

Significance of the Alkene Size and Nature of Metal ion in Metal-Alkene Complexes

A Theoretical Study

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Figure S2. The MP2/6-31G* structure and geometries (Å) of the various metal ion complexes of cycloalkenes. Along with structure name, point group and complexation energy (in kcal/mol) are also given.

Figure S3. The MP2/6-31G* structure and geometries (Å) of various metal ion complexes of methylsubstituted analogues of cycloalkenes. Along with structure name, point group and complexation energy (in kcal/mol) are also given.

Figure S4. The correlation plots of charge transfer (in amu) and the complexation energy (in kcal/mol) of the various metal ion-alkene complexes.

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Figure S6. Effective Ionic radius of metal ion verses $M-C_{\beta}$ distance of metal ion dimethyl substituted alkenes (8'-11').

Table S1. The MP2/6-31G* optimized coordinates of **Li⁺-A** (in Å)

Li⁺-1			
6	0.000000	0.675133	-0.354500
1	-0.927503	1.242482	-0.402583
1	0.927503	1.242482	-0.402583
6	0.000000	-0.675133	-0.354500
1	0.927503	-1.242482	-0.402583
1	-0.927503	-1.242482	-0.402583
3	0.000000	0.000000	1.954777
Zero-point correction = 0.053840			
Thermal correction to Energy = 0.058341			
Thermal correction to Enthalpy = 0.059286			
Thermal correction to Gibbs free Energy = 0.029258			
Total energy = -85.559286			
Nuclear repulsion energy = 43.245124			
Li⁺-2			
6	-0.061099	-0.198026	0.464053
1	-0.034295	-0.212416	1.556118
6	1.058020	-0.555450	-0.209596
1	1.056068	-0.653974	-1.295573
1	1.947960	-0.896939	0.317886
6	-1.380829	0.119544	-0.170200
1	-2.098455	-0.662267	0.100460
1	-1.798825	1.060649	0.201053
1	-1.312961	0.154158	-1.260394
3	1.514651	1.671460	-0.041699
Zero-point correction = 0.083027			
Thermal correction to Energy = 0.088737			
Thermal correction to Enthalpy = 0.089681			
Thermal correction to Gibbs free energy = 0.055232			
Total energy = -124.734240			
Nuclear repulsion energy = 84.274815			
Li⁺-3			
6	-0.150233	0.017420	0.000000
6	-0.242303	-1.338173	0.000000
1	-0.377630	-1.892273	0.929739
1	-0.377630	-1.892273	-0.929739
6	-0.150233	0.811488	1.277312
1	0.676362	1.529337	1.304095
1	-1.072297	1.400822	1.327344
1	-0.109031	0.174857	2.164608
6	-0.150233	0.811488	-1.277312
1	-1.072297	1.400822	-1.327344
1	0.676362	1.529337	-1.304095
1	-0.109031	0.174857	-2.164608
3	1.974399	-1.412943	0.000000
Zero-point correction = 0.111812			
Thermal correction to Energy = 0.118830			
Li⁺-3'			
6	0.178597	0.581742	0.679956
1	0.303981	1.550005	1.172994
6	0.178597	0.581742	-0.679956
1	0.303981	1.550005	-1.172994
6	0.178597	-0.615869	-1.589394
1	-0.481304	-0.471385	-2.450517
1	1.187454	-0.749583	-1.994876
1	-0.097007	-1.541612	-1.081495
6	0.178597	-0.615869	1.589394
1	1.187454	-0.749583	1.994876
1	-0.481304	-0.471385	2.450517
1	-0.097007	-1.541612	1.081495
3	-2.037528	0.944892	0.000000
Zero-point correction = 0.112017			
Thermal correction to Energy = 0.119289			
Thermal correction to Enthalpy = 0.120233			
Thermal correction to Gibbs free Energy = 0.081424			
Total energy = -163.905444			
Nuclear repulsion energy = 134.987262			
Li⁺-3''			
6	0.000000	0.678159	-0.135442
1	0.964655	1.193750	-0.181381
6	0.000000	-0.678159	-0.135442
1	-0.964655	-1.193750	-0.181381
6	-1.230407	1.539174	-0.225164
1	-1.237362	2.053022	-1.191897
1	-1.251118	2.326267	0.536778
1	-2.146553	0.946147	-0.155364
6	1.230407	-1.539174	-0.225164
1	1.251118	-2.326267	0.536778
1	2.146553	-0.946147	-0.155364
1	1.237362	-2.053022	-1.191897
3	0.000000	0.000000	2.103666
Zero-point correction = 0.111810			
Thermal correction to Energy = 0.119091			
Thermal correction to Enthalpy = 0.120035			
Thermal correction to Gibbs free Energy = 0.081711			
Total energy = -163.906925			
Nuclear repulsion energy = 133.477114			
Li⁺-4			
6	0.417144	0.090305	-0.095732

6	-0.748621	-0.601966	-0.205915
1	-0.678768	-1.644218	-0.546292
6	1.742555	-0.601096	-0.352558
1	2.257444	-0.127826	-1.195652
1	2.446204	-0.498747	0.490640
1	1.627933	-1.661508	-0.618519
6	-2.146506	-0.066333	-0.085744
1	-2.813086	-0.806616	0.363866
1	-2.198436	0.849570	0.504379
1	-2.540604	0.155040	-1.083368
6	0.512776	1.563939	0.192786
1	0.752656	2.094075	-0.735816
1	-0.414679	1.981782	0.584604
1	1.321079	1.780832	0.898506
3	0.525390	-1.477159	1.540209

