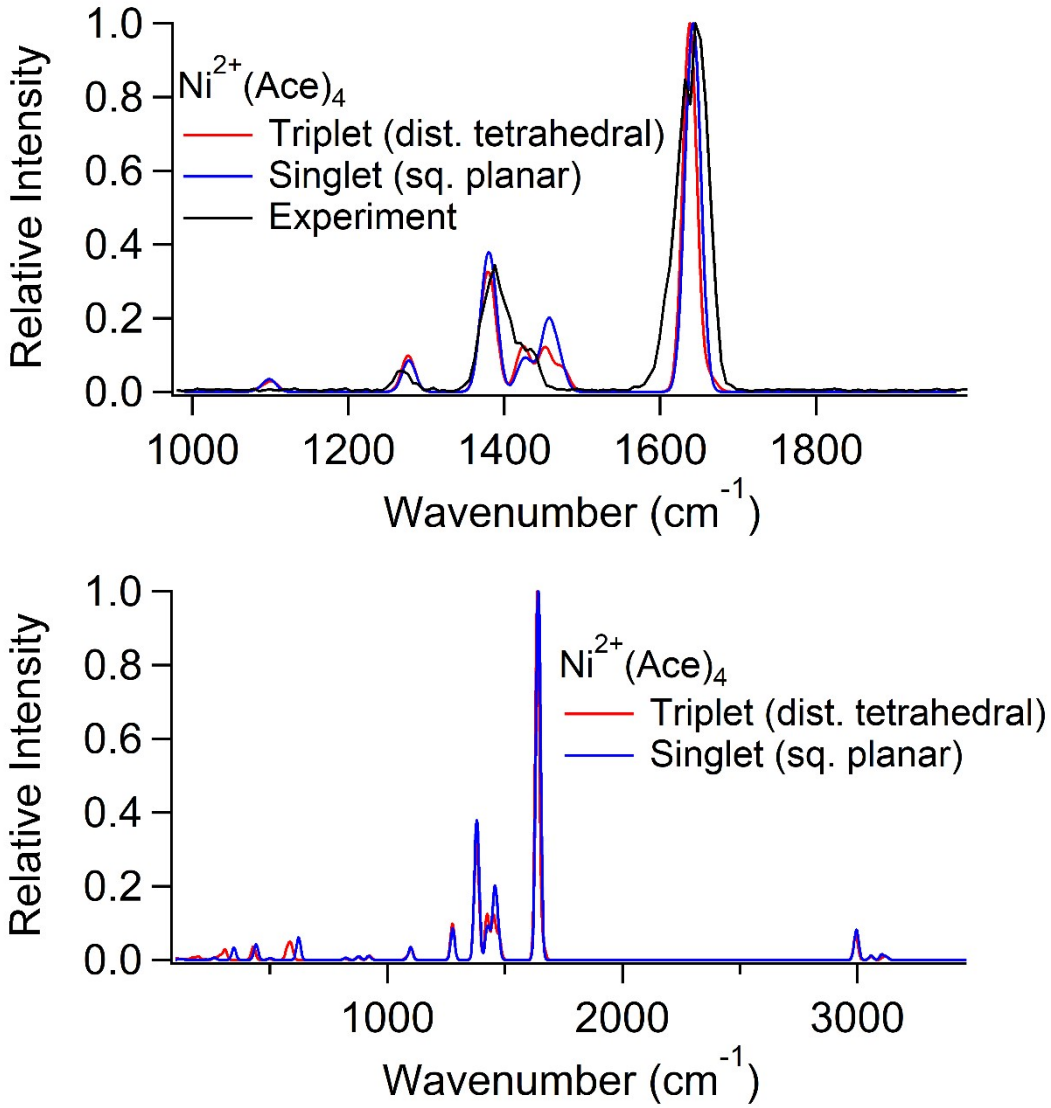


Figure S1. (top) Experimental photodissociation spectrum of $Ni^{2+}(Ace)_4$ (black). Simulated spectra of the lowest-lying isomer of $Ni^{2+}(Ace)_4$ in triplet state (red) and in singlet state (blue) at the B3LYP+D3/6-311+G(d,p) level of theory. (bottom) Simulated spectra of the lowest-lying isomer of $Ni^{2+}(Ace)_4$ in triplet state (red) and in singlet state (blue) from 100 cm^{-1} to 3500 cm^{-1} at the B3LYP+D3/6-311+G(d,p) level of theory.

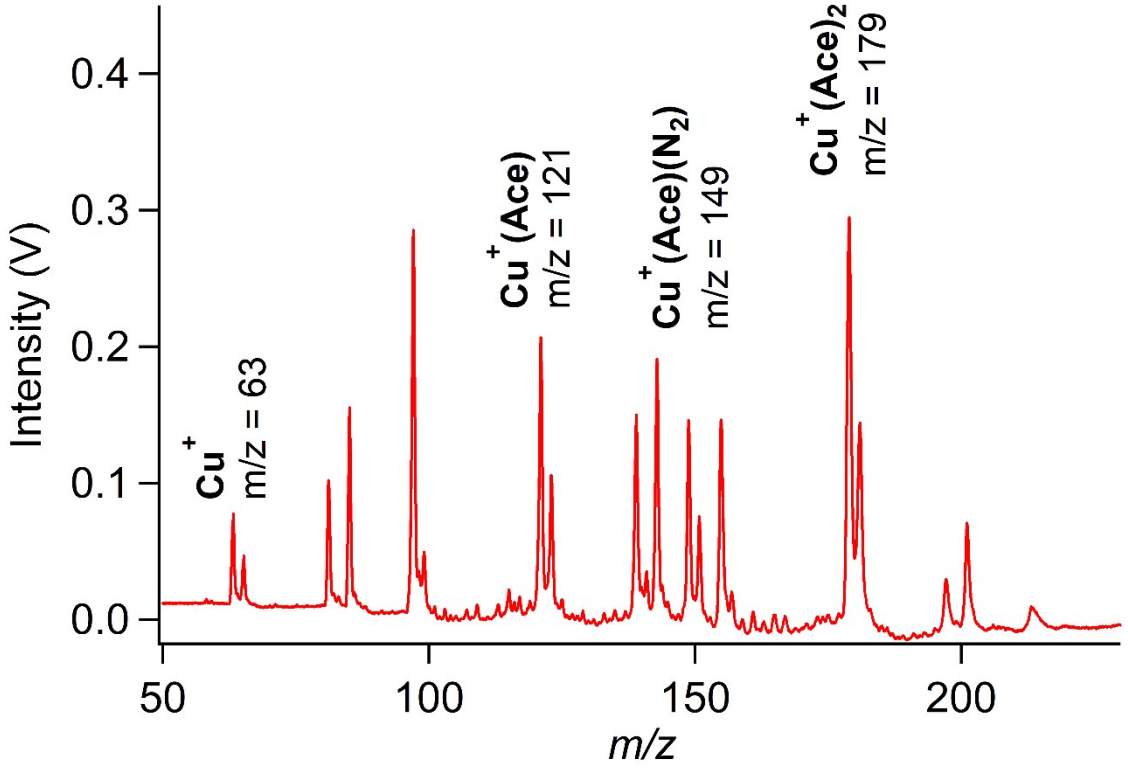


Figure S2. Mass spectrum of ions formed by ablating a copper rod in 0.08% acetone/10% N_2/He mixture. Copper-containing peaks are labeled. The labels indicate stoichiometry, not the structure. Other $M^+(Ace)_n$ (M=Al, Na, K) are also observed.

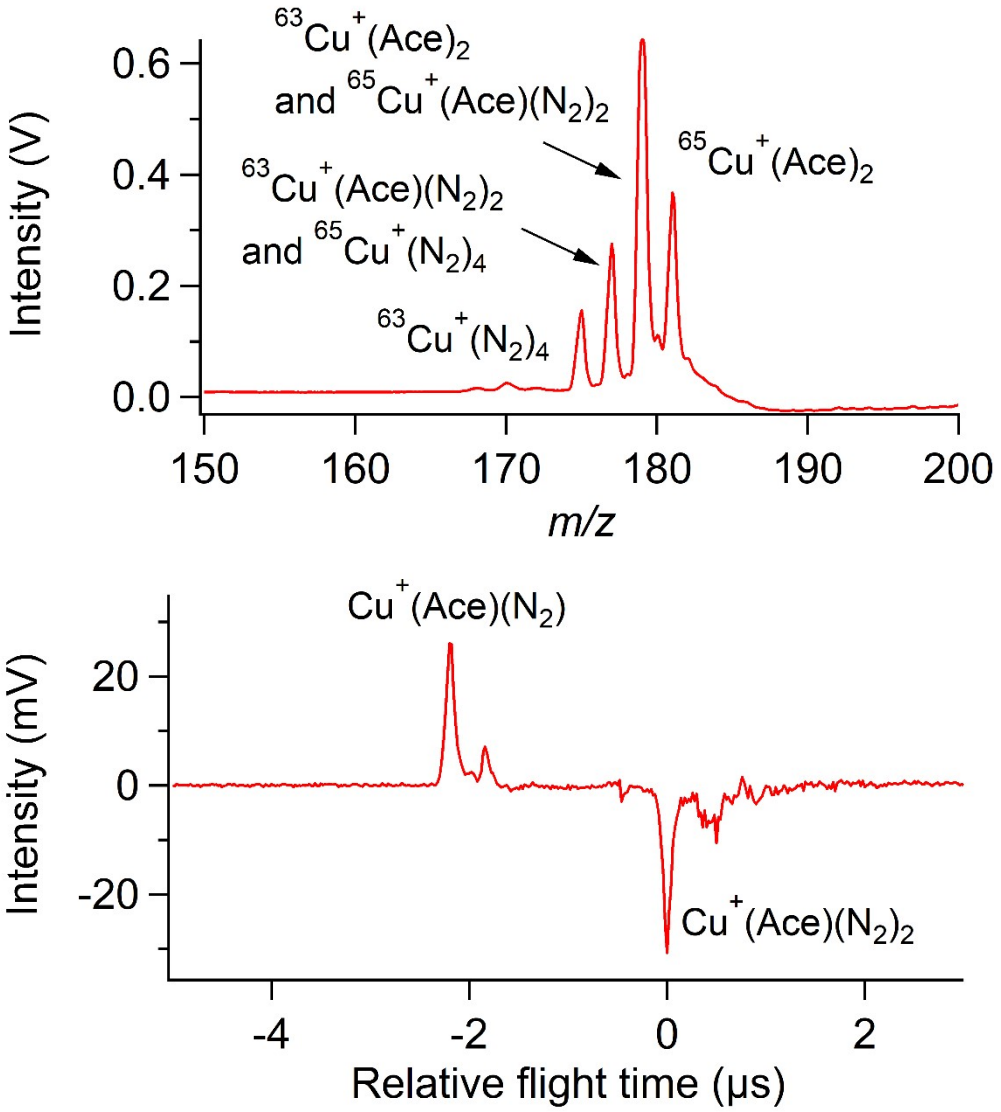


Figure S3. (top) Portion of the mass spectrum of ions formed by ablating a copper rod in 0.08% acetone/20% N_2/He. A mass gate is used to suppress the lighter ions. (bottom) Laser on – laser off difference mass spectrum measured at 1679 cm^{-1} showing loss of N_2 from $Cu^+(Ace)(N_2)_2$.

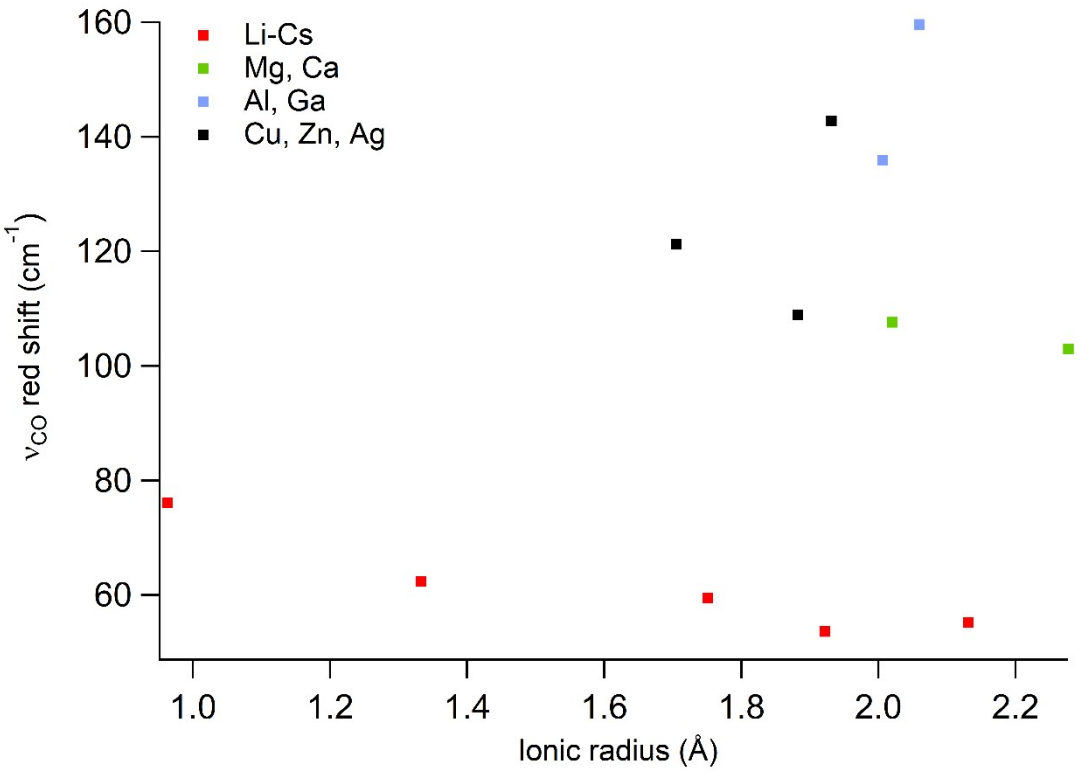


Figure S4. Correlation of red shift in C=O stretch frequency of M^+(Ace) with ionic radius.

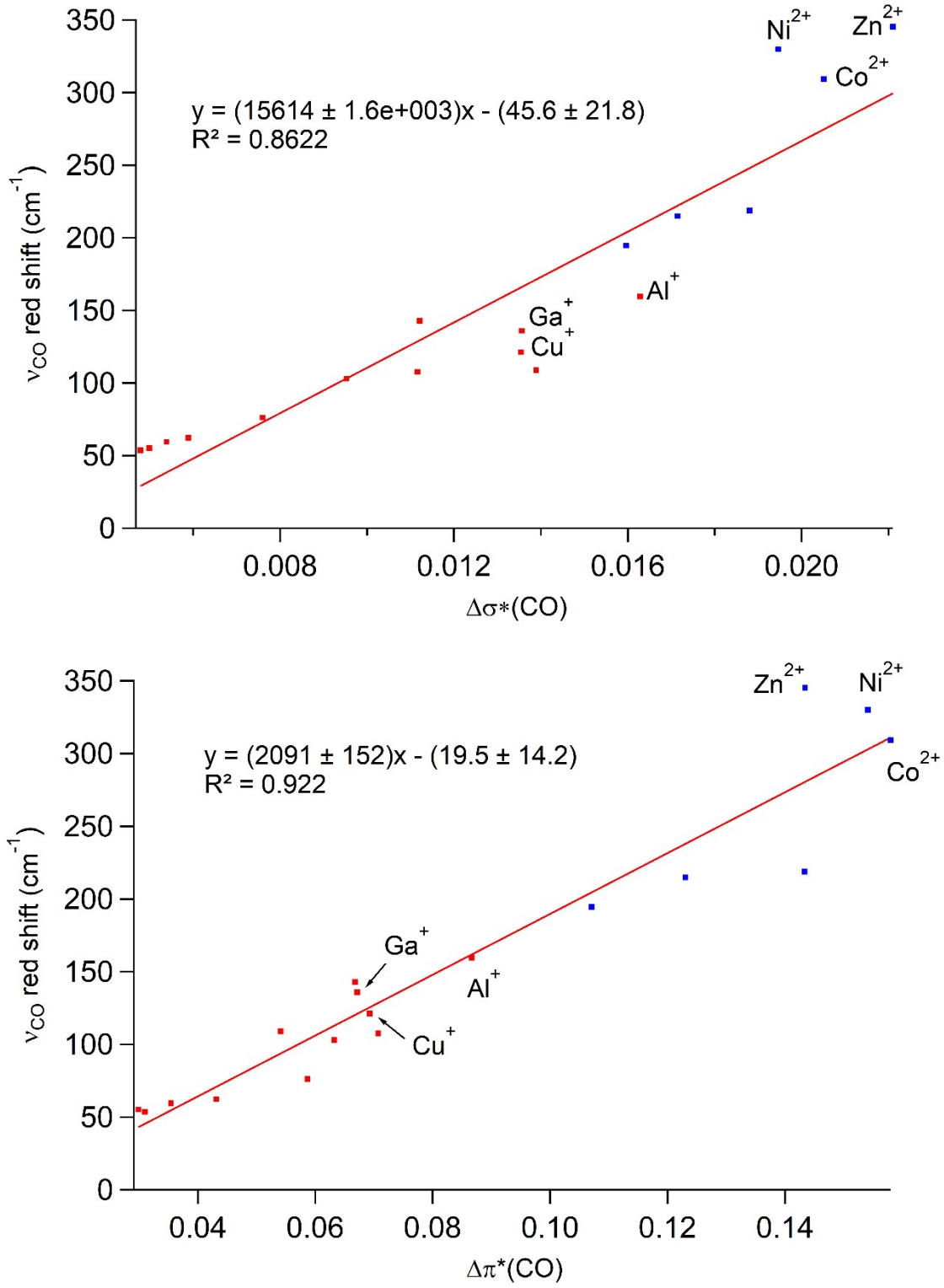


Figure S5. Correlation of red shift in C=O stretch frequency with change in populations in antibonding orbitals Δσ*(CO) (top) and Δπ*(CO) (bottom). Cations are shown in red and dications in blue.

