Supporting Information (11 pages)

Rubisco-Inspired Biomimetic Approaches to Reversible CO_2 Capture from Air.

Metal Dependence of the H_2O/CO_2 Replacement Penalty

Rainer Glaser

Department of Chemistry, University of Missouri, Columbia, Missouri 65211, USA and Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

Table of Content: Cartesian Coordinates of Metal Formates ML_2 and of their Complexes with H_2O and CO_2

MgL_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.333173	-0.000677	0.000120
2	1	0	3.429433	-0.001444	0.000307
3	6	0	-2.333159	-0.000509	0.000259
4	1	0	-3.429406	-0.001044	0.000694
5	8	0	1.711813	-0.791372	-0.787253
6	8	0	1.712928	0.791369	0.786922
7	8	0	-1.711845	-0.789680	0.789151
8	8	0	-1.712990	0.789392	-0.788681
9	12	0	0.000054	0.000995	-0.000366

Rotational constants (GHZ): 6.3407258 1.3240596 1.3232012
Standard basis: 6-31G(d) (6D, 7F)

$MgL_2{\cdot}OH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.299320	-0.565630	-0.054270
2	1	0	3.359732	-0.851020	-0.079210
3	6	0	-2.288448	-0.586821	0.106981
4	1	0	-3.342867	-0.886103	0.182157
5	8	0	1.544646	-0.930856	-1.016479
6	8	0	1.865283	0.117989	0.928170
7	8	0	-1.502676	-0.860514	1.073679
8	8	0	-1.892487	0.024237	-0.938281
9	12	0	0.001904	0.009274	-0.037301
10	8	0	0.002706	2.072600	-0.079335
11	1	0	0.561287	2.571245	0.539840
12	1	0	-0.806011	2.581648	-0.253480

Rotational constants (GHZ): 2.7927588 1.2614388 1.1118136
Standard basis: 6-31G(d) (6D, 7F)

$MgL_2{\cdot}OCO$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.653458	-0.791687	0.180292
2	1	0	3.624444	-1.290204	0.293637
3	6	0	-0.973520	2.081443	0.041613
4	1	0	-1.669402	2.929526	0.075328
5	8	0	2.064477	-0.343066	1.222128
6	8	0	2.145126	-0.678232	-0.981748
7	8	0	-0.050173	2.074619	-0.837509
8	8	0	-1.111838	1.130228	0.880445
9	12	0	0.579345	0.288711	-0.038993
10	6	0	-1.976675	-1.360678	-0.146978
11	8	0	-0.840406	-1.341902	-0.497613
12	8	0	-3.098030	-1.426437	0.170471

Rotational constants (GHZ): 1.5710996 0.8996599 0.6764321
Standard basis: 6-31G(d) (6D, 7F)

CaL_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.677201	0.005121	0.006103
2	1	0	-3.777843	0.008764	0.012378
3	6	0	2.677192	0.004106	0.004926
4	1	0	3.777793	0.011983	0.013480
5	8	0	-2.073574	0.805856	0.793152
6	8	0	-2.088063	-0.799877	-0.787783
7	8	0	2.080312	-0.795277	0.798586
8	8	0	2.081335	0.795524	-0.797443
9	20	0	0.000001	-0.006296	-0.007206

Rotational constants (GHZ): 6.2219123 0.9753151 0.9743787
Standard basis: 6-31G(d) (6D, 7F)

$CaL_2 \cdot OH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.797213	-0.273407	0.112185
2	1	0	-3.894009	-0.354506	0.183489
3	6	0	2.526652	-0.766718	0.047882
4	1	0	3.593226	-1.043777	0.056742
5	8	0	-2.118971	-0.451004	1.175830
6	8	0	-2.294310	-0.008265	-1.027364
7	8	0	1.766628	-1.355777	-0.780013
8	8	0	2.136881	0.126782	0.873544
9	8	0	0.762267	2.164213	-0.233021
10	1	0	0.638900	3.116444	-0.359342
11	1	0	1.617945	2.014902	0.217255
12	20	0	-0.117633	-0.064995	-0.056518

Rotational constants (GHZ): 2.6150121 0.9139317 0.8130209
Standard basis: 6-31G(d) (6D, 7F)