Zero-point correction = 0.140426

Thermal correction to Energy = 0.149060

Thermal correction to Enthalpy = 0.150004

Thermal correction to Gibbs free Energy = 0.108180

Total energy = -203.079299

Nuclear repulsion energy = 196.441018

Li⁺-5

6	0.676698	0.083850	-0.050616
6	-0.688880	0.073341	-0.034944
6	-1.530831	1.322818	0.010454
1	-0.948863	2.234190	0.134177
1	-2.087652	1.408788	-0.929597
1	-2.273612	1.270524	0.813179
6	1.515856	-1.166567	-0.261399
1	0.950516	-2.095835	-0.391870
1	2.098143	-1.051198	-1.182588
1	2.273369	-1.299442	0.527884
6	1.507235	1.343839	0.021747
1	1.685277	1.731337	-0.987555
1	1.038338	2.135394	0.606563
1	2.485893	1.135118	0.463120
6	-1.528467	-1.184895	-0.210025
1	-1.766685	-1.327088	-1.270554
1	-1.066592	-2.137467	0.095148
1	-2.481252	-1.089382	0.319166
3	0.127816	-1.249751	1.650541

Zero-point correction = 0.169018

Thermal correction to Energy = 0.179255

Thermal correction to Enthalpy = 0.180200

Thermal correction to Gibbs free Energy = 0.134297

Total energy = -242.248469

Nuclear repulsion energy = 268.115482

Li⁺-6

6	-1.099771	-0.126647	-0.000507
6	-0.201426	0.803561	0.000196
6	0.305776	-0.665787	0.000322

1	0.658995	-1.141089	-0.923357
1	0.657968	-1.141230	0.924273
1	-2.126997	-0.453560	-0.000148
1	0.039687	1.858781	0.000814
3	2.247623	0.270110	-0.000549

Zero-point correction = 0.057992

Thermal correction to Energy = 0.063067

Thermal correction to Enthalpy = 0.064011

Thermal correction to Gibbs free Energy = 0.031096

Total energy = -123.477161

Nuclear repulsion energy = 76.704787

Li⁺-7

6	0.182186	0.806090	0.680167
6	0.182186	0.806090	-0.680167
6	0.182186	-0.713786	-0.785137
6	0.182186	-0.713786	0.785137
1	1.087915	-1.135518	-1.229565
1	-0.662002	-1.209567	-1.296309
1	1.087915	-1.135518	1.229565
1	-0.662002	-1.209567	1.296309
1	0.287574	1.592615	1.423935
1	0.287574	1.592615	-1.423935
3	-1.933142	0.132433	0.000000

Zero-point correction = 0.089378

Thermal correction to Energy = 0.094809

Thermal correction to Enthalpy = 0.095753

Thermal correction to Gibbs free Energy = 0.061563

Total energy = -162.687769

Nuclear repulsion energy = 131.963481

Li⁺-8

6	-0.217391	-1.228773	0.000000
6	0.245472	-0.406356	1.219698
6	0.245472	1.009253	0.678512
6	0.245472	1.009253	-0.678512
6	0.245472	-0.406356	-1.219698
1	-1.321433	-1.333338	0.000000
1	1.272832	-0.672704	1.501180
1	-0.366250	-0.554206	2.116308
1	0.378881	1.895778	1.296365
1	0.378881	1.895778	-1.296365
1	1.272832	-0.672704	-1.501180
1	-0.366250	-0.554206	-2.116308
1	0.158365	-2.254115	0.000000
3	-1.998277	0.795860	0.000000

Zero-point correction = 0.120605

Thermal correction to Energy = 0.126810

Thermal correction to Enthalpy = 0.127755

Thermal correction to Gibbs free Energy = 0.091050

Total energy = -201.901657

Nuclear repulsion energy = 193.515023

Li⁺-9			
6	0.577295	-1.074565	0.778915
6	0.577295	-1.074565	-0.778915
6	-0.479509	-0.125921	-1.388508
6	-0.479509	1.204012	-0.678202
6	-0.479509	1.204012	0.678202
6	-0.479509	-0.125921	1.388508
1	0.417369	-2.089273	1.151810
1	1.573432	-0.818827	-1.191329
1	-0.311159	-0.011954	-2.462326
1	-0.564845	2.132780	-1.242062
1	-0.564845	2.132780	1.242062
1	-1.471768	-0.581727	1.273598
1	1.573432	-0.818827	1.191329
1	0.417369	-2.089273	-1.151810
1	-1.471768	-0.581727	-1.273598
1	-0.311159	-0.011954	2.462326
3	1.764867	0.898562	0.000000
Zero-point correction = 0.150924			
Thermal correction to Energy = 0.157933			
Thermal correction to Enthalpy = 0.158877			
Thermal correction to Gibbs free Energy = 0.120539			
Total energy = -241.070954			
Nuclear repulsion energy = 263.951793			