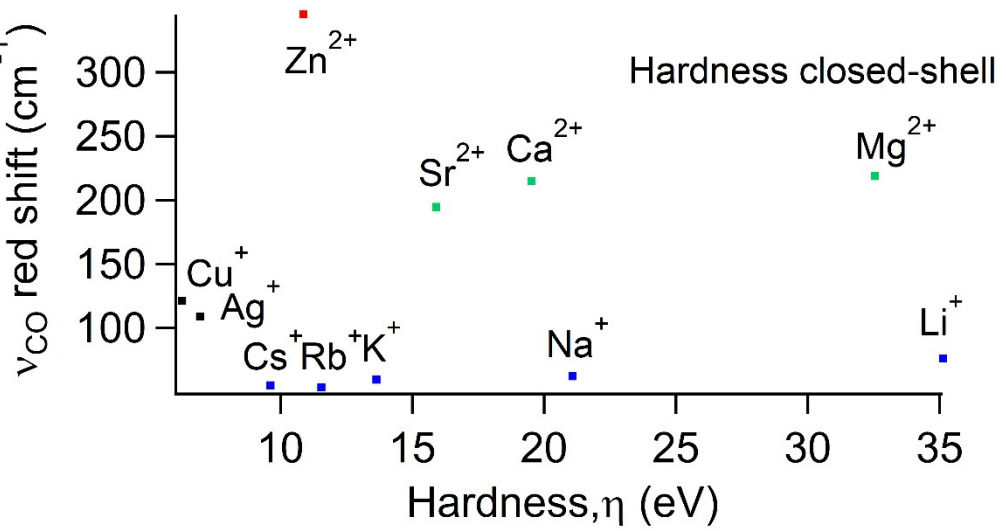


Figure S6. Correlation of red shift in C=O stretch frequency with hardness for closed-shell ions.

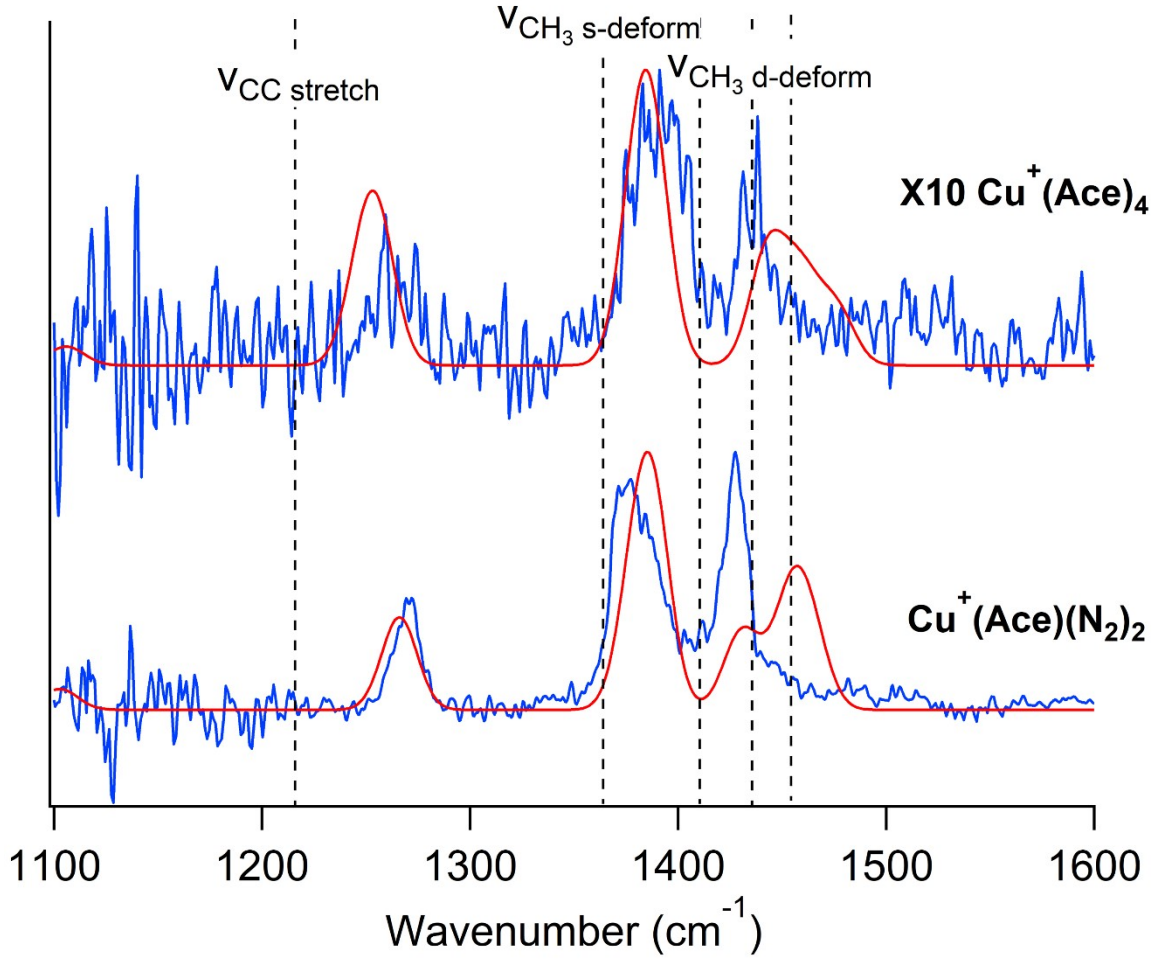


Figure S7. Experimental photodissociation spectrum of $Cu^+(Ace)(N_2)_2$ (blue) and ten times zoom in experimental photodissociation spectrum of $Cu^+(Ace)_4$ (blue). Simulated spectra of the lowest-lying isomer of $Cu^+(Ace)(N_2)_2$ and $Cu^+(Ace)_4$ at the B3LYP+D3/6-311+G(d,p) level of theory (red).

Table S1: Energies, unscaled vibrational frequencies, intensities (km/mol), and geometries (xyz coordinates) of $Cu^{+}(Ace)_n(N_2)_k$ (n = 1 and 4, k = 0–2) and $M^{2+}(Ace)_4$ (M = Co, Ni, Cu, and Zn) calculated at the B3LYP+D3/6-311+G(d,p) level of theory.

Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
Cu	1	-1640.176877	-1640.176877

Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
N_2	1	-109.5596937	-109.5541247

Frequency	Intensity
2444.4701	0

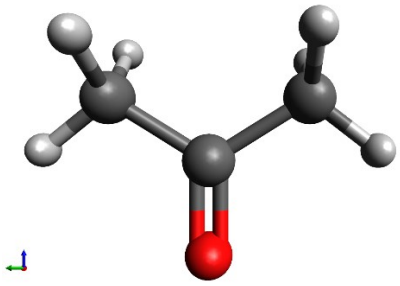
Atom	Standard Orientation		
N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	-1.09557600

Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
C_3H_6O	1	-193.2225414	-193.1393914

Frequency	Intensity
27.1	0
130.1	0.04
389.2	1.5
491.6	0.41
540.6	13.2
785.4	1.77
883.7	0.02
888.3	9.24
1085.1	0
1116.2	2.56
1232.2	74.62
1385.8	22.72
1387.5	61.06
1460.3	1.3
1463.9	2.23
1470.6	28.63
1487.4	24.02
1787.1	210.38
3021	1.43
3027.9	6.88
3077	0.24

3084.4	19.96
3137.5	12.32
3138.7	7.28

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	0.00000000	-1.28890000	-0.80043500
O	0.00000000	-1.28890000	-2.01182700
C	0.00000000	-2.57780000	0.00000000
H	-0.83942800	-2.59138200	0.70227200
H	-0.06190700	-3.43433400	-0.66992100
H	0.91588300	-2.64369400	0.59661100
H	-0.91588300	0.06589400	0.59661100
H	0.83942800	0.01358200	0.70227200
H	0.06190700	0.85653400	-0.66992100

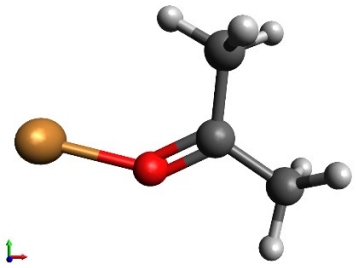


Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
Cu^{+}(Ace)	1	-1833.488851	-1833.404157

Frequency	Intensity
94.1	5.9
106.1	0.83
115.2	5.66
140.3	7.07
283.1	3.32
428.5	4.87
496	0.53
588.3	19.05
825.7	0.3
886.8	1.44
931.5	5.68
1093	1.28
1110.1	10.53
1283.2	31.88
1389.4	41.73

1399.5	79.19
1437.4	36.48
1448.8	7
1468.3	40.43
1477.9	31.52
1665.9	284.67
3020	9.59
3026.5	11.64
3085.9	0.73
3091.3	3.16
3125.3	6.79
3158.4	0.99

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-0.13629500	-1.48547600	0.00703200
O	-1.24649400	-2.04732300	0.01638900
Cu	-3.06647600	-1.50319300	0.00189500
C	1.09038300	-2.33134400	0.00432700
H	1.84234500	-1.92384300	0.68490800
H	0.85682600	-3.36528300	0.25023500
H	1.52541800	-2.29025600	-1.00260300
H	0.34441100	0.31811500	0.99161200
H	0.76611500	0.31712600	-0.71185200
H	-0.94923600	0.49033200	-0.22257400

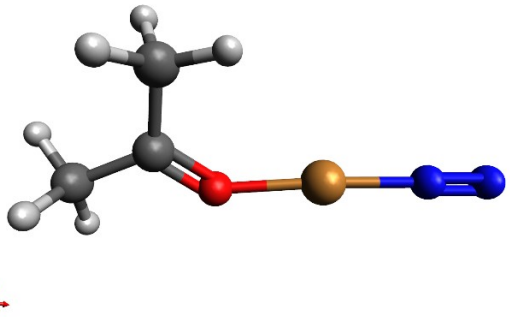


Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)(N_2)$	1	-1943.090828	-1942.998146

Frequency	Intensity
48.7	0.6
50.4	0.64
98.7	2.26
108.2	0.56
122	2.53

154.5	5.85
256.4	4.26
273.3	0.55
275.8	1.62
373.7	2.17
443.4	3.2
497.2	0.42
593.6	20.44
829.2	0.59
886.6	1.74
931.6	5.46
1096.1	1.55
1111.7	10.99
1286.3	36.31
1390.8	51.1
1400.9	83.88
1439	40.72
1449.8	5.79
1468.3	40.93
1478.8	30.23
1676.3	375.69
2427.7	13.67
3020.6	10.02
3027.1	11.06
3086	0.28
3091.7	2.44
3130.9	6.64
3157.8	0.84

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	0.06809100	-1.49029200	-0.00586600
O	1.15394800	-2.09733800	-0.01715700
Cu	2.98538900	-1.70885100	-0.00739500
N	4.85029500	-1.44495900	0.00045800
N	5.93683300	-1.29356600	0.00499900
C	-1.19456200	-2.27960900	0.00115100
H	-1.93242000	-1.83738400	-0.67302000
H	-1.00870100	-3.32230800	-0.24869300
H	-1.62193000	-2.22280800	1.01066000
H	-0.33258800	0.33166700	-0.99125200
H	-0.75005500	0.35149300	0.71285900
H	0.97085900	0.44634800	0.21857100

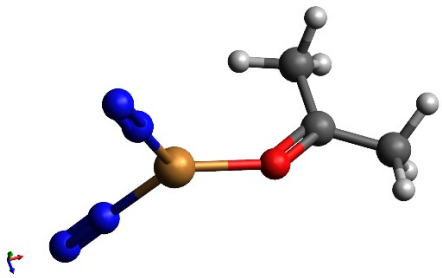


Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)(N_2)_2$	1	-2052.658306	-2052.559437

Frequency	Intensity
11.6	0.69
22.2	0.79
39.1	0.19
45	0.36
92.1	2.56
92.6	1.54
100.2	2.75
133.3	2.05
177.8	0.02
184.6	0.1
205.9	0.42
217.2	0.85
229.8	3.87
247.9	1.85
280.1	1.33
422	5.14
496.1	0.54
571.7	21.35
822.9	0.46
887	1.24
925.8	4.99
1094	1.03
1113.7	8.48
1279	38.17
1393.2	43.3
1402	77.28
1444.4	29.6
1453.1	5.61
1468.6	41.61
1478.9	27.34

1698.5	350.89
2422.5	12.18
2430.2	4.11
3023.6	4.86
3029.9	7.03
3085.9	0.14
3092.4	1.84
3128.1	8.82
3155.6	1.13

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-0.12728800	0.13845900	1.48408600
O	-1.23402200	0.19775100	2.03525700
Cu	-3.13113100	0.13700300	1.60221200
N	-4.21641400	-1.53127700	1.49265400
N	-4.80539800	-2.45503800	1.44212900
N	-4.17776500	1.84685300	1.42368100
N	-4.73640900	2.78629200	1.33669800
C	1.11197400	0.20838700	2.31350400
H	1.84336900	0.88182900	1.85882000
H	0.88403700	0.51393700	3.33279200
H	1.57276600	-0.78688800	2.32880000
H	0.36050100	0.95099700	-0.40930600
H	0.74808700	-0.75368900	-0.25825500
H	-0.95852100	-0.24593000	-0.45898300



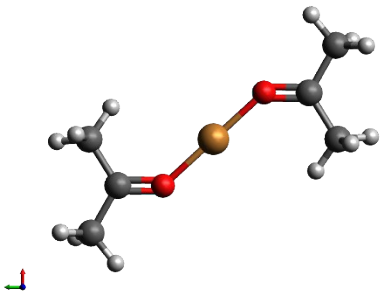
Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)_2$	1	-2026.792808	-2026.622632

Frequency	Intensity
9	4.13
38.6	3.77
39.9	2.69
90.2	0.07

93.5	0.39
102.4	0.32
103.2	0.83
110.7	0.74
136	0.15
170.8	3.18
199.9	10.28
232.4	0
334.9	1.01
422.7	0
443.8	11.02
495.6	0.18
496.7	0.69
589.3	0
610.2	36.04
824.1	0.01
827	1.73
889.4	2.97
889.5	0
931	1.03
931.2	8.82
1095.4	0.03
1096.2	1.09
1112.8	2.74
1113	14.73
1283.1	0.35
1283.2	73.46
1393.3	89.12
1393.5	0.02
1402.5	144.2
1402.5	10.53
1443.8	72.45
1443.8	0.11
1453.1	11.3
1453.2	0.9
1469.5	64.26
1469.7	2.12
1480.5	16.1
1480.8	41.49
1685.6	687.75
1693.5	0.02
3023.1	1.04
3023.1	10.13
3029.4	11.15
3029.4	0

3086.4	0.28
3086.4	0.02
3092.5	0.23
3092.5	2.44
3131.5	11.41
3131.6	0.1
3155.9	0.02
3155.9	2.45

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-1.27597500	-0.77670400	-0.05199500
O	-1.29015200	-2.01672100	-0.06766800
Cu	0.00000000	-3.38441300	-0.06371500
O	1.29015200	-4.75210500	-0.06766800
C	1.27597500	-5.99212200	-0.05199500
C	0.00000000	-6.76882600	0.00000000
H	0.03293200	-7.61840600	-0.68627300
H	-0.10825900	-7.18360300	1.00936100
H	-0.86113500	-6.13618500	-0.21815000
C	2.57247100	-6.73035800	-0.08203200
H	2.56534300	-7.55282000	0.63800100
H	2.68498900	-7.18499100	-1.07395400
H	3.40913200	-6.05922800	0.10175100
C	-2.57247100	-0.03846800	-0.08203200
H	-2.56534300	0.78399400	0.63800100
H	-2.68498900	0.41616500	-1.07395400
H	-3.40913200	-0.70959800	0.10175100
H	-0.03293200	0.84958000	-0.68627300
H	0.10825900	0.41477700	1.00936100
H	0.86113500	-0.63264100	-0.21815000



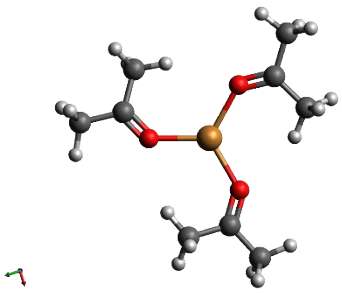
Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)_3$	1	-2220.044301	-2219.789693

Frequency	Intensity
14.9	0.07
16.6	0.06
25.6	6.92
31.9	2.23
36	0.97
39	0.79
81.4	0.09
81.9	0.13
100.3	0.82
103.7	0.51
104.9	0.77
110.7	3.32
123.3	0.96
125.2	2.57
137.8	7.35
141.7	4.33
143.7	0.61
166.1	7.88
198.8	0.01
218.9	8.95
221	8.78
415.4	0.03
418.7	11.16
419	10.98
495.3	0.36
495.7	0.32
495.9	0.8
577.8	0.62
579.8	26.22
580	26.3
813.9	0.28
814.3	0.55
814.5	0.68
888.8	1.36
889.1	1.25
889.3	0.48
927.7	6.68
927.7	3.52
928.5	5.72
1094.9	1.48
1095	1.52
1096	0.01
1116.8	0.79
1117	2.68

1117.4	15.08
1275.1	73.57
1275.2	75.19
1275.5	3.17
1395.3	63.99
1395.5	66.03
1395.6	0.36
1403.1	6.71
1403.3	87.41
1403.4	99.33
1452	49.37
1453	47.69
1453.4	3.32
1458.9	2.45
1459	3.71
1459.4	1.42
1472.6	2.64
1473.2	39.21
1473.5	38.2
1488.3	10.91
1488.8	5.67
1489.8	42.3
1700.9	505.97
1701	507.46
1710.8	0.09
3024.4	2.97
3024.6	3.87
3024.7	5.5
3031	0.06
3031.1	0.07
3031.2	0.09
3085.5	1.62
3085.7	2.14
3085.7	0.45
3091.5	0.68
3091.6	0.28
3091.6	1.54
3140.2	0.36
3140.3	0.19
3140.3	0.12
3150.6	0.4
3150.6	5.14
3150.6	4.86

Atom	Standard Orientation

C	0.00000000	0.00000000	0.00000000
C	0.25885300	-1.43060500	0.36732200
O	-0.65810400	-2.24826000	0.48401200
Cu	-2.66987200	-2.08339400	0.33137900
O	-3.52944400	-0.25009000	0.24971800
C	-4.69831800	0.13073600	0.35695900
C	-5.81740200	-0.82544200	0.64347000
H	-6.12172600	-0.69330900	1.68849100
H	-6.69216300	-0.59480700	0.03061000
H	-5.50278700	-1.85815700	0.49233000
C	-5.02527800	1.58495700	0.20624600
H	-5.56784100	1.72523600	-0.73582800
H	-5.69611900	1.91404100	1.00448600
H	-4.11960900	2.18854000	0.19309500
O	-3.83426400	-3.73994800	0.28536700
C	-3.57140100	-4.94530200	0.25540300
C	-4.68228600	-5.95045700	0.26707700
H	-4.51106900	-6.72393300	-0.48642800
H	-4.68523000	-6.45630700	1.23956400
H	-5.64527400	-5.46815800	0.10963400
C	-2.15872500	-5.44546100	0.20261200
H	-1.96697600	-5.82722700	-0.80704600
H	-1.44846700	-4.64864600	0.42353400
H	-2.01993800	-6.28625300	0.88680500
C	1.67575700	-1.86355600	0.58950700
H	2.32319300	-1.48885200	-0.20795300
H	2.03620200	-1.41411000	1.52202500
H	1.74492900	-2.94733200	0.66272500
H	0.60605500	0.67305600	0.61147200
H	0.31540000	0.15009500	-1.03923400
H	-1.05812000	0.24608500	0.08999100