$CaL_2 \cdot OCO$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.127480	-0.610674	0.117937
2	1	0	4.149974	-1.015594	0.178290
3	6	0	-1.599876	1.899637	0.061103
4	1	0	-2.506408	2.524937	0.085687
5	8	0	2.573213	-0.230613	1.201150
6	8	0	2.576116	-0.553102	-1.028790
7	8	0	-0.723962	2.153525	-0.825047

8	8	0	-1.496817	0.964274	0.923560
9	6	0	-2.134797	-1.580891	-0.126791
10	8	0	-0.991275	-1.558452	-0.448497
11	8	0	-3.263822	-1.654773	0.163945
12	20	0	0.630598	0.363767	-0.023402

Rotational constants (GHZ): 1.5025871 0.6705917 0.5304857
Standard basis: 6-31G(d) (6D, 7F)

ZnL_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.301650	0.000804	0.000311
2	1	0	-3.395733	0.001220	0.000292
3	6	0	2.301650	0.000747	0.000210
4	1	0	3.395733	0.001074	0.000463
5	8	0	-1.672841	0.785303	-0.783551
6	8	0	-1.673463	-0.785015	0.783352
7	8	0	1.672699	0.785649	0.783511
8	8	0	1.673609	-0.785130	-0.782932
9	30	0	-0.000001	-0.000602	-0.000231

Rotational constants (GHZ): 6.4205732 1.3705159 1.3697932
Standard basis: 6-31G(d) (6D, 7F)

$ZnL_2 \cdot OH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.304103	-0.511608	0.112840
2	1	0	-3.368423	-0.753642	0.216136
3	6	0	2.299805	-0.504669	-0.059168
4	1	0	3.367712	-0.743059	-0.125774
5	8	0	-1.492507	-0.921056	1.008674
6	8	0	-1.909175	0.169519	-0.882967
7	8	0	1.535123	-0.864802	-1.018796
8	8	0	1.854650	0.116786	0.951651
9	8	0	0.051236	2.007234	-0.026407
10	1	0	-0.781996	2.499116	-0.117371
11	1	0	0.600521	2.432835	0.653566
12	30	0	-0.003555	-0.046634	-0.040194

Rotational constants (GHZ): 2.9564022 1.2687735 1.1279775
Standard basis: 6-31G(d) (6D, 7F)

$ZnL_2 \cdot OCO$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.425260	-1.019478	0.155116

2	1	0	3.335978	-1.619152	0.253390
3	6	0	-0.971526	2.087408	0.012079
4	1	0	-1.635859	2.957844	0.009486
5	8	0	1.959410	-0.424077	1.185598
6	8	0	1.848427	-0.929540	-0.973051
7	8	0	0.017383	2.057932	-0.791495
8	8	0	-1.199070	1.122865	0.810407
9	6	0	-2.114866	-1.364426	-0.117618
10	8	0	-0.963384	-1.376670	-0.404515
11	8	0	-3.254203	-1.391098	0.144853
12	30	0	0.499939	0.265499	-0.011157

Rotational constants (GHZ): 1.5312173 0.9173514 0.6669930
Standard basis: 6-31G(d) (6D, 7F)

CuL_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.261088	0.000006	0.000025
2	1	0	-3.354971	0.000006	0.000428
3	6	0	2.261087	-0.000009	0.000207
4	1	0	3.354966	-0.000020	0.000298
5	8	0	-1.619584	1.102750	-0.000100
6	8	0	-1.619595	-1.102744	0.000276
7	8	0	1.619581	1.102712	0.000197
8	8	0	1.619551	-1.102711	-0.000178
9	29	0	0.000014	-0.000001	-0.000127

Rotational constants (GHZ): 6.4958714 1.6135527 1.2925000
Standard basis: 6-31G(d) (6D, 7F)

$CuL_2 \cdot OH_2$, HB2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.270789	-0.371502	0.218086
2	1	0	-3.356497	-0.493000	0.297862
3	6	0	2.270750	-0.371273	0.218160
4	1	0	3.356483	-0.492381	0.298083
5	8	0	-1.675434	0.513634	0.917137
6	8	0	-1.609374	-1.112632	-0.578377
7	8	0	1.609573	-1.113199	-0.577777
8	8	0	1.675044	0.514177	0.916581
9	8	0	0.000019	1.817740	-0.958802
10	1	0	-0.773604	2.266904	-0.574264
11	1	0	0.773024	2.266184	-0.572152
12	29	0	0.000076	-0.139615	0.006307