Li⁺-10			
6	-0.124703	-1.527910	0.678338
6	-0.124703	-1.527910	-0.678338
6	0.422439	-0.429713	-1.562522
6	0.422439	-0.429713	1.562522
6	-0.124703	0.984652	-1.306728
6	-0.124703	0.984652	1.306728
6	0.323284	1.646258	0.000000
1	-0.477996	-2.431875	1.177071
1	-0.477996	-2.431875	-1.177071
1	1.514544	-0.397215	-1.444358
1	0.237746	-0.697099	2.606898
1	0.196592	1.623297	-2.136577
1	-1.232810	1.009660	1.409409
1	1.419207	1.683775	0.000000
1	-0.018128	2.687457	0.000000
1	0.196592	1.623297	2.136577
1	1.514544	-0.397215	1.444358
1	-1.232810	1.009660	-1.409409
1	0.237746	-0.697099	-2.606898
3	-1.964447	-0.262221	0.000000
Zero-point correction = 0.180620			
Thermal correction to Energy = 0.188689			
Thermal correction to Enthalpy = 0.189633			
Thermal correction to Gibbs free Energy = 0.148672			
Total energy = -280.241862			
Nuclear repulsion energy = 337.963582			

Li⁺-11			
6	1.268456	-1.303744	0.303603
6	-0.005565	-1.763672	0.240736
6	-0.103105	1.718805	-0.316193
6	-1.045095	-1.209832	-0.689117
6	-1.290427	1.128633	0.477377
6	-1.965782	-0.143348	-0.075430
1	-0.556159	-0.792769	-1.575133
1	-0.303717	1.583756	-1.385354
1	-2.067198	1.900590	0.507949
1	-0.111556	2.801018	-0.147988
1	-1.672875	-2.034953	-1.041213
1	-1.070855	1.048008	1.565604
1	-2.659233	0.170646	-0.862701
1	-2.588131	-0.590543	0.709410
6	1.798045	-0.137858	-0.503084
1	1.513847	-0.250895	-1.555462
1	2.891108	-0.168714	-0.474257
6	1.347363	1.266030	-0.035019
1	1.610066	1.434883	1.033432
1	1.997923	1.989303	-0.538680
1	1.974417	-1.822675	0.958583
1	-0.280816	-2.622573	0.856365
3	0.433282	0.008282	1.844072
Zero-point correction = 0.210673			
Thermal correction to Energy = 0.219659			
Thermal correction to Enthalpy = 0.220603			
Thermal correction to Gibbs free Energy = 0.177586			
Total energy = -319.403949			
Nuclear repulsion energy = 421.308498			

Li⁺-6'			
6	-0.000998	-0.012462	0.660851
6	-0.000998	-0.012462	-0.660851
6	0.564656	1.236123	0.000000
1	1.641769	1.411182	0.000000
1	0.034219	2.207756	0.000000
6	-0.000998	-0.769006	1.936964
1	-0.484214	-0.211633	2.743920
1	-0.489973	-1.738275	1.817964
1	1.039046	-0.937387	2.238600
6	-0.000998	-0.769006	-1.936964
1	-0.489973	-1.738275	-1.817964
1	-0.484214	-0.211633	-2.743920
1	1.039046	-0.937387	-2.238600
3	-1.723231	1.372175	0.000000
Zero-point correction = 0.116806			
Thermal correction to Energy = 0.124775			
Thermal correction to Enthalpy = 0.125719			
Thermal correction to Gibbs free Energy = 0.084793			
Total energy = -201.837579			
Nuclear repulsion energy = 181.552174			

Li⁺-7'			
6	0.024403	-0.172682	0.685210
6	0.024403	-0.172682	-0.685210
6	0.273146	1.332004	-0.783362
6	0.273146	1.332004	0.783362
1	-0.477445	1.962568	-1.299143
1	1.235027	1.606833	-1.226567
1	-0.477445	1.962568	1.299143
1	1.235027	1.606833	1.226567
6	0.024403	-1.232826	1.733083
1	-0.646643	-0.987178	2.562338
1	-0.267706	-2.200767	1.317917
1	1.030753	-1.333892	2.154148
6	0.024403	-1.232826	-1.733083
1	1.030753	-1.333892	-2.154148
1	-0.267706	-2.200767	-1.317917
1	-0.646643	-0.987178	-2.562338
3	-1.870467	0.928974	0.000000
Zero-point correction = 0.146796			
Thermal correction to Energy = 0.155265			
Thermal correction to Enthalpy = 0.156209			
Thermal correction to Gibbs free Energy = 0.114851			
Total energy = -241.044460			
Nuclear repulsion energy = 255.341910			
Li⁺-8'			
6	0.006696	1.919774	0.000000
6	-0.290307	1.018298	1.212139
6	-0.032799	-0.385550	0.683122
6	-0.032799	-0.385550	-0.683122
6	-0.290307	1.018298	-1.212139
1	1.065925	2.251768	0.000000
1	-1.348281	1.095811	1.498458
1	0.285726	1.271121	2.111323
1	-1.348281	1.095811	-1.498458
1	0.285726	1.271121	-2.111323
1	-0.564074	2.851169	0.000000
6	-0.032799	-1.566880	-1.606945
1	0.269018	-2.490426	-1.108420
1	-1.044677	-1.716557	-2.000900
1	0.618755	-1.403944	-2.471686
6	-0.032799	-1.566880	1.606945
1	-1.044677	-1.716557	2.000900
1	0.269018	-2.490426	1.108420
1	0.618755	-1.403944	2.471686
3	2.055917	0.358663	0.000000
Zero-point correction = 0.177790			
Thermal correction to Energy = 0.187170			
Thermal correction to Enthalpy = 0.188115			
Thermal correction to Gibbs free Energy = 0.144169			
Total energy = -280.2518144			
Nuclear repulsion energy = 334.750998			