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)_4$	1	-2413.293002	-2412.954072

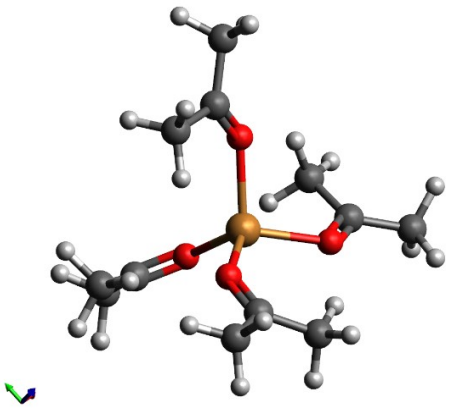
Frequency	Intensity
14.8	0.14
15.9	0.76
16.6	0.62
23.3	1.59
27.2	0.48
29.4	0.61
42.9	1.84
50.3	1.63
53.5	2.15
69.6	0.13
89.9	0.71
90.7	3.19
94.4	1.33
94.7	0.74
104.6	10.63
107.3	1.97
107.6	4.25
121.5	2.53
125.4	0.06
127	2.2
130.1	7.4
135	3.98
141	5.67
146.2	5.14
160.6	2.3
170.1	1.08
171.6	1.16
176.5	8.85
178.2	0.91
405.2	3.01
409.2	5.27
410.5	6.29
414.5	8.56
492.6	1.12
494	0.27
495.6	1.01
506.6	0.4
560.7	15.69
568	9.26
568.3	16.54
569.7	18.78
802.9	0.66
808.2	0.56

808.8	1.31
811.2	1.08
888.7	0.14
889	0.57
889.8	1.24
890.2	0.8
921.9	5.03
922.5	4.53
923.9	5.6
951.1	6.94
1083.4	4.75
1092.9	0
1093.7	0.58
1094.5	0.18
1115.3	3.25
1116.1	4.29
1117.2	4.84
1117.8	8.86
1259.7	72.46
1266.1	30.02
1268.2	66.47
1271.1	53.78
1392.7	75.33
1393.9	23.51
1394.8	37.7
1395.6	40.77
1396.1	16.08
1401	34.94
1402.6	88.5
1403.2	58.99
1455.2	13.48
1456.9	31.26
1457.5	46.71
1459	27.72
1459.6	0.24
1460.6	4.79
1462.1	2.98
1465.7	4.7
1472.7	34.32
1473.1	25.5
1474.4	17.74
1476.8	17.5
1486.6	10.79
1487.6	0.93

1490.5	19.19
1491.5	33.41
1710.3	380.62
1714.2	354.31
1717.5	285.37
1729	137.02
3023.8	4.7
3024.5	0.95
3024.9	2.52
3025.5	1.06
3030.7	0.81
3031	0.16
3031.2	0.99
3034.1	5.27
3079.4	1.13
3083	2.43
3084	1.01
3084.1	1.76
3089	2.05
3090	1.83
3090.2	2.99
3095.4	0.64
3138.7	1.49
3139.1	6.79
3141.2	0.65
3145.8	4.64
3147.3	3.84
3147.6	6.45
3147.7	4.9
3148.8	2.94

Atom	Standard Orientation		
Cu	0.00000000	0.00000000	0.00000000
O	-1.92063900	-0.71405800	0.40846300
C	-2.35701700	-1.82235300	0.72128800
C	-3.82447400	-2.00782000	0.97933800
H	-4.20153700	-2.88339500	0.44336400
H	-3.97441800	-2.20747300	2.04631900
H	-4.38459700	-1.11813100	0.69632300
C	-1.45911700	-3.01758500	0.84935200
H	-1.64178400	-3.67853500	-0.00621500
H	-0.41024900	-2.72377900	0.85417200
H	-1.70557600	-3.59255800	1.74575400
O	1.53050400	-1.42636000	0.35804800

C	2.73440400	-1.22970300	0.20214400
C	3.22588100	0.10087200	-0.30112300
H	2.90699500	0.87104100	0.40793600
H	4.30664300	0.13684300	-0.43153400
H	2.72159600	0.32028400	-1.24670900
C	3.73148000	-2.30444600	0.51208200
H	4.31201000	-2.53284500	-0.38822900
H	4.44675700	-1.93629800	1.25528600
H	3.23844100	-3.20329800	0.87808700
O	0.56628200	1.56917000	1.27809300
C	-0.07105200	2.40297700	1.91642200
C	-1.57153800	2.47133700	1.84386200
H	-2.00402700	2.59536700	2.84001500
H	-1.85260200	3.35980500	1.26691200
H	-1.97654600	1.58279600	1.35996300
C	0.63882400	3.39364700	2.79398300
H	0.26178900	4.40504000	2.61813500
H	0.42387400	3.15678800	3.84204800
H	1.71425400	3.35494000	2.62941100
O	0.25803500	0.54456600	-2.00413500
C	-0.51449900	0.97504200	-2.85686700
C	-0.02750900	1.26264700	-4.24781700
H	-0.46939900	0.53397000	-4.93663700
H	-0.36431800	2.24936700	-4.57806200
H	1.05777100	1.19471500	-4.29903200
C	-1.96284000	1.23519400	-2.54647800
H	-2.60660400	0.86053400	-3.34637000
H	-2.23992300	0.78750700	-1.59205600
H	-2.11984700	2.31879400	-2.49818500



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)

$Cu^{+}(Pin)(Ace)_2$	1	-2413.191971	-2412.845947

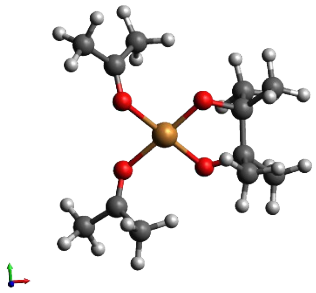
Frequency	Intensity
24.6	2.1
36	3.01
41	2.67
44.5	0.81
48.9	1.13
56.4	2.43
62.7	3.21
82	0.68
136.3	1.36
139.3	1.61
150.3	1.2
154	1.18
169.7	0.62
198.1	0.26
208.9	0.09
214.3	0.06
220	2.23
226.3	5.93
233.4	1.81
237.2	5.28
272.7	2.5
294.7	2.54
307.9	0.25
323.2	0.63
353.2	2.93
354.8	2.94
378.9	0.02
395	10.19
420.2	5.04
428.2	28.93
447.8	1.01
496.1	5.54
502.6	2.84
508.7	0.48
514.1	0.57
549.4	5.35
600.1	12.77
606.8	11.98
625.9	20.12
685.6	36.05
712	18.64
806.4	7.99

818.8	1.09
820.4	3.24
864.7	26.96
883.8	0.99
889	5.41
918.7	2.48
941.7	1.01
944.3	0.49
960.1	5.02
961.3	15.88
965.2	5.87
1010.5	3.65
1018.3	8.33
1083.5	4.69
1093	2.7
1113.3	9.26
1113.7	7.73
1133	13.94
1155.7	101.59
1185.9	19.67
1210.4	2.7
1253	17.46
1272.2	37
1278	35.67
1308.7	1.86
1385.9	50.48
1386	29.71
1387.6	42.56
1389.5	53.56
1397.1	10.85
1399	0.19
1412.5	23.95
1421.9	6.06
1450.7	63.46
1454.8	42.2
1456.2	4.08
1456.8	10.22
1463.8	19.1
1465.9	11.5
1470.4	8.65
1471.2	0.59
1484.6	21.27
1487.9	11.88
1489.9	5.85
1500.6	14.22

1504.6	10.05
1506.9	10.82
1517.3	2.68
1527.3	0.28
1671.8	602.23
1683.4	184.68
3023	8.99
3026.6	8.52
3027.7	2.15
3033.3	3.17
3035	4.31
3037.1	4.09
3039.5	18.43
3041.3	0.53
3080.4	0.16
3083.3	0.47
3097.1	8.56
3100.7	6.83
3101.4	2.39
3103.9	13.49
3110.3	1.24
3111.8	38.12
3114.8	0.91
3115.9	30.37
3137.6	0.77
3138.4	20.09
3152	1.32
3152.2	3.51
3157.2	3.36
3158.1	3.34

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-0.78128300	-0.54492300	1.15140900
O	-0.61776600	-1.70662600	1.55207300
Cu	0.71905900	-3.00780500	1.01784400
O	-0.73859400	-4.17619700	0.49195300
C	-1.03373200	-5.32516100	0.85195800
C	-0.32085900	-6.00909100	1.97290600
H	-0.73937000	-5.62429700	2.91151700
H	-0.47091600	-7.08777100	1.95399700
H	0.73938500	-5.75724200	1.93989100
C	-2.15194500	-6.02442200	0.15526800
H	-1.73426000	-6.88471500	-0.38124200
H	-2.85282600	-6.42901900	0.89181900

H	-2.66091000	-5.36440800	-0.54400500
O	2.06275100	-1.88883700	1.39871000
C	3.34158500	-2.34745500	0.87731300
C	4.39879600	-1.58645100	1.67690800
H	5.39472600	-1.94226900	1.39592100
H	4.34572700	-0.51976700	1.45032000
H	4.26177400	-1.71862600	2.74892900
C	3.43007000	-1.99077700	-0.60886800
H	4.42003500	-2.20842300	-1.01350400
H	2.69006700	-2.54736200	-1.18743500
H	3.24469200	-0.92203200	-0.73232100
C	3.28500600	-3.87278900	1.12659800
O	1.96507800	-4.23161200	0.62878700
C	4.26584400	-4.71239500	0.30870200
H	5.29115400	-4.43695400	0.57388200
H	4.13181400	-5.77198100	0.53474800
H	4.12234700	-4.56724200	-0.76079900
C	3.37186500	-4.23608200	2.61116500
H	2.68464000	-3.62706900	3.20181400
H	3.11125100	-5.28876300	2.73787700
H	4.38190500	-4.09256800	2.99900700
C	-1.77420300	0.32000800	1.84969300
H	-1.27142000	1.23162600	2.19113500
H	-2.53716100	0.63928100	1.13132000
H	-2.23421900	-0.19764000	2.68864300
H	-0.35005300	0.98072700	-0.31571800
H	1.04704200	0.04955200	0.31461500
H	-0.04319000	-0.70382200	-0.83584900



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Co^{2+}(Ace)_3$	4	-1961.940501	-1961.686144

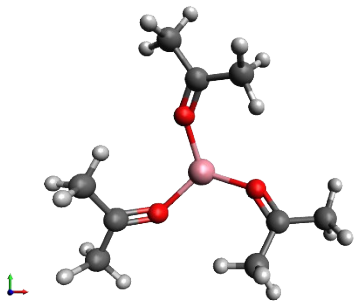
Frequency	Intensity
26.2	0.4

27.2	1.13
27.9	3.16
33.2	1.29
33.6	1.23
40.1	1.33
81.6	1.14
95.1	0.39
95.9	0.16
100.8	1.73
114.4	1.58
115.7	2.8
119.3	3.61
122.4	3.28
123.6	6.5
142.6	0.72
142.7	0.23
186.5	24.44
240.3	0
313.9	18.39
314	18.37
435.5	0.24
452.1	26.95
452.1	26.84
500.3	0.7
500.4	1.16
501.2	1.08
564.3	0.29
569.9	57.88
570.1	57.71
833.6	0.07
835	2.3
835.5	2.27
881	7.47
882.2	0.01
882.7	7.53
931.7	3.29
932.4	5.7
932.8	5.27
1097.4	0.25
1098	8.16
1098.1	7.64
1106.6	3.69
1106.9	6.42
1107.6	32.23
1295.4	55

1295.5	55.98
1295.9	2.23
1381.9	140.37
1382	137.69
1383.2	2.58
1392.2	19.58
1392.6	107.72
1392.7	127.98
1428.8	73.54
1430.4	76.25
1430.9	5.04
1446.5	8.4
1447.1	1.71
1447.4	14.47
1464.5	113.89
1464.8	95.74
1465	2.76
1475.7	7.81
1476.3	17.78
1477	67.46
1622.6	693.61
1622.8	694.31
1646.7	4.29
3012.3	25.92
3012.4	24.27
3012.6	28.87
3021.4	34.67
3021.6	22.85
3022	13.55
3078.9	1.9
3079.1	1.54
3079.2	1.47
3085.6	7.19
3085.7	5.95
3085.8	9.02
3137.7	5.33
3137.8	3.4
3138.4	4.16
3158.6	2
3159	2.13
3159.2	2.08

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	1.42071700	0.36476200	-0.24122600

O	1.76651800	1.56527200	-0.35807000
Co	1.12828500	3.36234900	-0.43878100
O	-0.74725800	3.70502900	-0.34437000
C	-1.61633600	4.60449400	-0.24401400
C	-1.22578200	6.03383000	-0.12631200
H	-1.51753500	6.54428000	-1.05340800
H	-1.79213200	6.51821300	0.67455700
H	-0.15415100	6.15454200	0.03176900
C	-3.04882100	4.22049600	-0.24081400
H	-3.42010300	4.32362100	0.78858100
H	-3.63628600	4.91738100	-0.84485600
H	-3.19463700	3.19425800	-0.57198600
O	2.36570500	4.81155900	-0.32836800
C	3.57930000	5.10870800	-0.21297800
C	3.97918100	6.53469800	-0.28699300
H	4.73399500	6.76336200	0.47050900
H	4.46700400	6.69415500	-1.25900300
H	3.12344800	7.20171100	-0.20478400
C	4.60679800	4.05439100	-0.00696300
H	4.97701400	4.13713700	1.02333900
H	4.20509500	3.05389700	-0.16780900
H	5.47122500	4.23277900	-0.65291800
C	2.45379400	-0.69341400	-0.35024300
H	2.29265000	-1.46945600	0.40307000
H	2.32526100	-1.18515300	-1.32490200
H	3.46094200	-0.28627100	-0.28797700
H	-0.29521500	-0.83115600	-0.64687800
H	-0.08540900	-0.37294600	1.02908000
H	-0.66967200	0.84960200	-0.13384200



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Co^{2+}(Ace)_4$	4	-2155.206576	-2154.866887

Frequency	Intensity

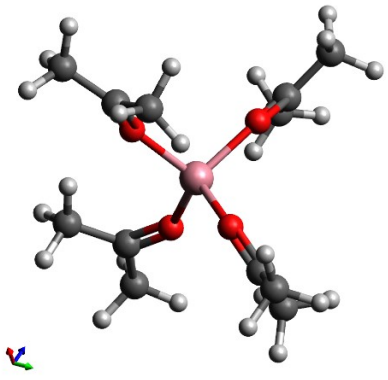
10.7	0.17
20.8	0.56
24.4	1.01
28.9	0.88
32.7	0.57
34.4	0.88
41.4	2.54
45.8	1.74
48.7	2.12
87.8	0.59
93.3	1.6
97.9	0.86
102.9	1.2
107.9	0.56
109.4	1.72
115.4	0.58
119.3	1.38
123.3	0.39
126.9	1.6
129.2	2.44
133.9	2.13
141.6	1.84
160.2	3.48
177.1	8.12
186.8	18.67
224.6	0.01
273.4	30.56
284.2	25.67
288.5	26.28
420.2	1.76
424.1	17.93
426.7	23.55
428.8	19.31
501.3	0.91
502.4	1.58
503.2	0.22
503.9	1.46
557.7	18.23
563.3	3.56
568.1	52.53
571.1	36.66
823.2	0.65
824.7	0.69
824.9	1.5

825.8	1.7
881.8	3.01
882.5	3.96
883.1	3.3
883.3	1.09
924.1	4.08
926.1	3.51
926.8	4.88
928.6	4.39
1092.7	4.83
1094.1	4.98
1094.3	1.77
1094.8	4.67
1110.9	2
1112.1	3.38
1112.5	18.41
1113.3	19.82
1283.3	22.12
1285.4	56.85
1287.5	52.97
1287.9	29.59
1389.3	103
1389.4	94.97
1390	94.12
1391	3.03
1397.8	19.74
1398.3	87.79
1398.4	52.88
1398.5	143.99
1437.9	49.57
1439.2	83.37
1440.8	43.07
1440.9	37.05
1449.6	5.51
1450	3.14
1450.8	3.65
1451.6	5.22
1466.4	56.51
1466.6	76.22
1468.6	25.58
1468.9	41.87
1479.2	25.28
1480.8	26.58
1482	14.76

1482.8	40.35
1648.7	623
1652.2	619.33
1656.5	593.65
1684.6	37.26
3020.9	14.39
3021.2	8.32
3021.3	19.3
3022.6	12.22
3028	14.08
3028.3	14.38
3028.5	11.73
3029.7	12.1
3082	0.44
3083.5	0.38
3084.1	0.18
3084.8	0.39
3089.8	2.17
3090.3	2.6
3090.7	2.59
3091.1	2.44
3142.1	4.14
3143.8	5.18
3147.3	2.03
3148.3	1.91
3157	1.61
3157.3	2.04
3158.3	1.56
3158.5	1.74

Atom	Standard Orientation		
Co	0.00000000	0.00000000	0.00000000
O	-1.66862900	-1.01151500	-0.32182900
C	-2.11416700	-2.09629600	-0.74923000
C	-3.58549100	-2.32781500	-0.74557400
H	-3.90831400	-2.76243400	-1.69601300
H	-3.81557000	-3.07877400	0.02137400
H	-4.13765900	-1.41523700	-0.53045800
C	-1.21267900	-3.16567900	-1.26723900
H	-1.31183900	-3.19547400	-2.36011500
H	-0.17048200	-2.98682400	-1.00679500
H	-1.53511800	-4.14691700	-0.90944100
O	1.60105500	-1.12902300	-0.28186500
C	2.81102900	-1.04599600	-0.57537000