Rotational constants (GHZ): 2.9646664 1.3496672 1.1574216
Standard basis: 6-31G(d) (6D, 7F)

$CuL_2 \cdot OH_2$, HB2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.233169	-0.490462	-0.050822
2	1	0	-3.314528	-0.668758	-0.064790
3	6	0	2.297344	-0.328631	-0.027700
4	1	0	3.391057	-0.385337	-0.040385
5	8	0	-1.619771	-0.418649	1.065474
6	8	0	-1.600313	-0.346828	-1.145105
7	8	0	1.661909	-0.106622	-1.111165
8	8	0	1.665906	-0.481794	1.066705
9	8	0	-0.135281	2.012834	0.186313
10	1	0	-0.316749	2.494995	-0.638691
11	1	0	-0.821853	2.291378	0.816628
12	29	0	0.030945	-0.141008	-0.003428

Rotational constants (GHZ): 2.9787251 1.2722569 1.2344922
Standard basis: 6-31G(d) (6D, 7F)

$CuL_2 \cdot OCO$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.716521	-2.267583	0.191371
2	1	0	0.752650	-3.360231	0.241290
3	6	0	0.735190	2.262216	0.191062
4	1	0	0.780411	3.354533	0.240793
5	8	0	-0.069179	-1.617651	0.958711
6	8	0	1.455775	-1.641661	-0.636526
7	8	0	1.469784	1.629998	-0.636262
8	8	0	-0.056356	1.618953	0.957993
9	6	0	-2.321391	0.008470	-0.438420
10	8	0	-1.353876	0.004925	-1.122916
11	8	0	-3.292878	0.012073	0.216095
12	29	0	0.636512	-0.002276	0.067485

Rotational constants (GHZ): 1.3227718 1.1430026 0.7318694
Standard basis: 6-31G(d) (6D, 7F)

NiL_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.181640
2	1	0	0.000000	0.000000	3.275231
3	6	0	0.000000	0.000000	-2.181640
4	1	0	0.000000	0.000000	-3.275231
5	8	0	0.000000	1.091719	1.519138
6	8	0	0.000000	-1.091719	1.519138
7	8	0	0.000000	1.091719	-1.519138
8	8	0	0.000000	-1.091719	-1.519138

9	28	0	0.000000	0.000000	0.000000

Rotational constants (GHZ): 6.6275632 1.7826270 1.4047807
Standard basis: 6-31G(d) (6D, 7F)

$NiL_2 \cdot OH_2$, HB2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.196690	-0.333487	0.149871
2	1	0	-3.289415	-0.391432	0.172626
3	6	0	2.196563	-0.333894	0.150015
4	1	0	3.289263	-0.392118	0.173003
5	8	0	-1.566162	0.498322	0.887711
6	8	0	-1.516681	-1.089764	-0.617025
7	8	0	1.516532	-1.090083	-0.616899
8	8	0	1.566126	0.498192	0.887663
9	8	0	0.000576	1.961602	-0.929930
10	1	0	-0.766047	2.322332	-0.453074
11	1	0	0.767498	2.320294	-0.452042
12	28	0	-0.000131	-0.217176	0.066715

Rotational constants (GHZ): 2.8643019 1.4722997 1.2181705
Standard basis: 6-31G(d) (6D, 7F)

$NiL_2 \cdot OH_2$, HB2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.189794	-0.355347	0.051570
2	1	0	-3.283497	-0.412081	0.063016
3	6	0	2.194874	-0.318947	0.045421
4	1	0	3.289481	-0.320930	0.047210
5	8	0	-1.536469	-0.114318	1.120262
6	8	0	-1.538398	-0.518024	-1.032464
7	8	0	1.540427	-0.516370	-1.031324
8	8	0	1.537514	-0.113113	1.119158
9	8	0	0.048869	2.064474	-0.283065
10	1	0	-0.349937	2.483680	-1.063114
11	1	0	-0.267612	2.578590	0.477735
12	28	0	0.005912	-0.239453	0.026881