Li⁺-9'			
6	0.786117	1.699250	0.777454
6	0.786117	1.699250	-0.777454
6	0.786117	0.272665	-1.361458
6	-0.235974	-0.622263	-0.683373
6	-0.235974	-0.622263	0.683373
6	0.786117	0.272665	1.361458
1	1.649341	2.254300	1.153987
1	-0.068726	2.267540	-1.196286
1	0.610933	0.313399	-2.441007
1	1.784490	-0.164567	1.225010
1	-0.068726	2.267540	1.196286
1	1.649341	2.254300	-1.153987
1	1.784490	-0.164567	-1.225010
1	0.610933	0.313399	2.441007
6	-1.030819	-1.545291	-1.569112
1	-0.357689	-2.295028	-2.001130
1	-1.822833	-2.077739	-1.041027
1	-1.474498	-1.004308	-2.412177
6	-1.030819	-1.545291	1.569112
1	-1.474498	-1.004308	2.412177
1	-1.822833	-2.077739	1.041027
1	-0.357689	-2.295028	2.001130
3	-1.435774	1.253492	0.000000
Zero-point correction = 0.208046			
Thermal correction to Energy = 0.218215			
Thermal correction to Enthalpy = 0.219159			
Thermal correction to Gibbs free Energy = 0.173705			
Total energy = -319.417506			
Nuclear repulsion energy = 420.381917			
Li⁺-10'			
6	-0.387020	-0.855691	0.682982
6	-0.387020	-0.855691	-0.682982
6	0.684704	-0.105075	-1.465615
6	0.684704	-0.105075	1.465615
6	0.684704	1.428000	-1.313925
6	0.684704	1.428000	1.313925
6	1.285425	1.947344	0.000000
1	1.677874	-0.474063	-1.175872
1	0.566958	-0.348087	2.526026
1	1.270088	1.857937	-2.134004
1	-0.326301	1.848918	1.515370
1	2.343185	1.660301	0.000000
1	1.267139	3.043385	0.000000
1	1.270088	1.857937	2.134004
1	1.677874	-0.474063	1.175872
1	-0.326301	1.848918	-1.515370
1	0.566958	-0.348087	-2.526026
6	-1.336432	-1.654143	1.545064
1	-0.781150	-2.468592	2.024856
1	-1.743400	-1.039916	2.356895
1	-2.167521	-2.098075	0.997817

6 -1.336432 -1.654143 -1.545064
 1 -0.781150 -2.468592 -2.024856
 1 -2.167521 -2.098075 -0.997817
 1 -1.743400 -1.039916 -2.356895
 3 -1.355811 1.099639 0.000000

Zero-point correction = 0.237934

Thermal correction to Energy = 0.249008

Thermal correction to Enthalpy = 0.249952

Thermal correction to Gibbs free Energy = 0.202425

Total energy = -358.584691

Nuclear repulsion energy = 509.748514

Li⁺-11'

6 -1.172002 -0.616903 -0.256236
 6 -1.022001 0.738677 -0.277802
 6 2.198094 -0.701528 0.069244
 6 0.151018 1.378758 -0.979329
 6 1.906326 0.626369 0.798284
 6 1.304053 1.763983 -0.040902
 1 0.534426 0.729041 -1.769655
 1 2.513618 -0.466922 -0.954429
 1 2.856671 0.997272 1.198740
 1 3.069353 -1.159777 0.550016
 1 -0.199643 2.290113 -1.478272
 1 1.336793 0.475451 1.742121
 1 2.108107 2.179728 -0.658664
 1 0.992918 2.574158 0.629595
 6 -0.137330 -1.558666 -0.858696
 1 0.183789 -1.212989 -1.846160
 1 -0.621243 -2.527502 -1.023163
 6 1.122955 -1.804352 0.000982
 1 0.849338 -2.140913 1.027261
 1 1.615852 -2.698587 -0.397260
 6 -2.330766 -1.334939 0.410644
 1 -2.806931 -1.999011 -0.318307
 1 -2.006751 -2.010152 1.225172
 1 -3.099401 -0.670448 0.805386
 6 -2.004163 1.726017 0.307411
 1 -2.607235 2.157825 -0.499690
 1 -2.693332 1.301971 1.039871
 1 -1.473439 2.558688 0.780452
 3 -0.216663 -0.560810 1.635131

Zero-point correction = 0.267576

Thermal correction to Energy = 0.279748

Thermal correction to Enthalpy = 0.280692

Thermal correction to Gibbs free Energy = 0.230527

Total energy = -397.748127

Nuclear repulsion energy = 609.021502

Table S2. The MP2/6-31G* optimized coordinates of Na⁺-A (in Å)

Na⁺-1

6 0.000000 0.673857 -1.080875
 1 -0.926392 1.241583 -1.129396
 1 0.926392 1.241583 -1.129396
 6 0.000000 -0.673857 -1.080875
 1 0.926392 -1.241583 -1.129396
 1 -0.926392 -1.241583 -1.129396
 11 0.000000 0.000000 1.589826