C	3.44373400	0.25380500	-0.94206300
H	4.07735800	0.57229900	-0.10427000
H	4.11450800	0.12665400	-1.79577900
H	2.70562600	1.02778500	-1.14769500
C	3.64560700	-2.27951100	-0.55829500
H	3.85659500	-2.56571800	-1.59715900
H	4.61694700	-2.08280100	-0.09656000
H	3.13816700	-3.10149400	-0.05723400
O	0.22492400	0.67995200	1.83948900
C	-0.18636100	0.67058500	3.01443900
C	-1.37275500	-0.13780700	3.42460000
H	-1.01790700	-0.99483300	4.01092800
H	-2.01943700	0.43782200	4.09180800
H	-1.93842500	-0.49995700	2.56699800
C	0.52450400	1.48528300	4.03961000
H	-0.11525600	2.33541900	4.30961400
H	0.66578800	0.91007100	4.95897200
H	1.47557600	1.85847700	3.66540300
O	0.04926100	1.61908000	-1.15237300
C	-0.67573200	2.51175000	-1.63265000
C	-0.05936400	3.56947400	-2.48145700
H	-0.32932400	3.36942500	-3.52688700
H	-0.47590300	4.55163600	-2.24306000
H	1.02491800	3.57596800	-2.39057700
C	-2.14653800	2.55295400	-1.38113200
H	-2.68770300	2.78377800	-2.30254400
H	-2.51737200	1.62568900	-0.94571800
H	-2.35310700	3.38338500	-0.69412300



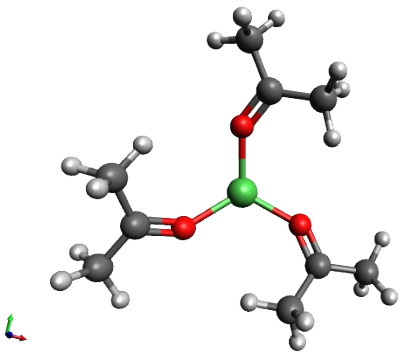
Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Ni^{2+}(Ace)_3$	3	-2087.46374	-2087.208946

Frequency	Intensity
21.4	0.14
24.1	0.11
32	2.58
44.8	4.54
47.2	0.85
47.5	0.76
88.3	0.87
101.4	1.82
106.9	3.07
110.9	3.43
119.8	2.06
124	1.76
130.3	1.01
136.1	1.58
137	0.74
154.3	5.66
155.2	5.73
200.7	15.06
259	5.42
315.6	15.62
316.1	14.64
435.1	3.01
449.3	19.76
449.5	19.72
499	1.3
499.3	0.82
503.3	0.54
577.2	1.53
588.1	50.68
588.5	49.52
830.5	0.41
831.7	2.14
836	1.96
880.3	4.64
884	6.26
884	2.54
930.4	4.42
935.8	4.92
935.9	5.34
1096	4.07
1096.1	1.82
1097.3	2.72
1105.4	4.38
1106.2	18.33

1108.5	18.42
1295.2	50.85
1295.6	49.33
1296.4	13.42
1378.5	136.11
1378.8	114.25
1380	32.1
1389.7	57.6
1390.4	99.94
1390.6	72.17
1429	63.5
1429.2	59.26
1430.1	23.65
1446.1	12.09
1446.3	7.54
1447.7	4.9
1464	20.44
1464.4	74.44
1464.7	95.29
1476	26.81
1478.8	38.18
1479.3	28.09
1612.6	589.41
1613.3	587.97
1633.3	48.1
3010.8	37.57
3011	30.44
3012.9	27.95
3021	23.32
3021.2	18.85
3023.5	23.62
3078	1.33
3078.7	2.31
3078.8	2.33
3085.3	8.27
3086.4	4.51
3086.5	10.04
3146	4.11
3146.4	3.35
3148.3	3.84
3158.7	2.3
3159.1	2.49
3159.3	2.5

Atom	Standard Orientation

C	0.00000000	0.00000000	0.00000000
C	0.12132100	-1.35276700	-0.60298300
O	1.23052500	-1.79466900	-0.99168000
Ni	3.00288700	-1.21717100	-1.33773100
O	3.37437300	0.60524000	-0.95917700
C	4.32253800	1.34669600	-0.60186800
C	5.62212400	0.77868900	-0.15840300
H	6.37922800	1.03524900	-0.91080000
H	5.94696400	1.25748900	0.77004500
H	5.57906700	-0.30338000	-0.04221800
C	4.11955600	2.81604100	-0.62563400
H	4.03703300	3.16072300	0.41468700
H	4.99963700	3.31663800	-1.03956700
H	3.21900300	3.09233500	-1.17037500
O	4.38532100	-2.45972300	-0.96354100
C	4.54940200	-3.64053500	-0.56941500
C	5.89645900	-4.24797000	-0.69265100
H	6.14433900	-4.82096800	0.20537300
H	5.85675200	-4.97586800	-1.51565800
H	6.65966700	-3.50450300	-0.91356100
C	3.42710000	-4.42130700	0.01312900
H	3.59805200	-4.49893400	1.09511700
H	2.46219900	-3.94889300	-0.16803100
H	3.43622600	-5.44579100	-0.36880200
C	-1.07666900	-2.21346200	-0.75364100
H	-1.70666400	-2.15635400	0.13858600
H	-1.67820000	-1.80144800	-1.57653900
H	-0.81213200	-3.24241300	-0.98889300
H	-0.88802500	0.51025100	-0.38283700
H	-0.16394500	-0.12697700	1.07842900
H	0.89338500	0.60215000	-0.16201600



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)

$Ni^{2+}(Ace)_4$	3	-2280.762336	-2280.421795

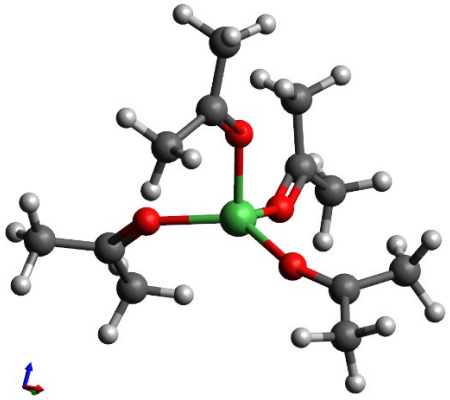
Frequency	Intensity
17.6	0.98
21	0.63
26.8	1.24
29.6	0.05
35	2.33
35.7	0.85
42.4	2.61
54.4	2.24
63.8	1.84
92	2.75
96.7	0.91
98.4	0.39
104.1	1
110.1	1.5
115.9	1.64
123.7	0.5
127.1	1.41
133.5	0.53
137.1	0.19
142.2	0.53
147.1	0.44
166.3	3.06
174.2	5.43
182.6	4.09
198	12.84
229	1.72
267.9	9.9
291.5	17.86
312	40.08
425.5	0
428	6.53
434.2	31.62
435.7	15.9
498.5	0.69
501.2	1
502	0.48
503.1	2.72
578.8	26.45
579.8	15.69
593	40.96
598.8	24.09
823.1	0.41

825.7	0.67
826.5	2.67
828.6	1.4
883	3.48
884.6	3.59
885.5	3.14
886.3	2.06
930.3	3.78
932.2	4.25
933.6	4.34
936.3	4.67
1094.1	2.39
1095.4	2.78
1096.4	4.33
1099.2	1.26
1109.9	2.52
1111.4	2.99
1112.5	22.44
1114	14.35
1287.8	24.06
1289.2	53.36
1290.6	36.09
1291.5	32.94
1387.1	74.33
1388.1	86.72
1388.7	111.75
1389.9	20.92
1397.2	58.99
1397.9	45.33
1398.6	113.53
1399.1	65.5
1434.8	53.74
1437.8	59.44
1438.7	35.31
1443.3	32.72
1448.8	5.48
1449.9	10.07
1449.9	4.87
1453.4	5.59
1465.4	53.15
1466.8	31.71
1467.3	36.06
1469	50.67
1484	24.76
1484.7	18.6

1489.9	26.1
1492.7	36.57
1650.6	551.23
1655	510.04
1657.7	502.19
1681	57.53
3019	11.88
3019.4	14.71
3020.3	13.26
3021.7	16.65
3025.7	18.22
3026.6	15.28
3026.8	9.37
3029	8.67
3080.6	0.39
3080.8	0.97
3080.8	0.67
3082.6	0.83
3089.6	1.58
3089.9	3.66
3092.5	2.1
3094.1	3.06
3138	3.14
3141.8	4.42
3146.3	2.92
3155.5	1.89
3156.3	1.68
3157.6	2.1
3157.9	2.28
3158.2	1.5

Atom	Standard Orientation		
Ni	0.00000000	0.00000000	0.00000000
O	-1.62199100	-0.18059400	1.06192400
C	-2.83183800	-0.44684300	0.93741100
C	-3.69702900	-0.49189600	2.14564700
H	-4.36181900	0.38161300	2.12344300
H	-4.34971800	-1.36927400	2.11617300
H	-3.10782200	-0.47355900	3.06026100
C	-3.42211900	-0.72525700	-0.40508500
H	-4.40514200	-0.25889900	-0.50345100
H	-2.75869400	-0.39771000	-1.20522200
H	-3.58572300	-1.80727800	-0.48367900
O	-0.59747500	1.27394300	-1.39176500
C	-0.51580700	2.51206100	-1.50994000

C	0.08116400	3.37003500	-0.44486400
H	0.67007800	4.17978300	-0.88129600
H	-0.74140500	3.84725700	0.10316100
H	0.69200900	2.79366000	0.24898500
C	-1.04585800	3.15535500	-2.74370300
H	-1.62875100	4.04597300	-2.49198800
H	-0.19270200	3.50849400	-3.33729400
H	-1.63559200	2.46053000	-3.33840000
O	1.89351900	0.56073300	0.08685800
C	2.94048100	0.06750000	0.55349800
C	4.20154000	0.85420800	0.49157900
H	4.72468900	0.81481200	1.45153500
H	4.86937300	0.37651400	-0.23695500
H	4.01753400	1.88360600	0.19103700
C	2.95633800	-1.28518100	1.18360100
H	3.85229900	-1.84037400	0.89593600
H	3.01715000	-1.14960300	2.27116300
H	2.06009900	-1.85781600	0.94365800
O	0.15385200	-1.77602400	-0.81129900
C	0.14889200	-2.32572300	-1.92866400
C	0.33645100	-3.80126500	-2.00663400
H	-0.60879400	-4.25319600	-2.33271900
H	1.07113600	-4.05090100	-2.77794500
H	0.62424700	-4.22101000	-1.04480800
C	-0.03457200	-1.54369300	-3.18503100
H	-0.72521100	-2.05710400	-3.85897400
H	-0.36836900	-0.52774800	-2.98277500
H	0.93004000	-1.51119500	-3.70707300



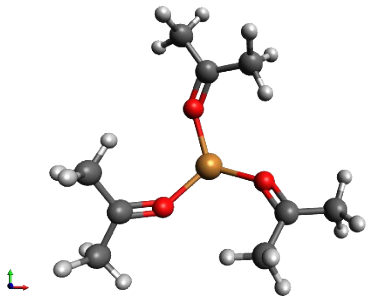
Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{2+}(Ace)_3$	2	-2219.637784	-2219.38312

Frequency	Intensity
13.4	1.67
26	0.39
34.4	2.31
42.2	1.63
44.5	5.16
55	1.12
92.1	0.24
99.6	1.15
102.6	2.49
114.5	1.92
118.1	0.93
127.1	1.33
131.8	0.28
136.5	0.43
145.4	0.23
173.5	1.01
192.7	9.32
203.4	7.19
242.3	0.59
277.8	5.73
332.5	15.6
429.1	1.62
434.2	3.87
455.4	23.96
496.5	0.38
501.6	0.58
503.3	0.99
575.2	31.58
595.6	14.68
610.2	28.91
823.3	0.59
830.1	0.72
832.5	5.3
879.9	1.5
884.3	4.78
884.5	7.22
929.8	4.6
935.7	5.39
936	4.88
1089.2	1.96
1091.6	1
1095.6	0.71
1102.6	3.19
1103.7	19.12

1105.4	19
1285.5	29.41
1287	43.71
1294.3	21.87
1372	63.6
1372.8	36.08
1379.2	59.13
1381.6	76.67
1387.6	69.97
1390.8	86.55
1427	22.06
1428	55.19
1430.6	28.35
1444	14.21
1444.1	4.75
1444.5	23.95
1462.3	54.24
1464.1	48.11
1467.7	64.24
1473.6	34.74
1476.2	31.24
1488	32.2
1610.9	359.05
1614.8	654.33
1625.2	41.07
3010.5	37.75
3012.5	24.99
3014.2	26.98
3020.4	30.29
3021.7	34.26
3022.2	26.36
3078.2	4.01
3079.4	3.43
3079.4	1.83
3085.4	9.2
3087.2	8.15
3090.1	5.86
3119	7.21
3150.5	2.44
3152	4.74
3159.6	3.2
3159.9	3.92
3160	3.66

Atom	Standard Orientation

C	0.00000000	0.00000000	0.00000000
C	0.82958000	0.06310800	-1.23422700
O	1.33939100	1.12930600	-1.64629600
Cu	1.24891000	2.97030400	-1.04642900
O	-0.59912300	3.24534500	-0.71155600
C	-1.50613400	3.87877800	-1.30299700
C	-1.29885600	4.47537900	-2.65036600
H	-1.92059200	3.93046600	-3.37157000
H	-1.65462500	5.51003400	-2.66512500
H	-0.25678900	4.43325400	-2.97319200
C	-2.81550600	4.03233500	-0.62098000
H	-2.88952500	5.07322700	-0.27567700
H	-3.63865600	3.88712000	-1.32620500
H	-2.90460400	3.36862600	0.23665700
O	2.97384400	3.66154800	-0.93604500
C	4.20276200	3.48615300	-1.09879000
C	5.11990500	4.63369900	-0.89154700
H	6.01672500	4.31082600	-0.35507900
H	5.45925600	4.96730000	-1.88265500
H	4.62843000	5.46066300	-0.38287300
C	4.73279900	2.15345300	-1.49046800
H	5.22887300	1.72176700	-0.61084700
H	3.94159900	1.48652400	-1.82943400
H	5.50748600	2.26395900	-2.25414200
C	1.09129400	-1.17896000	-2.01096500
H	1.34173500	-2.00185400	-1.33481200
H	0.15375800	-1.46412400	-2.50750600
H	1.86527900	-1.03403500	-2.76175100
H	-0.85229300	-0.66869200	-0.14303500
H	0.61573500	-0.45600000	0.78714800
H	-0.33352300	0.98347900	0.32852300



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{2+}(Ace)_4$	2	-2412.929454	-2412.588807

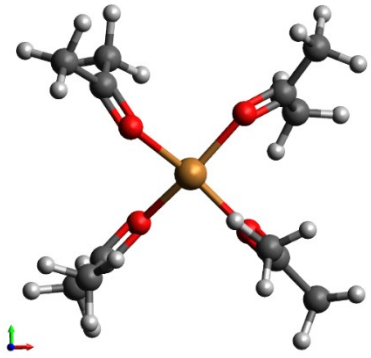
Frequency	Intensity
9.4	0.15
30.7	0
32	6.57
40.4	1.76
45.3	0
46.7	0.78
50.5	2.91
52.2	0
64.5	5.16
78.1	0
78.8	0.13
95.7	0
105.6	0
109.4	1.36
112.9	0
119.6	1.62
121.1	0
128.4	1.36
129	0
141.4	0.17
151	0
181.1	0
198.3	2.08
221.8	6.47
226.3	12.64
233.6	0
237.2	0
308.8	31.92
311	29.87
421.4	0
424.6	0
429.7	17.05
435	25.54
500.2	0
501.3	1.66
503.1	0
503.9	2.58
581.6	0
588.9	0
597.9	19.05
601.8	47.3
823.3	0
825.4	1.78

826.8	0
828.6	2.13
883.8	0
884.2	5.96
884.7	0
885.2	7.74
925.9	0
926	6.31
931.2	0
931.3	8.56
1092.7	0
1094.9	1.58
1095.3	0
1095.4	1.31
1108.4	0
1110.3	28.09
1110.9	12.07
1112.1	0
1285.3	23.91
1286.3	0
1286.6	85.48
1287.4	0
1386.2	0
1387.2	117
1387.9	108.4
1389.5	0
1396.5	17.76
1397.1	0
1397.8	0
1398	273.16
1437.3	71.5
1437.4	0
1438.9	0
1439	34.66
1448.7	0
1449	12.3
1450.7	0
1450.8	30.84
1469.1	96.87
1469.3	0
1470.3	96.94
1470.7	0
1478.1	0
1478.3	48.45
1486.3	0

1486.6	77.73
1649.1	0
1655	682.44
1664.8	817.67
1681.1	0
3020.4	0
3020.4	28.72
3022.3	0
3022.3	23.94
3028	24.39
3028.1	0
3031.2	35.87
3031.3	0
3082.7	0
3082.7	0.72
3083.7	0
3083.7	0.72
3090.7	0
3090.7	4.59
3091.6	0
3091.6	8.18
3135	0
3135	19.36
3150.6	5.7
3150.6	0
3157.5	2.86
3157.5	0
3158.1	3.38
3158.1	0

Atom	Standard Orientation		
Cu	0.00000000	0.00000000	0.00000000
O	-1.75076800	0.62979700	0.62909200
C	-2.64251500	1.36887000	0.17278900
C	-3.78266100	1.74081100	1.05695600
H	-3.67505900	2.80096600	1.32085000
H	-4.73131700	1.65605500	0.51959900
H	-3.79232700	1.14496400	1.96747500
C	-2.61404500	1.87665600	-1.23057100
H	-2.89142800	2.93340500	-1.26206800
H	-1.64313900	1.72947300	-1.70064600
H	-3.38720000	1.34576000	-1.79997300
O	0.53920800	1.85153600	-0.39826200
C	1.40213600	2.62169200	0.05737300
C	2.21371800	2.27717700	1.26253000

H	3.27488200	2.46103700	1.07329000
H	1.92756500	2.95003900	2.07923900
H	2.05627600	1.24628500	1.57948500
C	1.62721100	3.93165900	-0.61591600
H	1.69422900	4.73786800	0.11977400
H	2.60169900	3.89206200	-1.11941900
H	0.85403700	4.13874100	-1.35293900
O	1.75076800	-0.62979700	-0.62909200
C	2.64251500	-1.36887000	-0.17278900
C	3.78266100	-1.74081100	-1.05695600
H	4.73131700	-1.65605500	-0.51959900
H	3.67505900	-2.80096600	-1.32085000
H	3.79232700	-1.14496400	-1.96747500
C	2.61404500	-1.87665600	1.23057100
H	2.89142800	-2.93340500	1.26206800
H	3.38720000	-1.34576000	1.79997300
H	1.64313900	-1.72947300	1.70064600
O	-0.53920800	-1.85153600	0.39826200
C	-1.40213600	-2.62169200	-0.05737300
C	-1.62721100	-3.93165900	0.61591600
H	-2.60169900	-3.89206200	1.11941900
H	-1.69422900	-4.73786800	-0.11977400
H	-0.85403700	-4.13874100	1.35293900
C	-2.21371800	-2.27717700	-1.26253000
H	-3.27488200	-2.46103700	-1.07329000
H	-2.05627600	-1.24628500	-1.57948500
H	-1.92756500	-2.95003900	-2.07923900