Rotational constants (GHZ): 2.9183698 1.3824703 1.3123321
Standard basis: 6-31G(d) (6D, 7F)

$NiL_2 \cdot OCO$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.709583	-2.185626	-0.153129
2	1	0	-0.725361	-3.279210	-0.166984
3	6	0	-0.697315	2.188936	-0.152964
4	1	0	-0.706873	3.282595	-0.166669

5	8	0	0.104285	-1.527459	-0.887556
6	8	0	-1.498854	-1.522358	0.596896
7	8	0	-1.490396	1.530064	0.596934
8	8	0	0.112938	1.526277	-0.887385
9	6	0	2.307304	-0.005453	0.449424
10	8	0	1.448179	-0.004478	1.262205
11	8	0	3.173259	-0.006450	-0.343552
12	28	0	-0.670196	0.001597	-0.115238

Rotational constants (GHZ): 1.4300954 1.1563679 0.7717149
Standard basis: 6-31G(d) (6D, 7F)

CoL_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.207248	-0.000024	0.000374
2	1	0	-3.301219	-0.000109	-0.001008
3	6	0	2.207251	0.000028	0.000445
4	1	0	3.301221	0.000115	-0.000869
5	8	0	-1.547674	1.093591	0.001769
6	8	0	-1.547574	-1.093604	-0.000336
7	8	0	1.547576	1.093603	-0.000676
8	8	0	1.547678	-1.093589	0.002177
9	27	0	-0.000002	-0.000001	-0.000982

Rotational constants (GHZ): 6.6047987 1.7299547 1.3708881
Standard basis: 6-31G(d) (6D, 7F)

$CoL_2 \cdot OH_2$, HB2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.250775	-0.319493	0.189019
2	1	0	-3.342650	-0.397068	0.243927
3	6	0	2.250570	-0.319978	0.189117
4	1	0	3.342425	-0.397869	0.243952
5	8	0	-1.620673	0.489822	0.951429
6	8	0	-1.594494	-1.025932	-0.641111
7	8	0	1.594125	-1.025946	-0.641338
8	8	0	1.620665	0.489228	0.951924
9	8	0	0.000803	1.682410	-1.021045
10	1	0	-0.770724	2.176675	-0.691576
11	1	0	0.772019	2.175972	-0.690030
12	27	0	-0.000120	-0.170279	0.067631

Rotational constants (GHZ): 3.1287946 1.3608125 1.2284349
Standard basis: 6-31G(d) (6D, 7F)

$CoL_2 \cdot OH_2$, HB2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.229051	-0.399025	-0.000486
2	1	0	3.319781	-0.510817	-0.002751
3	6	0	-2.263540	-0.294932	-0.000440
4	1	0	-3.359263	-0.305892	-0.003829
5	8	0	1.585552	-0.336411	-1.099404
6	8	0	1.592423	-0.316760	1.101129
7	8	0	-1.620416	-0.279956	1.099975
8	8	0	-1.614127	-0.290783	-1.097626
9	8	0	0.034409	1.935878	-0.009802
10	1	0	0.510885	2.303005	0.754579
11	1	0	0.477838	2.296068	-0.796626
12	27	0	-0.020927	-0.196828	0.003704

Rotational constants (GHZ): 3.1460765 1.3054287 1.2936963
Standard basis: 6-31G(d) (6D, 7F)

$CoL_2 \cdot OCO$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.787342	2.189764	-0.186978
2	1	0	-1.426861	3.077689	-0.234493
3	6	0	1.991552	-1.386650	-0.168925
4	1	0	2.691327	-2.228328	-0.205469
5	8	0	-0.955417	1.229569	-1.013949
6	8	0	0.125418	2.097483	0.695357
7	8	0	2.134593	-0.465268	0.699819
8	8	0	1.018946	-1.319161	-0.993609
9	6	0	-1.887654	-1.240634	0.431537
10	8	0	-1.009984	-0.772302	1.078911
11	8	0	-2.766800	-1.716649	-0.176626
12	27	0	0.535635	0.346163	-0.086410