Zero-point correction = 0.053353

Thermal correction to Energy = 0.058135

Thermal correction to Enthalpy = 0.059079

Thermal correction to Gibbs free Energy = 0.026970

Total energy = -239.971085

Nuclear repulsion energy = 65.919127

Na⁺-2

6 0.757495 0.300982 0.464402
 1 0.742099 0.326381 1.556150
 6 0.061345 1.242173 -0.209986
 1 0.122975 1.321723 -1.294769
 1 -0.471576 2.033992 0.313053
 6 1.656067 -0.719169 -0.168925
 1 2.694268 -0.499062 0.099631
 1 1.451812 -1.731159 0.195236
 1 1.579567 -0.705354 -1.259285
 11 -1.906235 -0.517312 -0.011178

Zero-point correction = 0.082528

Thermal correction to Energy = 0.088555

Thermal correction to Enthalpy = 0.089499

Thermal correction to Gibbs free Energy = 0.052927

Total energy = -279.144473

Nuclear repulsion energy = 115.900165

Na⁺-3

6 -0.195830 0.644029 0.000000
 6 -1.261188 -0.193251 0.000000
 1 -1.758434 -0.472938 0.928295
 1 -1.758434 -0.472938 -0.928295
 6 0.390945 1.183318 1.276989
 1 1.477862 1.050757 1.308489
 1 0.210515 2.262344 1.328460
 1 -0.054760 0.725556 2.163903
 6 0.390945 1.183318 -1.276989
 1 0.210515 2.262344 -1.328460
 1 1.477862 1.050757 -1.308489
 1 -0.054760 0.725556 -2.163903
 11 0.390945 -2.185084 0.000000

Zero-point correction = 0.111305

Thermal correction to Energy = 0.118662

Thermal correction to Enthalpy = 0.119606
 Thermal correction to Gibbs free Energy = 0.079530

Total energy = -318.318556

Nuclear repulsion energy = 177.119605

Na⁺-3'

6	-0.646704	-0.365738	0.678407
1	-0.778046	-1.331115	1.174164
6	-0.646704	-0.365738	-0.678407
1	-0.778046	-1.331115	-1.174164
6	-0.646704	0.833966	-1.584964
1	-0.003588	0.682084	-2.457354
1	-1.659164	0.991562	-1.971834
1	-0.342517	1.751887	-1.078817
6	-0.646704	0.833966	1.584964
1	-1.659164	0.991562	1.971834
1	-0.003588	0.682084	2.457354
1	-0.342517	1.751887	1.078817
11	1.917048	-0.891597	0.000000

Zero-point correction = 0.111540

Thermal correction to Energy = 0.119128

Thermal correction to Enthalpy = 0.120072

Thermal correction to Gibbs free Energy = 0.079236

Total energy = -318.314575

Nuclear repulsion energy = 176.019037

Na⁺-3''

6	0.000000	0.676499	-0.621006
1	0.962775	1.194056	-0.667859
6	0.000000	-0.676499	-0.621006
1	-0.962775	-1.194056	-0.667859
6	-1.231363	1.535320	-0.713618
1	-1.250647	2.041878	-1.683819
1	-1.250797	2.327290	0.043331
1	-2.145133	0.939822	-0.631378
6	1.231363	-1.535320	-0.713618
1	1.250797	-2.327290	0.043331
1	2.145133	-0.939822	-0.631378
1	1.250647	-2.041878	-1.683819
11	0.000000	0.000000	1.990448

Zero-point correction = 0.111376

Thermal correction to Energy = 0.118929

Thermal correction to Enthalpy = 0.119873

Thermal correction to Gibbs free Energy = 0.079761

Total energy = -318.316130

Nuclear repulsion energy = 175.327807

Na⁺-4

6	-0.511167	-0.454028	-0.137588
6	0.705822	-0.214803	-0.694316
1	0.713393	0.298308	-1.661924
6	-1.777265	-0.007372	-0.831994
1	-2.351310	-0.885346	-1.147762

1	-2.439722	0.556668	-0.163006
1	-1.572938	0.588960	-1.727107
6	2.041533	-0.739515	-0.238461
1	2.838792	-0.009226	-0.407427
1	2.052971	-1.027387	0.814421
1	2.304909	-1.627335	-0.823479
6	-0.728493	-1.292607	1.095836
1	-1.116118	-2.273300	0.797650
1	0.181437	-1.460736	1.673623
1	-1.484874	-0.846756	1.750556
11	0.226444	2.085100	0.521236

Zero-point correction = 0.140053

Thermal correction to Energy = 0.149132

Thermal correction to Enthalpy = 0.150076

Thermal correction to Gibbs free Energy = 0.105401

Total energy = -357.487090

Nuclear repulsion energy = 246.748226

Na⁺-5

6	0.399454	0.105044	0.682979
6	0.399454	0.105044	-0.682979
6	0.593504	1.353994	-1.513211
1	0.334906	2.276873	-0.994502
1	1.644948	1.429707	-1.813738
1	0.007647	1.303856	-2.436608
6	0.399454	-1.151459	1.532132
1	0.197207	-2.077067	0.989065
1	1.385443	-1.272043	1.995669
1	-0.307815	-1.067830	2.367374
6	0.593504	1.353994	1.513211
1	1.644948	1.429707	1.813738
1	0.334906	2.276873	0.994502
1	0.007647	1.303856	2.436608
6	0.399454	-1.151459	-1.532132
1	1.385443	-1.272043	-1.995669
1	0.197207	-2.077067	-0.989065
1	-0.307815	-1.067830	-2.367374
11	-2.112147	-0.443449	0.000000