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Zn^{2+}(Ace)_3$	2	-2358.518203	-2358.263302

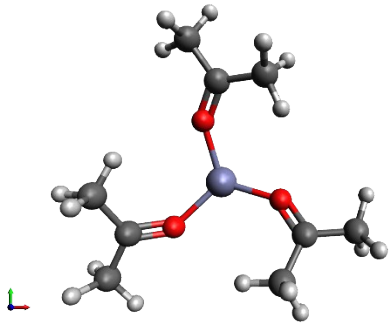
Frequency	Intensity
17	0.01

17.3	0.01
27.2	3.88
43.8	4.85
49.9	0.99
50.6	0.95
99.6	0.11
100.4	0.23
107.3	3.66
125.2	0.06
130.6	0.25
135.1	1.92
138.9	1.66
143.8	3.53
146.3	2.41
150.3	7.58
150.9	7.22
198.5	25.34
248.3	0.01
308.6	20.38
308.7	20.09
434.7	0.01
447	27.56
447.2	28.05
502.3	0.18
502.6	1.15
502.9	0.77
586.1	0.03
598.2	48.26
598.4	48.31
829.9	0
831.7	1.5
831.9	1.6
880.5	7.33
880.7	8.16
880.9	0.78
937.8	1.99
938.1	5.83
938.2	9.77
1095.2	1.54
1095.2	17.47
1095.2	18.75
1107.4	2.65
1107.7	3.08
1108.5	37.98
1300.6	53.23

1300.7	54.33
1302.2	0.16
1380.8	159.23
1381	160.54
1382.3	0.82
1394.5	8.38
1394.7	124.75
1394.9	164.11
1425.2	98.59
1426.6	100.1
1427.6	4.33
1445.5	5.81
1445.8	1.65
1446.6	14.78
1467.7	68.19
1467.9	66.91
1468.1	37.73
1482	4.99
1482.8	35.81
1483.4	67.85
1609.4	656.55
1609.4	652.51
1632.3	0.01
3008.1	38.89
3008.1	43.74
3008.2	14.09
3017.9	29.66
3018	23.03
3018.3	11.13
3079	2.63
3079	3.51
3079.1	0.5
3085.2	4.44
3085.3	7.81
3085.4	8.68
3136.7	3.4
3136.7	3.63
3136.9	0.2
3159.1	1.67
3159.3	1.7
3159.3	1.7

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-0.09256900	-1.45540300	-0.27907700

O	0.93255500	-2.18432900	-0.34482200
Zn	2.83611500	-1.91249000	-0.25215800
O	3.55032600	-0.12492600	-0.21914300
C	4.69512900	0.39625200	-0.28487800
C	5.91623500	-0.42300500	-0.49057200
H	6.27345700	-0.24183900	-1.51341900
H	6.71981800	-0.08584400	0.17026000
H	5.73072700	-1.48936600	-0.35788700
C	4.80517300	1.86766400	-0.15173100
H	5.18112100	2.07934500	0.86000200
H	5.55329500	2.26764500	-0.84119200
H	3.84314700	2.35979200	-0.28015400
O	4.02783500	-3.42429400	-0.21900000
C	3.90310600	-4.67738600	-0.19161300
C	5.13100600	-5.50566500	-0.22596900
H	5.03841900	-6.36970400	0.43723800
H	5.22505900	-5.91283300	-1.24338000
H	6.02037200	-4.92217200	0.00378400
C	2.57061600	-5.32930100	-0.12776100
H	2.45309600	-5.75577100	0.87764500
H	1.75487800	-4.63182400	-0.32062900
H	2.52538400	-6.17629300	-0.81826900
C	-1.41679500	-2.08609800	-0.48752600
H	-2.15989200	-1.67133000	0.19863100
H	-1.75386300	-1.81617900	-1.49911200
H	-1.36646200	-3.17044700	-0.41127900
H	-0.67173500	0.55993500	-0.65675000
H	-0.36843800	0.16983500	1.02083000
H	1.02016800	0.37662400	-0.08121000



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Zn^{2+}(Ace)_4$	1	-2551.778197	-2551.438795

Frequency	Intensity

10.9	0.59
14.5	0.7
20	0.29
23.8	1.3
30.8	0.06
33.7	1.85
38.5	1.58
43.8	1.65
45.9	1.7
86.3	0.18
94.3	0.78
94.9	0.84
103.9	2.95
108	1.51
111	2.13
117.9	3.03
118.6	1.26
123.2	0.68
123.7	0.3
127	2.24
127.9	0.74
148	10.01
153.8	5.59
167.3	6.7
182.4	33
226.6	0.05
266.5	32.27
268.4	25.62
268.7	25.63
419.3	0.63
420.9	17.15
421.9	18.28
423.5	19.61
501.2	1.26
501.6	0.97
502.2	0.3
502.8	1.73
561.4	14.56
565.1	11.72
567.8	49.46
570.9	35.22
822.5	0.47
823.1	1.02
823.2	1.19

823.8	1.37
880.9	4.29
881.3	3.74
881.6	2.71
881.8	0.83
925.6	4.85
927.8	4.67
929	4.49
929.3	5.6
1091.3	7.22
1091.9	6.32
1093.2	4.96
1093.3	6.37
1111.1	1.07
1111.7	12.08
1112.7	12.6
1113.3	21.15
1284.7	32.36
1285.6	25.71
1287	65.27
1287.7	40.32
1389	96.18
1389.1	104.26
1389.6	103.68
1390.5	0.43
1398.7	23.04
1399	124.61
1399.3	126.52
1399.3	39.86
1435.8	72.58
1436.9	74.4
1438.3	62.44
1439	32.96
1447.7	4.07
1448.7	0.69
1449.1	7.25
1449.6	2.59
1466.9	55.28
1467.8	60.3
1468	22.23
1469.5	26.61
1481	27.02
1482.6	48.08
1482.9	15.71

1484.5	25.75
1651.4	604.34
1654.4	594.56
1656.3	587.95
1685.2	12.8
3019.8	15.42
3020.4	12.7
3020.8	15.16
3021.2	12.34
3026.5	12.72
3027.5	16.49
3027.7	12.25
3028.2	12.37
3083.2	0.79
3083.2	0.21
3084	0.73
3085	0.53
3090.6	2.19
3091.1	2.37
3091.2	3.81
3091.5	2.48
3137.9	6.64
3143.5	4.23
3145.3	3.41
3146.9	1.75
3157.5	1.44
3157.6	1.39
3158.3	1.47
3159.1	1.51

Atom	Standard Orientation		
Zn	0.00000000	0.00000000	0.00000000
O	1.77475900	-0.82984000	-0.34079300
C	2.31860200	-1.95284100	-0.38757600
C	3.77109500	-2.03772600	-0.70397600
H	4.26831900	-2.75984800	-0.05040700
H	3.87721600	-2.43207500	-1.72336400
H	4.25361800	-1.06412500	-0.64579000
C	1.55913300	-3.21043200	-0.13163400
H	1.82661500	-3.57054600	0.87052300
H	0.48178400	-3.05837300	-0.18267800
H	1.86704100	-3.99632000	-0.82576900
O	-1.44813700	-1.25825600	-0.51738700
C	-2.68661600	-1.36157600	-0.40301200

C	-3.50621700	-0.32656900	0.29103300
H	-4.04329800	0.25098800	-0.47237400
H	-4.27459100	-0.79474200	0.91140200
H	-2.89786800	0.35063400	0.88951300
C	-3.36743700	-2.55314100	-0.98074200
H	-3.65405700	-3.21658400	-0.15380200
H	-4.29966500	-2.26736100	-1.47512400
H	-2.71633900	-3.09598600	-1.66307600
O	-0.21641400	1.69140800	-1.01169800
C	0.16195500	2.28640600	-2.04020300
C	1.13585900	1.67702000	-2.99225700
H	0.58065800	1.34131000	-3.87784500
H	1.85000500	2.42346300	-3.34841400
H	1.65983300	0.82769800	-2.55552900
C	-0.37918300	3.64317200	-2.32971000
H	0.41923200	4.37604000	-2.15363300
H	-0.64439600	3.73659400	-3.38656000
H	-1.22866000	3.88070000	-1.69258500
O	-0.22950900	0.42858000	1.92590800
C	0.31922400	1.06965700	2.84364000
C	-0.30507700	1.07603800	4.19549900
H	0.30888600	0.45318200	4.85940500
H	-0.28975700	2.08128400	4.62550700
H	-1.31753900	0.67838000	4.17169400
C	1.58208500	1.83529600	2.62804400
H	2.26237100	1.70899100	3.47393600
H	2.08056700	1.56024700	1.69860400
H	1.33101300	2.90328300	2.59715800

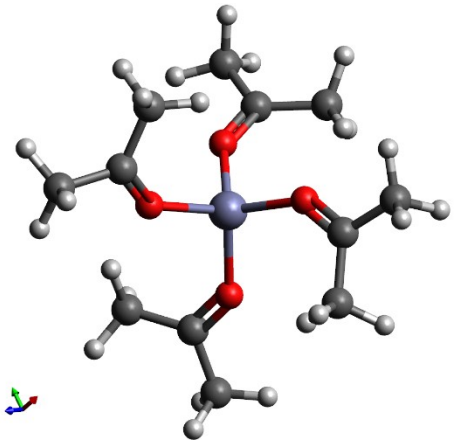


Table S2: Energies, unscaled vibrational frequencies, intensities (km/mol), and geometries (xyz coordinates) of $Cu^{+}(Ace)_n(N_2)_k$ (n = 1 and 4, k = 0–2) and $M^{2+}(Ace)_4$ (M = Co, Ni, Cu, and Zn) calculated at the ωB97X-D/6-311+G(d,p) level of theory.

Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
Cu	1	-1640.17928	-1640.17928

Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
N_2	1	-109.5178987	-109.5122277

Frequency	Intensity
2489.428	0

Atom	Standard Orientation		
N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	-1.09231200

Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
C_3H_6O	1	-193.1492361	-193.0653111

Frequency	Intensity
78.7	0.03
123.9	0.09
384.8	1.53
491.4	0.55
541.2	14.04
798	1.45
884.5	0.2
900.5	5.93
1085.5	0.02
1120.2	3.59
1246.6	65.33
1390.1	20.06
1398.9	78.38
1464.8	1.13
1466.9	10.01
1474.6	20.57
1490.6	24.67
1835.1	223.61
3045.2	1.58
3050.2	5.76
3114.8	1.26

3120.4	17.9
3167.4	10.89
3168.8	7.03

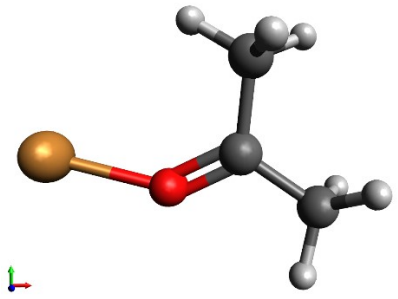
Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	0.00000000	-1.28480900	-0.79829600
O	0.00000000	-1.28480900	-2.00531300
C	0.00000000	-2.56961800	0.00000000
H	-0.76737200	-2.54216300	0.77867800
H	-0.16203100	-3.42154500	-0.65872300
H	0.96567400	-2.68018500	0.50387100
H	-0.96567400	0.11056700	0.50387100
H	0.76737200	-0.02745500	0.77867800
H	0.16203100	0.85192700	-0.65872300

Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
Cu^{+}(Ace)	1	-1833.413631	-1833.328221

Frequency	Intensity
89.8	5.85
98.9	5.42
126.1	0.73
137.3	8.35
283.3	4.4
428.5	5.98
499.3	0.62
581.4	22.79
833.2	0.35
889.1	1.87
937.1	4.04
1095.5	1.7
1115	12.72

1292.7	26.68
1397	35.5
1413.8	93.26
1443.7	43.11
1453.7	5.06
1473.4	30.45
1484.9	34.84
1726.1	354.08
3044.5	8.14
3050	9.6
3121.6	0.4
3126.1	3.53
3161.4	5.6
3187.4	0.76

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-0.18868200	-1.477407	0.00634800
O	-1.31115500	-1.99892700	0.01430500
Cu	-3.13901200	-1.49119100	0.00328500
C	1.01039700	-2.35669600	0.00695600
H	1.78336000	-1.95568700	0.66622800
H	0.75116700	-3.37766500	0.27894300
H	1.42794700	-2.35078400	-1.00732000
H	0.30654600	0.30385600	1.00794300
H	0.81282100	0.28311500	-0.67200100
H	-0.91428500	0.53040100	-0.26862900



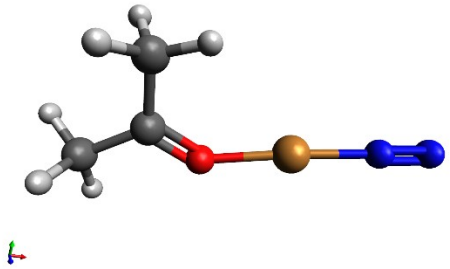
Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)(N_2)$	1	-1942.971511	-1942.878048

Frequency	Intensity
46.6	0.7

49.8	0.7
93.9	2.21
113.7	1.92
124.2	0.89
152.5	6.6
251.9	4.38
268.1	0.62
271.4	1.82
371.6	1.31
441.5	3.95
500	0.51
585.1	23.02
835.1	0.55
889.5	2.12
937.7	3.91
1097.5	1.49
1115.9	12.88
1294.7	28.81
1397.3	39.03
1414.7	97.09
1444.4	46.05
1454.1	4.59
1473.3	29.56
1485.4	34.31
1731.9	425.76
2488	3.83
3045.1	8.31
3050.4	9.64
3121.8	0.19
3126.5	2.95
3164.7	5.06
3187.4	0.73

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	0.10968100	-1.48528500	-0.00547700
O	1.20404400	-2.06317600	-0.01507900
Cu	3.03680000	-1.69324300	-0.00719000
N	4.90761400	-1.43892500	-0.00191100
N	5.99063300	-1.29508900	0.00112100
C	-1.13325400	-2.30052700	-0.00333700
H	-1.88558600	-1.86026100	-0.66139300
H	-0.92790200	-3.33382200	-0.27484400
H	-1.54833200	-2.27205400	1.01157700

H	-0.28762000	0.31806400	-1.00918700
H	-0.79866500	0.32579100	0.66958700
H	0.94094300	0.48038400	0.26915800

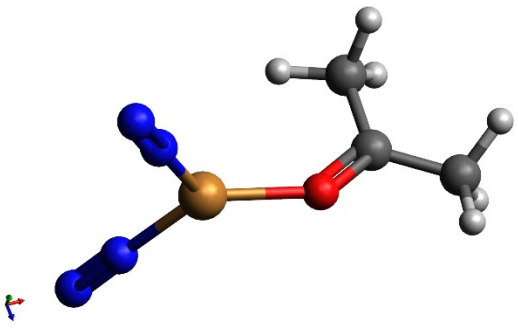


Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)(N_2)_2$	1	-2052.497232	-2052.397399

Frequency	Intensity
13.6	0.67
22.4	0.72
39.7	0.14
43.5	0.52
87.4	2.7
95.4	4.11
117.2	0.47
130.6	3.19
179.3	0.01
185	0.01
204.3	0.44
214.8	0.9
224.8	3.78
244.7	0.73
273.9	2.35
420.7	6
499.1	0.65
566.1	23.22
830.7	0.38
889.6	1.71
933	3.48
1096	1.09
1118.1	10.39
1288.4	31.37
1399.4	34.86
1415.5	91.28
1449.3	35.84

1457.3	4.86
1473.9	31.26
1485.4	31.03
1754.2	404.64
2482.4	1.51
2487.3	0.44
3047.6	4.3
3053	5.9
3122.3	0.21
3127.4	2.11
3162.9	6.86
3185.3	0.98

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	0.17832800	-0.11030300	1.47828200
O	1.29522600	-0.15718500	1.99535300
Cu	3.19682000	-0.11084300	1.58780000
N	4.29401900	1.56316300	1.47903700
N	4.88360800	2.48154000	1.43064700
N	4.25190400	-1.82707300	1.42469000
N	4.81123100	-2.76206900	1.34733700
C	-1.03460800	-0.16893900	2.34188900
H	-1.78898500	-0.82586700	1.90282700
H	-0.78233100	-0.48522100	3.35187000
H	-1.47444500	0.83448600	2.37790000
H	-0.32038000	-0.97748900	-0.37814200
H	-0.79716900	0.70589300	-0.24251200
H	0.92547800	0.28830400	-0.49905100

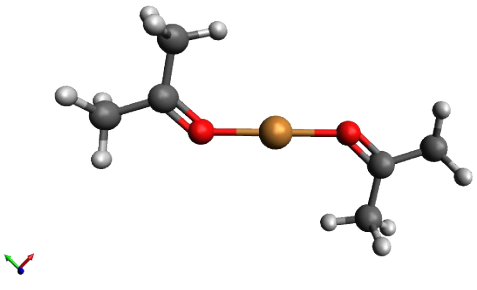


Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)_2$	1	-2026.642642	-2026.471123

Frequency	Intensity
11.2	3.75
35.9	3.77
39.3	2.87
85.1	0.17
85.6	0.2
100.2	1.05
122.3	0.42
125.1	0.23
134.7	0.25
157.3	2.95
197	11.21
231.5	0
333.6	1.49
419.4	0
441.7	12.42
498.4	0.21
499.6	0.74
585.3	0
604.8	42.58
831.1	0.03
833.7	1.47
891.1	0
891.2	3.79
937.3	1.12
937.4	5.76
1095.9	0.11
1096.9	1.3
1117.1	3.65
1117.3	17.49
1291.6	0.25
1291.7	58.63
1398.9	69.42
1399.1	0.02
1415.6	15.04
1415.6	169.06
1448.3	84.11
1448.4	0.35
1457	10.44
1457.1	0.08
1473.6	47.45
1473.6	1.01
1486	19.95
1486.3	43.44
1740.5	791.42

1749.6	0.07
3046.8	1.28
3046.8	8.65
3052.6	10.32
3052.7	0.02
3122.6	0.54
3122.6	0.01
3127.2	0.35
3127.2	3.41
3164.3	8.96
3164.3	0.13
3185.5	0.04
3185.5	2.02