Rotational constants (GHZ): 1.3594092 1.1498840 0.7538945
Standard basis: 6-31G(d) (6D, 7F)

FeL_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.252415	-0.000084	0.009958
2	1	0	3.347252	-0.000543	0.030460
3	6	0	-2.252334	0.000086	0.011125
4	1	0	-3.347266	0.000322	0.026920
5	8	0	1.601667	1.100640	0.009132
6	8	0	1.601170	-1.100723	-0.007752
7	8	0	-1.601236	1.100746	-0.007903

8	8	0	-1.601521	-1.100697	0.008979
9	26	0	-0.000043	0.000018	-0.007828

Rotational constants (GHZ): 6.5187945 1.6385701 1.3095140
Standard basis: 6-31G(d) (6D, 7F)

$FeL_2{\cdot}OH_2$, HB2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.292400	-0.260440	0.219738
2	1	0	-3.385370	-0.325789	0.288014
3	6	0	2.292704	-0.259981	0.219370
4	1	0	3.385697	-0.325053	0.287569
5	8	0	-1.660753	0.638047	0.873417
6	8	0	-1.645331	-1.069575	-0.516892
7	8	0	1.645589	-1.069911	-0.516080
8	8	0	1.661105	0.638920	0.872054
9	8	0	-0.000950	1.344609	-1.187292
10	1	0	-0.776749	1.899523	-0.981852
11	1	0	0.774181	1.900251	-0.981558
12	26	0	0.000121	-0.149351	0.098135

Rotational constants (GHZ): 3.4129422 1.3159061 1.2187829
Standard basis: 6-31G(d) (6D, 7F)

$FeL_2{\cdot}OH_2$, HB2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.270056	0.026246	0.364729
2	1	0	-3.362028	0.036349	0.474178
3	6	0	2.304330	0.019844	0.262409
4	1	0	3.401250	0.023564	0.263621
5	8	0	-1.630485	1.119486	0.223107
6	8	0	-1.636588	-1.079438	0.365710
7	8	0	1.665789	-1.080928	0.329710
8	8	0	1.659442	1.116581	0.188673
9	8	0	-0.037530	-0.115931	-1.770740
10	1	0	-0.511465	-0.919230	-2.053047
11	1	0	-0.527074	0.635652	-2.151658
12	26	0	0.024179	0.010345	0.192784

Rotational constants (GHZ): 3.4193744 1.2893535 1.2576702
Standard basis: 6-31G(d) (6D, 7F)

$FeL_2{\cdot}OCO$, short

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.284014	-0.676704	0.185121
2	1	0	-3.378724	-0.710658	0.231176
3	6	0	2.283141	-0.679430	0.185207

4	1	0	3.377807	-0.714713	0.231310
5	8	0	-1.625892	0.036990	1.016816
6	8	0	-1.652696	-1.339697	-0.697952
7	8	0	1.651064	-1.341666	-0.697891
8	8	0	1.625843	0.035063	1.016868
9	6	0	0.001361	2.091737	-0.446370
10	8	0	0.000625	1.066352	-1.053004
11	8	0	0.002076	3.124972	0.095274
12	26	0	-0.000391	-0.601706	0.098188

Rotational constants (GHZ): 1.3054317 1.2944767 0.7936884
Standard basis: 6-31G(d) (6D, 7F)

FeL_2·OCO, long

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.758486	-2.223071	-0.134336
2	1	0	-0.753837	-3.317369	-0.136044
3	6	0	-0.754802	2.224035	-0.134265
4	1	0	-0.748347	3.318325	-0.135952
5	8	0	0.089839	-1.559687	-0.823577
6	8	0	-1.610922	-1.569348	0.555321
7	8	0	-1.608319	1.571707	0.555371
8	8	0	0.092434	1.559268	-0.823519
9	6	0	2.480128	-0.001574	0.414196
10	8	0	1.630813	-0.001496	1.235937
11	8	0	3.332667	-0.001662	-0.394404
12	26	0	-0.758114	0.000479	-0.117023

Rotational constants (GHZ): 1.4064474 1.0400008 0.7002472
Standard basis: 6-31G(d) (6D, 7F)