Zero-point correction = 0.168367

Thermal correction to Energy = 0.179296

Thermal correction to Enthalpy = 0.180240

Thermal correction to Gibbs free Energy = 0.130227

Total energy = -396.654307

Nuclear repulsion energy = 329.140848

Na⁺-6

6	0.847876	-0.089907	0.658342
6	0.847876	-0.089907	-0.658342
6	0.847876	1.271400	0.000000
1	1.772935	1.844101	0.000000
1	-0.048566	1.889290	0.000000
1	1.038641	-0.634462	1.575063
1	1.038641	-0.634462	-1.575063

11 -1.733038 -0.819453 0.000000
Zero-point correction = 0.058035
Thermal correction to Energy = 0.063445
Thermal correction to Enthalpy = 0.064389
Thermal correction to Gibbs free Energy = 0.028859
Total energy = -277.886961
Nuclear repulsion energy = 106.046978

Na⁺-7

6 -0.676057 -0.420305 0.680239
6 -0.676057 -0.420305 -0.680239
6 -0.676057 1.095156 -0.782172
6 -0.676057 1.095156 0.782172
1 -1.588215 1.503106 -1.226598
1 0.181110 1.574158 -1.267748
1 -1.588215 1.503106 1.226598
1 0.181110 1.574158 1.267748
1 -0.807183 -1.207610 1.423645
1 -0.807183 -1.207610 -1.423645
11 1.877630 -1.076138 0.000000

Zero-point correction = 0.089042
Thermal correction to Energy = 0.094963
Thermal correction to Enthalpy = 0.095907
Thermal correction to Gibbs free Energy = 0.058766
Total energy = -317.097773
Nuclear repulsion energy = 168.605223

Na⁺-8

6 -0.198764 1.446348 0.000000
6 -0.653485 0.620469 1.218779
6 -0.653485 -0.792512 0.677515
6 -0.653485 -0.792512 -0.677515
6 -0.653485 0.620469 -1.218779
1 0.900651 1.543075 0.000000
1 -1.678998 0.884229 1.509425
1 -0.033523 0.768534 2.109403
1 -0.798376 -1.677162 1.296514
1 -0.798376 -1.677162 -1.296514
1 -1.678998 0.884229 -1.509425
1 -0.033523 0.768534 -2.109403
1 -0.590682 2.465632 0.000000
11 1.962550 -0.961225 0.000000

Zero-point correction = 0.120210
Thermal correction to Energy = 0.126771
Thermal correction to Enthalpy = 0.127715
Thermal correction to Gibbs free Energy = 0.088862
Total energy = -356.310464
Nuclear repulsion energy = 242.381115

Na⁺-9

6 0.245795 -1.293015 0.776022
6 0.245795 -1.293015 -0.776022
6 -0.795372 -0.334437 -1.388241

6 -0.795372 0.991620 -0.677466
6 -0.795372 0.991620 0.677466
6 -0.795372 -0.334437 1.388241
1 0.072461 -2.303787 1.155152
1 1.241423 -1.027894 -1.170179
1 -0.620948 -0.219507 -2.461562
1 -0.903760 1.919125 -1.241083
1 -0.903760 1.919125 1.241083
1 -1.793872 -0.780567 1.284411
1 1.241423 -1.027894 1.170179
1 0.072461 -2.303787 -1.155152
1 -1.793872 -0.780567 -1.284411
1 -0.620948 -0.219507 2.461562
11 1.831707 1.132294 0.000000

Zero-point correction = 0.150161
Thermal correction to Energy = 0.157787
Thermal correction to Enthalpy = 0.158732
Thermal correction to Gibbs free Energy = 0.117662

Total energy = -395.477379
Nuclear repulsion energy = 323.550723

Na⁺-10

6 0.812675 -1.197423 0.677784
6 0.812675 -1.197423 -0.677784
6 0.812675 0.015166 -1.575349
6 0.812675 0.015166 1.575349
6 -0.261273 1.073745 -1.296780
6 -0.261273 1.073745 1.296780
6 -0.093957 1.863768 0.000000
1 0.933792 -2.164895 1.170756
1 0.933792 -2.164895 -1.170756
1 1.798206 0.497365 -1.503609
1 0.720491 -0.318788 2.613755
1 -0.261249 1.780170 -2.134220
1 -1.268453 0.614062 1.329116
1 0.900390 2.327809 0.000000
1 -0.814564 2.689537 0.000000
1 -0.261249 1.780170 2.134220
1 1.798206 0.497365 1.503609
1 -1.268453 0.614062 -1.329116
1 0.720491 -0.318788 -2.613755
11 -1.794234 -1.428513 0.000000

Zero-point correction = 0.179894
Thermal correction to Energy = 0.188498
Thermal correction to Enthalpy = 0.189443
Thermal correction to Gibbs free Energy = 0.146125

Total energy = -434.647533
Nuclear repulsion energy = 404.341471

Na⁺-11

6 1.413550 0.510674 -0.780345
6 1.095374 -0.791020 -0.977968
6 -1.698853 0.860602 0.408131

6	-0.281894	-1.266946	-1.332979
6	-1.364094	-0.547977	0.926948
6	-1.155558	-1.643342	-0.127093
1	-0.790473	-0.489174	-1.911559
1	-2.228994	0.786758	-0.549450
1	-2.170940	-0.891218	1.584148
1	-2.412312	1.314206	1.104429
1	-0.201315	-2.139243	-1.989779
1	-0.498603	-0.466674	1.609515
1	-2.140598	-1.928029	-0.513405
1	-0.756394	-2.545279	0.357450
6	0.449200	1.664929	-0.895352
1	-0.126781	1.566560	-1.823748
1	1.033119	2.584766	-0.999239
6	-0.532733	1.851961	0.276060
1	0.025835	1.876446	1.227619
1	-0.962612	2.854785	0.173922
1	2.467572	0.764639	-0.620535
1	1.896369	-1.537240	-0.955035
11	1.756015	-0.507690	1.665569