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-1.26587500	-0.78733400	-0.05863900
O	-1.27218600	-2.02118500	-0.07842500
Cu	0.00000000	-3.40415800	-0.07454500
O	1.27218600	-4.78713100	-0.07842500
C	1.26587500	-6.02098200	-0.05863900
C	0.00000000	-6.80831600	0.00000000
H	0.06357300	-7.69381900	-0.63543000
H	-0.12554500	-7.16498900	1.02899000
H	-0.86664900	-6.20562200	-0.27297500
C	2.56310800	-6.75186400	-0.08697300
H	2.54918900	-7.58849200	0.61525100
H	2.68623800	-7.18257700	-1.08750600
H	3.39521200	-6.08198800	0.11909100
C	-2.56310800	-0.05645200	-0.08697300
H	-2.54918900	0.78017600	0.61525100
H	-2.68623800	0.37426100	-1.08750600
H	-3.39521200	-0.72632800	0.11909100
H	-0.06357300	0.88550300	-0.63543000
H	0.12554500	0.35667300	1.02899000
H	0.86664900	-0.60269400	-0.27297500



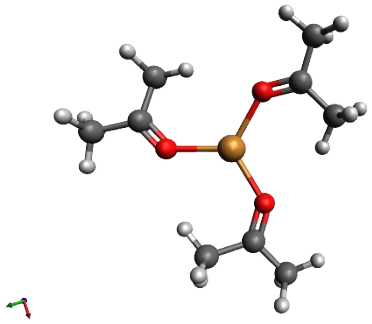
Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)_3$	1	-2219.821446	-2219.564956

Frequency	Intensity
16.2	0.12
18.1	0.09
26	6.29
30.3	2.11
32.4	1.36
38.2	0.61
82.2	0.09
83.7	0.25
103.7	3.61
109	1.08
110.2	5.23
112.6	4.77
122.5	0.44
124.3	0.49
127.8	2.26
131.4	1.6
135.7	0.83
162.9	9.69
198.3	0.02
218.2	9.83
221.9	9.68
409.7	0.05
412.8	11.15
413.5	11.39
497.9	0.44
498.9	0.41
499.1	0.79
575	3.31
576.4	28.37
577	28.97
822.5	0.14
823.1	0.51
823.2	0.5
890.9	2.01
891.6	0.16
891.8	1.95
933.3	3.87
933.5	2.84
934.8	3.38

1094.5	1.27
1094.6	1.24
1095.5	0.02
1121.3	0.88
1121.6	3.92
1122	18
1284.3	62.23
1284.4	59.6
1284.9	3.62
1400.5	43.81
1400.7	15.62
1400.8	40.84
1415.1	12.06
1415.4	120.89
1415.6	117.62
1455.6	54.72
1456.7	54.41
1457.1	3.97
1461.3	2.27
1461.7	2.33
1461.9	1.88
1474.7	4.12
1475.7	27.29
1475.9	27.42
1489.7	15.71
1490.7	10.28
1492	40.06
1755	569.32
1755.1	576.89
1766.5	0.13
3047.5	2.44
3047.7	2.88
3047.7	4.55
3053.8	0.21
3054	0.27
3054.3	0.3
3121.9	1.97
3122.1	1.63
3122.3	1.42
3126.5	0.7
3126.9	0.78
3127	0.72
3166.1	0.21
3166.1	0.16
3167.6	0.14

3181	1.67
3181	4.3
3181.6	3.02

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-0.19965600	-1.41755700	0.43521200
O	-1.31908800	-1.90389500	0.57324000
Cu	-3.18175200	-1.14564800	0.39792000
O	-3.44548700	0.85757600	0.30731400
C	-4.43144100	1.57988700	0.42822200
C	-5.78367800	1.02634000	0.75088700
H	-5.97977600	1.21505100	1.81253200
H	-6.56078900	1.54780500	0.18829000
H	-5.83022500	-0.04741500	0.56775400
C	-4.29644000	3.05914100	0.26071600
H	-4.76460000	3.34250200	-0.68833500
H	-4.83913300	3.58636200	1.04898900
H	-3.24989100	3.35702200	0.24781500
O	-4.79215600	-2.36426600	0.34082400
C	-4.91691000	-3.58580700	0.31108700
C	-6.28211800	-4.19478100	0.30921100
H	-6.34123700	-5.00629600	-0.41987100
H	-6.46095100	-4.64110900	1.29363500
H	-7.04432500	-3.44346200	0.11231100
C	-3.73523400	-4.50272000	0.27030800
H	-3.64084300	-4.88638300	-0.75185100
H	-2.81562700	-3.98355900	0.54096400
H	-3.89485300	-5.36724600	0.91826300
C	1.01218100	-2.25255900	0.69733200
H	1.75701400	-2.10772900	-0.08882200
H	1.46969700	-1.91093200	1.63228700
H	0.74909900	-3.30434100	0.79064100
H	0.81861800	0.46361900	0.55449900
H	0.29755400	-0.01004500	-1.05471600
H	-0.91504300	0.58347600	0.10432900



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Ace)_4$	1	-2412.996732	-2412.6553

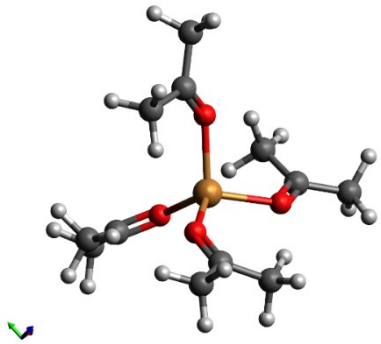
Frequency	Intensity
12.1	0.7
14.7	0.12
17.1	0.44
25	2.03
26.1	0.09
27.6	0.26
37.4	2.39
45.2	2.05
49.8	1.68
64.3	0.08
81	0.82
93.9	3.15
95.9	4.89
100	3.4
101.5	3.12
108.8	7.54
110.1	3.24
116.8	1.47
117.4	1.19
122.4	2.25
124.2	4.98
131	4.4
138.6	6.45
140.7	6.09
159.5	2.86
165.6	1.34
173.1	1.55
174.8	3.3
176.4	8
402.9	4.1
404.1	1.98

405.7	8.57
411.2	9.55
495.7	1.25
497.4	0.21
499.2	1.01
508.9	0.5
563.6	17.05
565.5	13.62
567.2	19.72
568.2	20.08
815.5	0.6
817.4	0.13
818	1.07
821	0.63
889.2	0.25
890.7	0.86
891.4	1.13
892.4	1.27
927.8	3.75
928.6	2.45
931.3	3.49
956.8	4.6
1086.2	3.81
1092.2	0.07
1093.7	0.52
1095.5	0.25
1120.6	0.08
1121.1	8.45
1122.4	5.58
1122.9	12.24
1272.7	62.46
1275.2	31.9
1277.8	53.92
1281.6	43.55
1397.1	15.45
1398.9	18.81
1400.7	47.12
1401.6	30.76
1403	75.54
1412.2	72.95
1414.3	76.54
1415.1	88.58
1457.2	15.2
1460.3	33.28

1461.5	42.97
1462.4	5.91
1463.2	20.27
1463.6	13.6
1465	6.94
1471.1	5.59
1474.9	20.91
1476	23.79
1477.1	16.38
1481.9	16.84
1489	6.08
1489.3	9.42
1493.4	22.32
1494.1	34.99
1766	474.03
1769.3	411.26
1772.5	308.93
1786.9	152.21
3046.9	0.71
3047.2	5.09
3047.7	2.4
3049.9	1.6
3053.5	2.71
3053.9	0.15
3053.9	0.29
3054	0.46
3118.1	0.94
3120	2.98
3120.9	1.49
3121	1.56
3125.1	1.49
3125.7	0.78
3125.8	3.55
3127.6	0.26
3163.9	1.7
3165.6	6.11
3166.8	0.73
3172.3	2.07
3176.8	4.44
3178	3.72
3178.1	5.86
3178.5	3.82

Atom	Standard Orientation

Cu	0.00000000	0.00000000	0.00000000
O	-1.80101700	-1.02784200	0.24210000
C	-2.08970900	-2.21865700	0.26601600
C	-3.50782900	-2.64374600	0.49522300
H	-3.79733600	-3.41622100	-0.22161300
H	-3.58053500	-3.09552700	1.49025900
H	-4.18464600	-1.79334200	0.43539200
C	-1.06158700	-3.28776200	0.06224400
H	-1.18231800	-3.68291800	-0.95287300
H	-0.05094100	-2.89491800	0.17074700
H	-1.23041400	-4.12194700	0.74694100
O	1.69033100	-1.26015900	0.02596100
C	2.86093800	-0.91542200	-0.07217600
C	3.21925300	0.53093800	-0.26053800
H	2.86486100	1.08927300	0.61125000
H	4.29007300	0.68661700	-0.38649700
H	2.67925200	0.91748500	-1.12933500
C	3.96096500	-1.92592300	-0.00206800
H	4.54106100	-1.89281600	-0.92969800
H	4.64951500	-1.65846000	0.80545700
H	3.56525600	-2.92718100	0.15682400
O	0.37419200	1.30686900	1.60230400
C	-0.35082800	1.90351800	2.38502500
C	-1.84669900	1.82875100	2.29151100
H	-2.29305600	1.73238900	3.28389100
H	-2.21140700	2.77288500	1.87199100
H	-2.15951700	1.00431900	1.65062100
C	0.23939700	2.74618800	3.47467600
H	-0.27348600	3.70901000	3.53910500
H	0.08143200	2.23886300	4.43235600
H	1.30658900	2.89119500	3.31761000
O	0.09417000	1.03601200	-1.81055000
C	-0.75212900	1.61243100	-2.47858100
C	-0.37878400	2.27402700	-3.76987000
H	-0.80036600	1.69157600	-4.59596400
H	-0.81783700	3.27293100	-3.83185400
H	0.70270000	2.32411600	-3.88111600
C	-2.18524800	1.69132200	-2.03995800
H	-2.86057600	1.54562400	-2.88598600
H	-2.39513200	0.96518300	-1.25419300
H	-2.37049100	2.70107500	-1.65725600



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{+}(Pin)(Ace)_2$	1	-2412.890862	-2412.541314

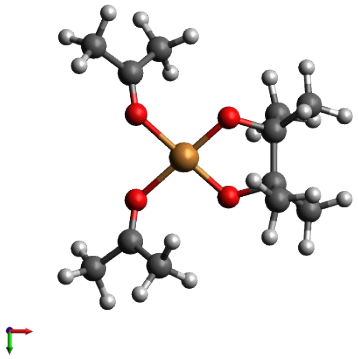
Frequency	Intensity
32.7	5.65
38.3	0.08
45	0.47
51.9	2.04
55.5	5.32
68.8	0.73
104.6	0.77
126.2	0.55
131.1	1.05
134.6	1.44
155.9	1.19
167.2	0.43
198.6	0.15
213.2	0.02
213.8	0.05
219.5	0.2
230	2.97
238.1	5.82
240.2	6.55
247.8	2.54
278.7	2.75
289.6	1.63
300.1	0.89
318.5	0.24
348.9	2.47
360	2.47
368.6	0
394.6	12.39
424.8	4.43
437.2	26.13

457.8	0.89
497.1	7.01
506.6	0.82
507.8	0.34
520.4	0.23
560.2	4.77
612.6	15.62
621	23.96
646.6	15.49
715.2	40.93
736.6	23.26
829.8	2.69
832.3	6.04
847.9	4.25
889.9	1.18
891.3	0.88
903.3	27.54
937.8	1.35
946.4	0.07
952.4	2.25
957.1	3.91
957.7	4.71
979.5	22.58
1008.4	2.68
1018.8	3.74
1093.6	2.75
1098	1.27
1116.9	8.76
1118.4	12.95
1149.6	10.16
1177.7	124.58
1195.2	24.25
1231.3	2.31
1272.3	13.55
1290.3	27.62
1292.3	27.83
1333.8	1.57
1395.6	24.23
1396.9	16.6
1403.5	90.57
1404.5	23.52
1406.4	73.63
1406.8	10.32
1415.5	20.56
1425.9	6.21

1450.5	75.64
1453.6	48.56
1457.9	18.71
1458.3	2.58
1470.2	18
1472	18.88
1476.2	0.05
1477.9	6.92
1486.1	26.52
1488	0.6
1494	21.98
1506	12.97
1507.5	15.27
1508.4	16.3
1513.5	8
1527.2	0.45
1725.8	731.15
1738	178.04
3052.3	5.11
3052.5	4.5
3052.8	5.41
3053.1	17.47
3056.5	9.8
3057.3	3.16
3060	4.68
3060.2	4.23
3121.8	0.14
3122.7	0.19
3130.1	3.42
3130.2	1.04
3134.8	4.95
3135.8	28.1
3138.4	2.01
3139.1	1.55
3139.6	15.16
3140.6	27.47
3161.7	0.01
3162.5	19.63
3174.6	5.92
3177.1	6.55
3188	1.86
3188.1	2.23

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000

C	-0.82867200	-0.64919600	1.05531800
O	-0.67113800	-1.82418300	1.40035400
Cu	0.70546300	-3.08000900	0.92386000
O	-0.67475800	-4.33147100	0.44620100
C	-0.83818000	-5.50495900	0.79386700
C	-0.01504000	-6.15126500	1.85556000
H	0.31042000	-5.43112800	2.60655200
H	-0.54893400	-6.98014700	2.31984600
H	0.88484500	-6.54216000	1.36835900
C	-1.89305900	-6.30661000	0.11542400
H	-1.47784300	-7.26924000	-0.19596800
H	-2.68172000	-6.52678900	0.84297100
H	-2.31155500	-5.77261200	-0.73460900
O	1.98667200	-1.92672900	1.31500600
C	3.28508800	-2.32016300	0.81778700
C	4.29998000	-1.54845700	1.65188800
H	5.31171100	-1.87290700	1.39091600
H	4.22583300	-0.47954400	1.44136300
H	4.14273300	-1.70256900	2.71891100
C	3.39782500	-1.92571300	-0.65319600
H	4.41028600	-2.08645000	-1.02925500
H	2.70758900	-2.49959100	-1.27645100
H	3.16809400	-0.86295500	-0.75671300
C	3.28293800	-3.84629900	1.03129400
O	1.98410200	-4.23617000	0.53234300
C	4.29677900	-4.62073500	0.19846000
H	5.30905900	-4.29893300	0.46057100
H	4.21962700	-5.68945000	0.40896300
H	4.14116400	-4.46631300	-0.86875800
C	3.39273600	-4.24099700	2.50243700
H	2.70338600	-3.66512900	3.12480600
H	3.15970700	-5.30303600	2.60590400
H	4.40523000	-4.08320600	2.87965900
C	-1.88614500	0.15303300	1.72978500
H	-1.47789300	1.12169500	2.03077000
H	-2.67885200	0.35927600	1.00244300
H	-2.29918300	-0.37619500	2.58548700
H	-0.55168400	0.79950200	-0.49482600
H	0.87014500	0.43824600	0.50089200
H	0.37199000	-0.72296800	-0.72557400



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Co^{2+}(Ace)_3$	4	-1961.711868	-1961.455138

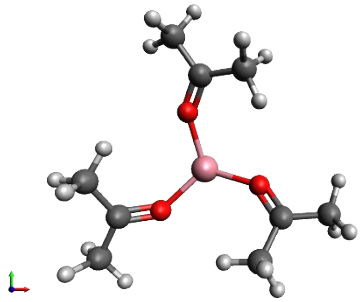
Frequency	Intensity
23.3	1.18
26.9	1.9
27.7	1.49
28.1	0.6
34.2	1.11
41	2.02
77.8	1.08
99.5	0.36
102.6	0.79
113	7.18
116.3	3.97
118.2	5.11
125.7	0.4
126	1.12
130.4	1.4
138.8	1.12
140.3	0.65
188.3	27.57
246.9	0.02
321.2	16.85
322.1	17.41
439.9	0.42
458.9	30.95
460.3	30.72
502.1	1.03
502.9	1.15
503.7	1.56
565.4	0.43
572.2	64.52

572.6	64.99
841.1	0.08
842.5	1.52
843.3	1.45
886.4	8.14
887.5	8
887.6	4.88
937.7	2.92
938.3	3.19
938.7	4.53
1101.7	0.88
1102.4	8.94
1102.8	8.9
1110.5	5.09
1110.9	11.57
1111.9	33.69
1305.2	38.63
1305.4	20.73
1305.7	24.25
1390.7	106.02
1390.8	102.16
1391.7	9.02
1408.4	22.4
1408.8	114.03
1409	159.77
1434.3	82.72
1435.9	85.34
1436.5	9.89
1449.4	9.84
1449.9	1.94
1450.5	14.94
1470.1	68.58
1470.9	52.19
1472.2	41.93
1482.6	22.55
1483.4	17.3
1484.2	68.52
1675.6	852.52
1675.9	855.12
1705.9	6.17
3037.5	20.81
3038	19.34
3038.1	24.82
3044.3	28.88
3044.7	34.58

3045	7.04
3114.7	0.52
3114.9	1.33
3114.9	0.72
3120.4	7.55
3120.8	8.32
3121.3	7.54
3169.1	4.96
3169.2	3.05
3170.8	4.22
3188.1	1.68
3188.3	1.85
3188.4	1.82

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	1.37335400	0.49141900	-0.26910800
O	1.60921700	1.71170900	-0.39001700
Co	0.88943100	3.47106100	-0.47000900
O	-0.99381900	3.72500800	-0.37782800
C	-1.93558100	4.53800400	-0.27091100
C	-1.68005700	5.99151300	-0.12371600
H	-1.97375600	6.47859800	-1.06216200
H	-2.32589800	6.41330000	0.65072300
H	-0.63341900	6.21113800	0.08472600
C	-3.32649900	4.03251500	-0.29000500
H	-3.69619300	4.04902800	0.74415800
H	-3.97404700	4.70609100	-0.85602800
H	-3.38438500	3.01572800	-0.67264700
O	2.05535300	4.97045600	-0.36083300
C	3.23195500	5.37118700	-0.24108200
C	3.51061700	6.82137700	-0.33645900
H	4.25761700	7.11969200	0.40294400
H	3.96359100	7.00437300	-1.32019700
H	2.60482600	7.41708200	-0.24668800
C	4.34485500	4.41896800	-0.00670600
H	4.66418800	4.53050900	1.03731000
H	4.05131800	3.38483900	-0.18529400
H	5.20981300	4.68705500	-0.61847900
C	2.48854300	-0.47256500	-0.39968500
H	2.39140200	-1.27680100	0.33330300
H	2.39894200	-0.94525900	-1.38713800
H	3.45862100	0.01440000	-0.32708700
H	-0.21692300	-0.87661000	-0.61560100
H	-0.03259900	-0.34436900	1.04146800

H	-0.75450500	0.77210000	-0.14829800



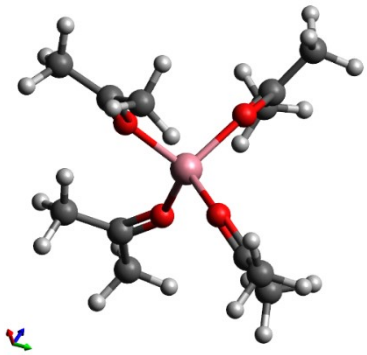
Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Co^{2+}(Ace)_4$	4	-2154.941587	-2154.598592