Zero-point correction = 0.209569

Thermal correction to Energy = 0.219204

Thermal correction to Enthalpy = 0.220149

Thermal correction to Gibbs free Energy = 0.174186

Total energy = -473.807329

Nuclear repulsion energy = 493.693388

Na⁺-6'

6	0.400588	-0.223642	0.660012
6	0.400588	-0.223642	-0.660012
6	0.957133	1.024836	0.000000
1	2.035844	1.193688	0.000000
1	0.408133	1.977009	0.000000
6	0.400588	-0.978496	1.938151
1	-0.097290	-0.427930	2.741640
1	-0.070641	-1.957344	1.821663
1	1.439235	-1.130376	2.252570
6	0.400588	-0.978496	-1.938151
1	-0.070641	-1.957344	-1.821663
1	-0.097290	-0.427930	-2.741640
1	1.439235	-1.130376	-2.252570
11	-1.849408	1.103386	0.000000

Zero-point correction = 0.116277

Thermal correction to Energy = 0.124694

Thermal correction to Enthalpy = 0.125639

Thermal correction to Gibbs free Energy = 0.082724

Total energy = -356.245036

Nuclear repulsion energy = 230.015474

Na⁺-7'

6	0.392633	-0.222793	0.684006
6	0.392633	-0.222793	-0.684006
6	0.665871	1.274736	-0.780953

6	0.665871	1.274736	0.780953
1	-0.082624	1.911076	-1.277870
1	1.635493	1.522898	-1.224358
1	-0.082624	1.911076	1.277870
1	1.635493	1.522898	1.224358
6	0.392633	-1.287873	1.731286
1	-0.288204	-1.055561	2.557675
1	0.123228	-2.262530	1.314359
1	1.394325	-1.375310	2.166479
6	0.392633	-1.287873	-1.731286
1	1.394325	-1.375310	-2.166479
1	0.123228	-2.262530	-1.314359
1	-0.288204	-1.055561	-2.557675
11	-2.088917	0.486366	0.000000

Zero-point correction = 0.146107

Thermal correction to Energy = 0.155275

Thermal correction to Enthalpy = 0.156219

Thermal correction to Gibbs free Energy = 0.111314

Total energy = -395.450415

Nuclear repulsion energy = 314.122250

Na⁺-8'

6	-0.337747	1.912048	0.000000
6	-0.625257	1.008586	1.210187
6	-0.356601	-0.389546	0.681975
6	-0.356601	-0.389546	-0.681975
6	-0.625257	1.008586	-1.210187
1	0.719891	2.231667	0.000000
1	-1.682897	1.077302	1.501257
1	-0.047246	1.266816	2.106354
1	-1.682897	1.077302	-1.501257
1	-0.047246	1.266816	-2.106354
1	-0.921574	2.835531	0.000000
6	-0.356601	-1.571372	-1.607149
1	-0.073239	-2.500634	-1.106939
1	-1.362667	-1.712098	-2.018797
1	0.308036	-1.415907	-2.464364
6	-0.356601	-1.571372	1.607149
1	-1.362667	-1.712098	2.018797
1	-0.073239	-2.500634	1.106939
1	0.308036	-1.415907	2.464364
11	2.182335	0.132503	0.000000

Zero-point correction = 0.177309

Thermal correction to Energy = 0.187087

Thermal correction to Enthalpy = 0.188031

Thermal correction to Gibbs free Energy = 0.142041

Total energy = -434.6583493

Nuclear repulsion energy = 403.303743

Na⁺-9'

6	1.020947	1.568893	0.774565
6	1.020947	1.568893	-0.774565
6	1.020947	0.147429	-1.361623

6	0.012456	-0.754692	-0.682184
6	0.012456	-0.754692	0.682184
6	1.020947	0.147429	1.361623
1	1.883424	2.122440	1.156804
1	0.153347	2.120076	-1.177007
1	0.840088	0.189883	-2.440849
1	2.021842	-0.289033	1.236378
1	0.153347	2.120076	1.177007
1	1.883424	2.122440	-1.156804
1	2.021842	-0.289033	-1.236378
1	0.840088	0.189883	2.440849
6	-0.757831	-1.701668	-1.567212
1	-0.067068	-2.434135	-2.001019
1	-1.534321	-2.259336	-1.040331
1	-1.215738	-1.176199	-2.413528
6	-0.757831	-1.701668	1.567212
1	-1.215738	-1.176199	2.413528
1	-1.534321	-2.259336	1.040331
1	-0.067068	-2.434135	2.001019
11	-1.792854	1.121187	0.000000

Zero-point correction = 0.207204
Thermal correction to Energy = 0.218032
Thermal correction to Enthalpy = 0.218976
Thermal correction to Gibbs free Energy = 0.170770
Total energy = -473.821728
Nuclear repulsion energy = 499.467575

Na⁺-10'