Frequency	Intensity
9.8	0.02
20.2	0.44
21.5	1.82
30.1	1.64
33	0.14
35.8	2.11
39.5	0.72
50.3	1.66
52.1	2.28
94.2	0.49
98.4	0.71
105.7	4.35
106.4	2.23
110.3	0.16
114.6	0.16
122.8	0.54
125.4	1.24
128	1.12
132.3	1.29
137.1	0.32
139	0.29
145.4	4.77
157.3	2.55
177.8	10.22
187.7	20.57
232.3	0.04
283.3	32.13

289.5	25.66
294.9	22.89
426.1	0.9
431.4	19.57
433.6	23.25
436.7	19.89
502.6	1.1
503.7	0.84
504.5	1.13
506.1	1.61
575	20.03
577.4	4.06
582.9	62.11
587.8	43.39
832.8	1
836.5	0.87
836.7	0.82
837.9	1.69
886	3.67
886.6	5.91
887.4	2.67
888.4	2.8
935.3	2.73
936.4	0.05
936.6	5.52
942.5	3.28
1097.7	4.77
1099.6	5.06
1100.2	2.01
1101.2	3.79
1115.5	8.16
1116.5	1.36
1118.2	24.16
1118.7	17.63
1298.7	11.06
1300.5	51.63
1302.1	41.16
1303.1	17.39
1395.7	81.41
1396.4	79.12
1396.9	72.07
1397.8	18
1413.1	41.6
1413.8	89.13
1414	93.35

1414.6	138.84
1440.7	72.17
1443.7	55.44
1445.1	46.79
1445.6	33.61
1452.5	2.82
1455.1	6.75
1455.6	7.15
1456.5	4.3
1472.2	37.44
1472.7	58.7
1474.1	29.3
1474.7	39.92
1486.7	17.05
1487.2	37.75
1488.5	25.24
1493.5	35.62
1697.3	720.2
1702.4	626.52
1707.2	643.64
1736.2	56.88
3043.2	14.27
3043.3	11.92
3044.2	10.41
3044.9	10.07
3048.6	13.46
3049.2	11.43
3049.9	13.85
3050.8	12.04
3116.1	0.11
3118	0.46
3118.4	0.1
3118.5	0.13
3122.6	3.29
3124.3	3.2
3124.6	3.17
3125.2	3.5
3167.5	3.42
3169.8	3.37
3170.8	1.63
3173.8	2.26
3185.1	1.75
3186.2	1.61
3187	1.32
3187.8	1.56

Atom	Standard Orientation		
Co	0.00000000	0.00000000	0.00000000
O	-1.76868800	-0.78936800	-0.36079300
C	-2.28956900	-1.85089500	-0.74496900
C	-3.76927400	-1.94332800	-0.82433700
H	-4.07291700	-2.43425600	-1.75242200
H	-4.11155200	-2.59460600	-0.01052600
H	-4.24059100	-0.96760700	-0.72645500
C	-1.46869000	-3.02937500	-1.13066100
H	-1.50565000	-3.11841700	-2.22340800
H	-0.43127600	-2.93222800	-0.81272800
H	-1.91115900	-3.94723400	-0.73650900
O	1.43250600	-1.34610800	-0.16987600
C	2.67338900	-1.34411600	-0.23826500
C	3.45286200	-0.07656200	-0.23270200
H	3.86187500	0.05429000	0.77683900
H	4.30911800	-0.14574300	-0.90652500
H	2.83701200	0.78728500	-0.48282400
C	3.39691000	-2.63714000	-0.31960400
H	3.76016700	-2.75406300	-1.34838800
H	4.28476300	-2.62068400	0.31723000
H	2.75151000	-3.47629800	-0.06888900
O	0.17461400	0.74624700	1.81045400
C	-0.44521900	0.91774100	2.87045300
C	-1.84707200	0.44368200	3.03942600
H	-1.82827800	-0.43573200	3.69414800
H	-2.44624800	1.19668600	3.55637400
H	-2.30616200	0.17506300	2.08821900
C	0.22384900	1.60991800	4.00105800
H	-0.21883700	2.60913400	4.09537900
H	0.01744300	1.09441800	4.94233500
H	1.29437800	1.70652500	3.83406800
O	0.38361700	1.50829700	-1.21657300
C	-0.19994900	2.37833500	-1.88094700
C	0.59978300	3.34286600	-2.67789400
H	0.51503200	3.05703000	-3.73384500
H	0.18354300	4.34973900	-2.59807900
H	1.64833100	3.32903100	-2.38818000
C	-1.68533500	2.48115300	-1.90084600
H	-2.04213500	2.63822100	-2.92167600
H	-2.16514200	1.60837900	-1.45828700
H	-1.96951200	3.37775500	-1.33747800



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Ni^{2+}(Ace)_3$	3	-2087.236437	-2086.979486

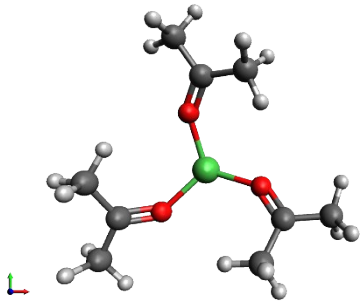
Frequency	Intensity
20.6	0.16
22.2	0.15
28.6	2.05
42.3	2.41
43.2	2.01
43.7	1.57
97.3	3.41
98.5	2.06
105.8	4.55
114.8	0.13
124.8	1.44
125.6	2.4
126.3	1.26
134.1	0.4
136	0.36
153.4	6.19
154.1	7.87
199.8	18.06
261.4	5.36
319.4	18.21
320.1	17.35
437.6	3.81
452.3	25.46
453.1	24.38
501.3	1.48
501.9	0.94
505.1	0.79

576.8	2.15
587	59.22
587.8	58.41
838.2	0.25
839.4	1.53
842.5	1.64
885.4	6.63
887.8	4.93
887.9	8.57
937.1	3.44
940.4	3.63
940.9	3.83
1099.7	2.79
1100.1	4.96
1100.3	5.2
1109.8	6.36
1110.7	19.06
1112.3	23.96
1306	36.24
1306.2	38.22
1306.8	7.8
1388.9	100.32
1389.3	106.18
1389.8	28.04
1406.9	70.77
1407.3	80.34
1407.4	123.81
1434	76.58
1434.4	82.24
1434.9	18.67
1448.9	12.15
1449.2	8.95
1450.1	6.86
1470.1	28.69
1470.6	65.38
1470.6	55.8
1483.3	36.2
1485.1	34.07
1485.6	34.82
1662.8	761.58
1663.8	757.38
1690.6	70.83
3036.2	28.94
3036.6	28.12
3037.9	23.31

3044.1	22.35
3044.5	19.91
3045.7	22.78
3113.9	1.08
3114.3	0.56
3114.5	0.91
3120.5	8.14
3120.6	6.73
3120.8	9.56
3173.4	3.89
3174	3.35
3176.2	3.97
3188.1	1.79
3188.4	2.07
3188.9	2.03

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	0.15701300	-1.32391400	-0.64912400
O	1.27141400	-1.72572000	-1.04877900
Ni	3.03994400	-1.15800900	-1.38585300
O	3.42095000	0.65577700	-1.01924400
C	4.33684800	1.42007400	-0.64537300
C	5.63000200	0.89388600	-0.14605200
H	6.39061400	1.10557800	-0.90837500
H	5.93969200	1.43942100	0.74896700
H	5.59987600	-0.17791200	0.04471900
C	4.10954500	2.88117600	-0.70593300
H	3.94066700	3.23194600	0.32113100
H	5.00807400	3.39425400	-1.05745700
H	3.24635800	3.13315000	-1.31834600
O	4.41064700	-2.40499300	-1.02689000
C	4.61251400	-3.56838100	-0.61621300
C	5.96083800	-4.15452900	-0.78040500
H	6.24318400	-4.72696700	0.10651500
H	5.90320000	-4.87781200	-1.60538200
H	6.70644400	-3.40050800	-1.02332700
C	3.53605800	-4.35842100	0.02881300
H	3.74594600	-4.38515800	1.10581000
H	2.54823300	-3.92962400	-0.13589100
H	3.56998700	-5.39577900	-0.31272500
C	-1.02015400	-2.20130200	-0.83051600
H	-1.66522100	-2.16790500	0.05089700
H	-1.61175100	-1.78578900	-1.65778000
H	-0.73459700	-3.22142800	-1.07808200

H	-0.91446100	0.48693700	-0.34712100
H	-0.13652700	-0.17395500	1.07511300
H	0.86408600	0.64526200	-0.15425600



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Ni^{2+}(Ace)_4$	3	-2280.463433	-2280.12025

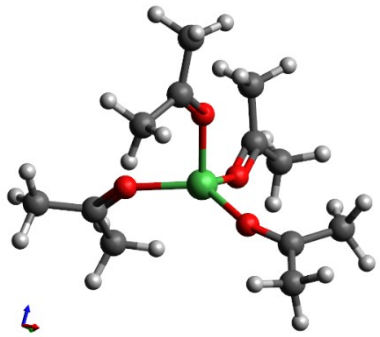
Frequency	Intensity
9.4	0.02
20.2	1.39
22.1	0.68
30.6	0.78
33.2	2.78
38.7	0.94
42.3	0.43
49	1.93
58.9	2.95
87.7	1.75
94	0.81
106.7	2.37
112	2.72
115.1	0.47
118.7	0.71
121.3	0.72
129.8	0.69
134.1	0.13
136.6	0.2
138.8	0.34
142.7	1.34
154.9	4.41
168.6	2.57
184.7	10.69
192.5	12.75

229	0.61
271.9	12.39
291	18.16
306.1	49.98
422.4	5.54
428.5	5.19
434.1	35.94
436.5	18.5
501.1	1.1
502.6	0.43
504	0.76
505.9	2.51
572.3	31.2
576.5	30.58
580.9	24.42
599.6	30.9
829.9	0.71
834.4	1.29
834.7	1.62
837.4	1.36
887.4	4.43
887.9	4.85
888.4	2.3
889.6	1.99
936.3	2.59
937.8	3.03
938.3	2.96
942.5	3.27
1093.6	2.26
1098.2	5.02
1099.1	2.54
1102.1	1.42
1114.2	12.18
1115.7	3.13
1117.1	26.82
1119	12.01
1296.8	5.31
1298.2	40.58
1299.4	53.16
1302.8	17.51
1395.2	63.79
1395.7	87.22
1396.5	69.06
1396.9	15.35
1411.5	63.56

1412.8	93.13
1412.8	18.12
1413.5	170.1
1439.9	65.5
1444	91
1444.7	16.09
1446.8	43.36
1452.7	5.87
1454.2	3.67
1456.5	6.38
1456.6	8.27
1470.8	54.27
1472	20.99
1472.6	32.54
1473.5	44.63
1485.6	25.18
1487.7	31.63
1490.2	14.57
1494.8	37.94
1703.4	393.64
1706.1	910.32
1708.6	642.44
1736.8	8.29
3043.6	16.51
3044.5	7.29
3044.6	17.42
3045.7	9.03
3049.5	7.19
3050.2	15.04
3050.6	16.83
3050.7	6.19
3115.6	0.16
3117.9	0.76
3118.7	0.16
3119	0.62
3122.2	2.36
3124.6	3.14
3126.5	2.77
3127.3	3.7
3165.7	2.66
3175.9	3.87
3178.8	3.23
3183.8	0.82
3185.2	5.34
3186.1	1.25

3187.1	1.51
3187.3	1.69

Atom	Standard Orientation		
Ni	0.00000000	0.00000000	0.00000000
O	-1.79138100	-0.57076100	-0.55641000
C	-2.88832800	-0.15397300	-0.95941500
C	-3.90172800	-1.12730400	-1.43958200
H	-4.89895000	-0.85309200	-1.08743800
H	-3.93369200	-1.06338500	-2.53460100
H	-3.64927400	-2.14514500	-1.15015500
C	-3.21891200	1.29750800	-0.97705100
H	-3.93364200	1.48955400	-0.16796500
H	-2.33770300	1.92242500	-0.83970800
H	-3.73309800	1.55795100	-1.90519100
O	-0.15903300	1.85919500	0.57015100
C	-0.31380600	2.54391900	1.59454400
C	-0.46456600	1.92819600	2.93925000
H	0.10650900	2.49190200	3.68065900
H	-1.51761500	2.02326700	3.23176300
H	-0.18259500	0.87699100	2.94454800
C	-0.35356000	4.02389400	1.46763800
H	-1.16177600	4.43831300	2.07570700
H	0.57713300	4.42514400	1.88752200
H	-0.44436800	4.33801600	0.42977500
O	1.80901100	-0.26346000	-0.67908700
C	2.90248500	0.27132400	-0.91748200
C	3.93837100	-0.48934700	-1.66009500
H	4.00488900	-0.06625400	-2.67027000
H	4.92089300	-0.34492100	-1.20372200
H	3.68893400	-1.54579800	-1.73094900
C	3.20363400	1.65851800	-0.47007400
H	3.84749900	1.58949700	0.41525600
H	3.77871900	2.19221900	-1.22945200
H	2.29795800	2.20708900	-0.21615400
O	0.15409500	-1.09469500	1.62886100
C	0.19694100	-2.32076700	1.80986800
C	0.32553000	-2.84369100	3.19415100
H	-0.63644100	-3.28660400	3.47949500
H	1.05748300	-3.65471500	3.22840900
H	0.58405200	-2.05672700	3.89937800
C	0.13780300	-3.28830000	0.67794600
H	-0.41139000	-4.18728800	0.96314700
H	-0.29949800	-2.85166000	-0.22039400
H	1.16471400	-3.60427000	0.45807100



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{2+}(Ace)_3$	2	-2219.413417	-2219.156532

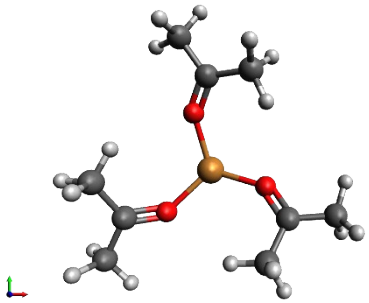
Frequency	Intensity
16.1	0.78
20.9	1.63
29.6	2.62
38.4	2.5
40.9	0.55
47.1	3.43
73.2	0.32
98.2	2.46
100.2	2.01
107.2	1.67
119.5	0.19
121.4	0.77
128.6	0.4
146.1	0.57
150.4	0.48
165	1.33
195.1	3.29
204.7	14.94
253.6	0.71
297	7.86
335.9	23.13
431.2	5.52
438.1	4.54
463	34.8
500.6	0.42
504	0.81
508.5	1.29
585.1	45.35

598	55.69
604.2	11.18
838.5	0.47
839.1	0.94
841.6	2.46
881.2	1.62
884.9	11.61
889.9	11.58
929.7	2.73
938	3.7
942.8	3.67
1093.3	0.1
1096.3	1.79
1101.8	1.06
1108.9	0.55
1109.8	33.07
1113.1	13.09
1302	22.42
1302.9	12.71
1305.5	30.38
1385.9	68.89
1387.3	58.2
1390.7	59.96
1401.9	82.14
1404.7	74.61
1405.4	103.64
1432.9	68.9
1433.4	58.56
1436.1	17.76
1447.1	8.13
1449.1	14.48
1451.4	13.8
1469.3	105.78
1470.3	10.56
1472.7	55.73
1478.6	35.79
1483.9	33.4
1486.5	39.29
1662.5	1074.32
1666	399.77
1686.7	42.49
3035.5	24.12
3035.9	31.8
3040.6	17.38
3041.9	35.55

3044.2	20.44
3048.5	26.36
3112.9	1.01
3113.5	0.73
3115.1	0.71
3119	8.24
3120.9	5.25
3121	11.43
3159.5	4.58
3165.2	3.69
3177.3	4.2
3187.7	2.16
3188.6	2.97
3189.1	2.53

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	0.43633300	-1.32619500	0.49938800
O	1.63894500	-1.56305800	0.73606300
Cu	3.40189200	-1.00930300	0.63521200
O	3.48107900	0.83478800	0.11203500
C	3.92213300	1.85939100	0.66991300
C	4.56506900	1.82452700	2.00905300
H	5.61767700	2.10808400	1.89587900
H	4.11873600	2.58904400	2.65185700
H	4.50181800	0.84885500	2.49178200
C	3.78022700	3.15597000	-0.03680700
H	2.99714000	3.73098600	0.47425600
H	4.69693200	3.74397700	0.05436000
H	3.50292200	3.01879000	-1.07983300
O	5.14834400	-1.59483100	0.96149400
C	6.22696100	-1.75689100	0.35228100
C	7.32463300	-2.46803600	1.04421700
H	7.82793700	-3.15266700	0.35667600
H	8.07466300	-1.71901700	1.33215600
H	6.97406400	-2.98549100	1.93462600
C	6.42115400	-1.26318100	-1.03393200
H	6.37313900	-2.13323100	-1.70198300
H	5.66091400	-0.54172200	-1.33486000
H	7.42221800	-0.84375400	-1.15689100
C	-0.55455600	-2.40021300	0.72875300
H	-1.47253200	-1.98957900	1.15587900
H	-0.82692600	-2.80534800	-0.25567800
H	-0.15072000	-3.20174000	1.34375000
H	-0.75687600	-0.12205000	-0.77870700

H	-0.49764800	0.51627600	0.83090900
H	0.83323400	0.60207400	-0.35926500



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Cu^{2+}(Ace)_4$	2	-2412.634387	-2412.290969

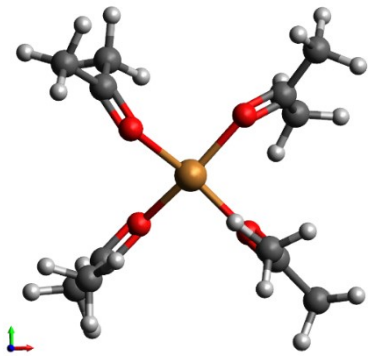
Frequency	Intensity
11	0.17
33.3	7.22
33.8	0
40.1	1.66
45.8	0
46.5	1.06
49.5	0
51.4	2.17
61.2	4.77
95	0
96.4	0
102.1	0.38
102.6	0
114.7	0
115.6	1.34
116.5	1.51
117.8	0
123.3	0.48
126.4	0
133.5	0.75
146.3	0
186.2	0
192.6	3.31
222.2	9.62
228.4	13.61
238.5	0

241.1	0
313	36.36
314.3	35.19
418.6	0
424.2	0
428.2	22.22
434.4	31.13
503	0
503.8	2.43
505.4	0
506.6	3.22
580.9	0
588.1	0
596.6	29.73
600.1	57.29
832.8	0
834.8	1.86
835.5	0
837	1.88
885.8	0
886.2	8.22
887	0
887.4	9.08
931.6	0
931.7	4.63
936.5	0
936.6	6
1094.2	0
1095.8	4.4
1096.7	0
1097.2	1.78
1112.6	0
1114.6	32
1115.5	18.95
1116.5	0
1295.7	26.95
1296.4	0
1298.3	56.73
1298.8	0
1394.8	0
1396	87.64
1396.2	128.1
1398.1	0
1411.7	35.35
1412.3	0

1413.3	0
1413.4	301.86
1442	83.8
1442.2	0
1443.1	51.99
1443.1	0
1452.9	0
1453	3.47
1453.6	0
1453.8	36.52
1472.8	101.09
1473.1	0
1474.6	74.79
1475	0
1483.1	0
1483.4	49.14
1489.8	0
1490.1	75.5
1699.6	0
1706	801.45
1715.5	990.58
1738.9	0
3044.1	0
3044.1	24.08
3045.5	0
3045.5	14.67
3049.6	26.92
3049.7	0
3051.7	37.01
3051.7	0
3117.7	0.21
3117.7	0
3119.2	0
3119.3	0.71
3123.5	0
3123.6	5.71
3125.2	0
3125.2	10.3
3162.9	0
3162.9	17.6
3174.3	0
3174.3	5.51
3187.2	2.25
3187.2	0
3187.4	0

3187.4 2.48

Atom	Standard Orientation		
Cu	0.00000000	0.00000000	0.00000000
O	-1.73213900	0.64717200	0.61665500
C	-2.63635300	1.36469600	0.16391500
C	-3.75835100	1.74961900	1.05899400
H	-3.63419800	2.80909200	1.31532700
H	-4.71418500	1.67167300	0.53524700
H	-3.76038700	1.15972300	1.97311800
C	-2.64496100	1.83930100	-1.24815200
H	-2.95883600	2.88455000	-1.29708600
H	-1.67970600	1.71496500	-1.73751000
H	-3.40999700	1.26990200	-1.78997900
O	0.56038500	1.83295400	-0.37552500
C	1.41518800	2.60623400	0.07736500
C	2.22484900	2.27572200	1.28367400
H	3.27797200	2.51093800	1.11107200
H	1.89617500	2.92501600	2.10319900
H	2.11133600	1.23581200	1.59053100
C	1.63694100	3.91105900	-0.59818900
H	1.75028500	4.71322000	0.13470700
H	2.58839300	3.84893000	-1.14078600
H	0.84110800	4.13455600	-1.30542500
O	1.73213900	-0.64717200	-0.61665500
C	2.63635300	-1.36469600	-0.16391500
C	3.75835100	-1.74961900	-1.05899400
H	4.71418500	-1.67167300	-0.53524700
H	3.63419800	-2.80909200	-1.31532700
H	3.76038700	-1.15972300	-1.97311800
C	2.64496100	-1.83930100	1.24815200
H	2.95883600	-2.88455000	1.29708600
H	3.40999700	-1.26990200	1.78997900
H	1.67970600	-1.71496500	1.73751000
O	-0.56038500	-1.83295400	0.37552500
C	-1.41518800	-2.60623400	-0.07736500
C	-1.63694100	-3.91105900	0.59818900
H	-2.58839300	-3.84893000	1.14078600
H	-1.75028500	-4.71322000	-0.13470700
H	-0.84110800	-4.13455600	1.30542500
C	-2.22484900	-2.27572200	-1.28367400
H	-3.27797200	-2.51093800	-1.11107200
H	-2.11133600	-1.23581200	-1.59053100
H	-1.89617500	-2.92501600	-2.10319900



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Zn^{2+}(Ace)_3$	1	-2358.306724	-2358.049848

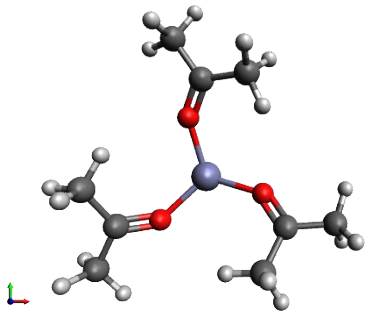
Frequency	Intensity
14.3	0.03
16.2	0.15
25.9	3.51
43	3.88
45.4	1.55
49.6	0.83
100.8	0.03
102.3	0.39
111.7	4.72
118.6	0.19
133.7	3.03
136.8	4.25
139.2	2.43
141	5.41
145.1	3.86
146.8	1.98
152.5	2.7
197.6	27.82
248.4	0.01
305.8	22.09
306.6	21.22
433.5	0.16
444	29.11
445.8	28.35
503.6	0.43
504.4	1.08
505.1	0.68
584.2	0.03
593.5	52.09

593.9	52.55
835.4	0
836.7	0.89
837.2	0.94
884.7	9.77
885.1	9.15
885.5	0.91
942.1	3.27
942.6	3.33
942.8	6.19
1097.2	7.81
1097.2	12.93
1097.4	10.17
1110.5	2.29
1110.9	9.15
1111.9	40.42
1308.7	39.39
1308.9	38.65
1309.9	0.8
1389.2	115.85
1389.6	117.12
1390.6	6
1409.3	5.63
1409.5	138.2
1410	181.78
1431	101.35
1432.7	104.68
1433.6	5.42
1447.9	3.42
1448.1	5.01
1449.3	14.96
1472.7	27.49
1473	50.93
1474	46.88
1487.5	8.5
1488.3	34.82
1488.9	70.39
1657.4	772.59
1657.6	766.96
1683.8	0.06
3034.7	10.4
3034.7	41.22
3034.8	28.14
3041.3	33.09
3041.4	14.59

3042.3	18.13
3114.1	1.49
3114.1	1.3
3114.3	1.32
3119.8	7.09
3120	7.56
3120.2	8.19
3165.3	2.89
3165.9	2.55
3168	2.64
3188.6	1.6
3189	1.69
3189.1	1.68

Atom	Standard Orientation		
C	0.00000000	0.00000000	0.00000000
C	-0.17813200	1.42906600	-0.35040100
O	-1.31280100	1.95424000	-0.43571200
Zn	-3.13995300	1.39881400	-0.32205600
O	-3.56665700	-0.46602600	-0.28215200
C	-4.59120300	-1.18326000	-0.36219600
C	-5.93406300	-0.60733500	-0.61074700
H	-6.20438000	-0.83918100	-1.64930300
H	-6.68235700	-1.10303200	0.01255900
H	-5.96588900	0.47256000	-0.46376400
C	-4.44012300	-2.64571700	-0.20480300
H	-4.77741600	-2.89964200	0.80979800
H	-5.10218000	-3.18140500	-0.88883900
H	-3.40593700	-2.96238900	-0.32186400
O	-4.54261400	2.69918500	-0.27324000
C	-4.64656500	3.94788000	-0.24875900
C	-6.00110600	4.54085800	-0.26203000
H	-6.04645600	5.42375800	0.37940500
H	-6.19043900	4.89494600	-1.28501800
H	-6.76506500	3.81423000	0.00632000
C	-3.45897100	4.83362600	-0.20765900
H	-3.39536200	5.25339800	0.80472900
H	-2.53099800	4.31019000	-0.43906100
H	-3.59761400	5.68568200	-0.87792900
C	1.00856900	2.27322600	-0.60620100
H	1.82288300	2.01769400	0.07554900
H	1.36714200	2.03093700	-1.61635900
H	0.77008800	3.33377200	-0.56283000
H	0.78417100	-0.44823700	-0.61506200
H	0.36625000	-0.04183800	1.03420000

H	-0.92396900	-0.57374300	-0.07686200



Molecule	Multiplicity	E (no zpe)	E (w/ zpe)
$Zn^{2+}(Ace)_4$	1	-2551.532334	-2551.189405

Frequency	Intensity
8.3	0.58
18.9	1.03
19.8	0.47
27.4	2.24
30.8	0.4
34.5	1.14
36.3	1.12
44.4	2
49.9	1.62
89.6	1.04
95.8	0.82
102.8	2.07
106.9	2.66
110.9	1.56
112.8	1.35
125	1.56
126.6	1.1
133.4	0.52
134.4	0.16
138.8	1.27
138.9	0.43
148.9	11.06
154.8	3.39
172.8	11.06
185.9	34.57
241.6	0.07
283.9	21.63

285	23.64
288.3	21.56
426.9	0.9
430.1	16.32
432.4	20.22
435.2	19.87
502.6	0.98
503.1	1.03
503.9	0.62
505.1	1.68
579.2	17.07
583.9	23.03
587.9	47.85
593.3	39.8
833.5	0.78
834.7	0.75
835.2	1.14
836.4	1.5
886.5	4.36
886.8	5.58
887.3	3.63
887.8	1.46
937.3	3.27
937.7	3.17
939.7	3.36
942	3.7
1097.5	6.46
1097.8	4.14
1099.7	5.16
1100	3.85
1115.6	2.53
1116	8.15
1117.8	25.44
1118.5	18.22
1299.2	8.98
1299.7	45.74
1301.6	43.2
1302.7	24.89
1395.3	83.59
1395.7	82.64
1396.2	69.11
1396.8	15.43
1413.4	38.73
1414	131.71
1414.3	81.73

1414.6	118.56
1439.3	74.06
1441.9	66.9
1443.3	42.64
1444.7	48.42
1451.3	3.42
1453.1	2.49
1453.7	7.66
1455	3.24
1471.8	41.02
1473	24.78
1473.5	43.56
1474.3	28.3
1489.2	25.84
1489.5	26.76
1492	16.9
1492.8	48.16
1699.8	653.11
1704.4	654.6
1707.6	583
1736.4	43.72
3042.3	15.1
3043.1	8.98
3043.3	10.66
3043.8	13.18
3048	11.24
3048.6	14.98
3048.8	17.22
3049.5	9.09
3117.1	0.26
3117.1	0.32
3118.1	0.29
3118.7	0.39
3123.5	3
3123.8	4.55
3124.8	2.7
3125.2	4.03
3161.3	4.39
3168.5	2.27
3172.2	1.82
3173.9	1.67
3185.3	1.59
3186.8	1.39
3187.7	1.35
3188	1.54

Atom		Standard Orientation	
Zn	0.00000000	0.00000000	0.00000000
O	1.67406900	-1.02548600	-0.21202500
C	2.03342900	-2.21399500	-0.28536000
C	3.47426800	-2.52134600	-0.46565100
H	3.77188900	-3.35653900	0.17328500
H	3.61773100	-2.86314600	-1.49850100
H	4.09880400	-1.64876500	-0.28608100
C	1.06216200	-3.33598100	-0.19194200
H	1.15378700	-3.77024200	0.81159700
H	0.03537100	-3.00737500	-0.34961900
H	1.32486500	-4.13120000	-0.89291900
O	-1.56489100	-1.08939300	-0.49383800
C	-2.79740700	-0.95718200	-0.40270000
C	-3.41364500	0.26433100	0.18221700
H	-3.76378200	0.88864600	-0.64905400
H	-4.29718800	0.00867700	0.77040700
H	-2.70744200	0.83535700	0.78506400
C	-3.67920900	-2.04276800	-0.89813900
H	-4.08833900	-2.56616300	-0.02469200
H	-4.53645700	-1.62787000	-1.43387900
H	-3.13497600	-2.75128200	-1.51894400
O	-0.01432700	1.62957600	-1.10303000
C	0.60819200	2.16474300	-2.03403700
C	1.79914700	1.52118800	-2.65326700
H	1.48665200	1.10197800	-3.61762300
H	2.56734800	2.26431700	-2.87722500
H	2.20434900	0.72453500	-2.02983900
C	0.15037800	3.47946500	-2.54945400
H	0.87019900	4.24000700	-2.22243100
H	0.17231400	3.49084200	-3.64218700
H	-0.83804700	3.73541000	-2.17425600
O	-0.23298700	0.56526300	1.87492600
C	0.45520400	1.10179700	2.75737300
C	-0.14880700	1.37134400	4.08590900
H	0.26560700	0.64548700	4.79676200
H	0.14613000	2.35844700	4.45023300
H	-1.23154700	1.26919200	4.06202200
C	1.87339900	1.48816600	2.51716100
H	2.48867200	1.26478900	3.39141100
H	2.28765200	1.00843500	1.62959900
H	1.90548500	2.57684400	2.38871600

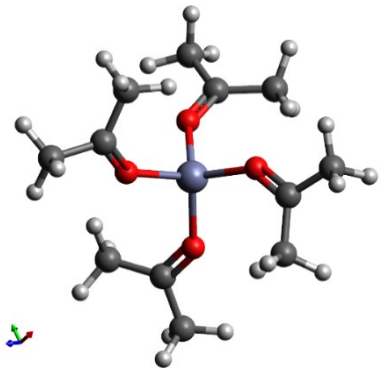


Table S3 Calculated bond lengths and angles of $M^{2+}(Ace)_4$, M = Co, Ni, Cu, and Zn, $Cu^{+}(Ace)_4$, $Cu^{+}(Ace)(N_2)_k$ (k=0–2) and $Al^{+}(Ace)(N_2)$.

Species	Bond Length (Å)				Bond Angle (degree)			
	r_{M-O}	$r_{C=O}$	r_{C-C}	r_{C-H}	r_{M-N}	L_1–M–L_3	L_2–M–L_4	C–C–C
C_3H_6O	N/A	*1.214* 1.211	*1.520* 1.517	*1.103* 1.089 to 1.095	N/A	N/A	N/A	*116.0* 116.3
$Co^{2+}(Ace)_4$	1.970 to 1.979	1.245 1.246 1.249	1.487 to 1.492	1.088 to 1.098	N/A	113.7	109.0	119.4 119.3
$Ni^{2+}(Ace)_4$	1.949 1.958 1.975	1.245 1.246 1.247	1.487 to 1.493	1.088 to 1.098	N/A	138.5	107.4	119.1 to 119.5
$Cu^{2+}(Ace)_4$	1.964 1.969	1.243 1.245	1.490 1.493	1.088 to 1.098	N/A	180.0	180.0	119.0 119.2
$Zn^{2+}(Ace)_4$	1.978 to 1.987	1.247 to 1.250	1.487 to 1.492	1.088 to 1.098	N/A	112.5	107.4	119.3
$Cu^{+}(Ace)_4$	2.088 2.101 2.109	1.222 to 1.226	1.495 to 1.502	1.088 to 1.096	N/A	111.8	105.7	117.8 117.9 118.8
$Cu^{+}(Ace)(N_2)_2$	1.945	1.234	1.490 1.493	1.088 to 1.096	2.004 2.021	N/A	N/A	118.7
$Cu^{+}(Ace)(N_2)$	1.869	1.237	1.486 1.489	1.087 to 1.096	1.888	N/A	N/A	119.0
$Cu^{+}(Ace)$	1.890	1.237	1.486 1.489	1.087 to 1.096	N/A	N/A	N/A	119.0
$Al^{+}(Ace)(N_2)$[a]	1.937	1.251	1.485	1.088 to 1.099	3.381	N/A	N/A	120.0

Calculations performed at zero Kelvin with the B3LYP+D3/6–311+G(d,p) level of theory unless indicated otherwise. [a] B3LYP+D3/6–311+G(d,p).[26]

Table S4: Properties of the metal cations and of the complexes calculated at the B3LYP+D3/6-311+G(d, p) (for Z < 37) and B3LYP+D3/Def2-TZVP (for Z ≥ 37) level of theory.

Species	q	Multi	IE($M^{(n-1)+}$)	Radii (Å)	q(M^+)	q(/Ace)	σ* (CO)	Δσ*(CO)	π*(CO)	Δπ*(CO)	ν_{CO}	$-\Delta\nu_{CO}$
Li^+(Ace)	1	1	5.392	0.96283	0.9632	0.0368	0.02309	0.0076	0.14694	0.05869	1711	76.1
Na^+(Ace)	1	1	5.139	1.332761	0.98444	0.01556	0.02138	0.00589	0.13143	0.04318	1724.8	62.3
K^+(Ace)	1	1	4.34	1.751214	0.98813	0.01187	0.02088	0.00539	0.12368	0.03543	1727.7	59.4
Rb^+(Ace)	1	1	4.177	1.921683	0.97983	0.02017	0.02028	0.00479	0.11925	0.031	1733.5	53.6
Cs^+(Ace)	1	1	3.894	2.131406	0.98301	0.01699	0.02048	0.00499	0.11815	0.0299	1731.9	55.2
Mg^+(Ace)	1	2	7.646	2.02058	0.94674	0.05326	0.02665	0.01116	0.159	0.07075	1679.5	107.6
Ca^+(Ace)	1	2	6.113	2.277188	0.95531	0.04469	0.02502	0.00953	0.15148	0.06323	1684.2	102.9
Al^+(Ace)	1	1	5.986	2.059452	0.93803	0.06197	0.03177	0.01628	0.1749	0.08665	1627.5	159.6
Ga^+(Ace)	1	1	5.999	2.005779	0.94266	0.05734	0.02905	0.01356	0.15541	0.06716	1651.2	135.9
Cu^+(Ace)	1	1	7.726	1.705265	0.89908	0.10092	0.02903	0.01354	0.15755	0.0693	1665.9	121.2
Zn^+(Ace)	1	2	9.394	1.931557	0.85901	0.14099	0.0267	0.01121	0.15505	0.0668	1644.3	142.8
Ag^+(Ace)	1	1	7.576	1.882244	0.90285	0.09715	0.02938	0.01389	0.14236	0.05411	1678.2	108.9
Mg^{2+}(Ace)	2	1	15.035	1.158021	1.92846	0.07154	0.03429	0.0188	0.2316	0.14335	1568.3	218.8
Ca^{2+}(Ace)	2	1	11.871	1.560916	1.91143	0.08857	0.03264	0.01715	0.2113	0.12305	1572.2	214.9
Sr^{2+}(Ace)	2	1	11.03	1.752159	1.92519	0.07481	0.03145	0.01596	0.19533	0.10708	1592.5	194.6
Co^{2+}(Ace)	2	4	17.083	1.575664	1.56568	0.43432	0.036	0.02051	0.24629	0.15804	1477.9	309.2
Ni^{2+}(Ace)	2	3	18.169	1.555686	1.45922	0.54078	0.03495	0.01946	0.24239	0.15414	1457.2	329.9
Cu^{2+}(Ace)	2	2	20.292	1.522092	1.18861	0.81139	0.02929	N/A	0.10684	N/A	1506.7	280.4
Zn^{2+}(Ace)	2	1	17.964	1.496894	1.63151	0.36849	0.03759	0.0221	0.23169	0.14344	1441.8	345.3