6	-0.695435	0.651021	0.681287
6	-0.695435	0.651021	-0.681287
6	-0.695435	-0.649442	-1.465220
6	-0.695435	-0.649442	1.465220
6	0.560407	-1.518876	-1.299487
6	0.560407	-1.518876	1.299487
6	0.617957	-2.320833	0.000000
1	-1.572299	-1.248935	-1.183996
1	-0.822187	-0.413347	2.527002
1	0.613208	-2.224654	-2.136318
1	1.468728	-0.895295	1.415098
1	-0.229193	-3.017824	0.000000
1	1.520911	-2.942853	0.000000
1	0.613208	-2.224654	2.136318
1	-1.572299	-1.248935	1.183996
1	1.468728	-0.895295	-1.415098
1	-0.822187	-0.413347	-2.527002
6	-0.806434	1.888864	1.544493
1	-1.781606	1.893054	2.045061
1	-0.059954	1.881078	2.349828
1	-0.722104	2.830197	0.998785
6	-0.806434	1.888864	-1.544493
1	-1.781606	1.893054	-2.045061
1	-0.722104	2.830197	-0.998785
1	-0.059954	1.881078	-2.349828

11	1.854157	1.071153	0.000000
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Zero-point correction = 0.236873
Thermal correction to Energy = 0.248589
Thermal correction to Enthalpy = 0.249533
Thermal correction to Gibbs free Energy = 0.199404
Total energy = -512.987800
Nuclear repulsion energy = 596.998212

Na⁺-11'

6	0.916678	0.727490	-0.568139
6	0.859697	-0.628276	-0.676511
6	-2.361581	0.587195	0.183235
6	-0.371683	-1.320104	-1.206164
6	-1.849021	-0.704552	0.840348
6	-1.336553	-1.792831	-0.109167
1	-0.910555	-0.666438	-1.895931
1	-2.778712	0.354586	-0.804754
1	-2.653964	-1.149925	1.436100
1	-3.203172	0.958465	0.778265
1	-0.062392	-2.192534	-1.794694
1	-1.087837	-0.430498	1.593968
1	-2.204913	-2.245109	-0.602229
1	-0.878074	-2.602348	0.475738
6	-0.237185	1.623238	-0.976457
1	-0.660463	1.301205	-1.933998
1	0.167548	2.625640	-1.157637
6	-1.368623	1.751557	0.058398
1	-0.935472	1.960130	1.051964
1	-1.945291	2.648655	-0.195576
6	2.132317	1.502715	-0.097987
1	2.560492	2.060039	-0.938705
1	1.858558	2.266103	0.644973
1	2.949975	0.891162	0.298911
6	1.991574	-1.579449	-0.343953
1	2.407253	-1.993861	-1.269473
1	2.839621	-1.130620	0.185318
1	1.630708	-2.443061	0.230500
11	1.150270	-0.110317	1.934149

Zero-point correction = 0.266660
Thermal correction to Energy = 0.279298
Thermal correction to Enthalpy = 0.280242
Thermal correction to Gibbs free Energy = 0.228318
Total energy = -552.149680
Nuclear repulsion energy = 704.408074

Table S3. The MP2/6-31G* optimized coordinates of $\text{K}^+\text{-A}$ (in Å)

$\text{K}^+\text{-1}$			
6	0.000000	0.671996	-1.710348
1	-0.925454	1.240372	-1.753960
1	0.925454	1.240372	-1.753960
6	0.000000	-0.671996	-1.710348
1	0.925454	-1.240372	-1.753960
1	-0.925454	-1.240372	-1.753960
19	0.000000	0.000000	1.449474
Zero-point correction = 0.053065			
Thermal correction to Energy = 0.058053			
Thermal correction to Enthalpy = 0.058997			
Thermal correction to Gibbs free Energy = 0.025280			
Total energy = -677.289959			
Nuclear repulsion energy = 81.828513			
$\text{K}^+\text{-2}$			
6	1.364951	0.262015	0.462193
1	1.389654	0.310908	1.552240
6	0.893983	1.322461	-0.220466
1	0.929951	1.356450	-1.308201
1	0.572326	2.227513	0.288561
6	1.955266	-0.965772	-0.166710
1	3.020032	-1.030337	0.077774
1	1.497645	-1.885795	0.213599
1	1.862765	-0.943557	-1.256156
19	-1.818819	-0.197232	-0.000943
Zero-point correction = 0.082247			
Thermal correction to Energy = 0.088495			
Thermal correction to Enthalpy = 0.089439			
Thermal correction to Gibbs free Energy = 0.051096			
Total energy = -716.462424			
Nuclear repulsion energy = 139.981371			
$\text{K}^+\text{-3}$			
6	1.105978	-0.378352	0.000000
6	1.133337	0.970635	0.000000
1	1.216870	1.534980	0.926919
1	1.216870	1.534980	-0.926919
6	1.133337	-1.176250	1.276729
1	0.313628	-1.903439	1.316599
1	2.060068	-1.757104	1.328977
1	1.088487	-0.536962	2.162517
6	1.133337	-1.176250	-1.276729
1	2.060068	-1.757104	-1.328977
1	0.313628	-1.903439	-1.316599
1	1.088487	-0.536962	-2.162517
19	-1.915476	0.836124	0.000000
Zero-point correction = 0.111035			
Thermal correction to Energy = 0.118625			

Thermal correction to Enthalpy = 0.119569
 Thermal correction to Gibbs free Energy = 0.077562

Total energy = -755.635763

Nuclear repulsion energy = 209.321374

$\text{K}^+\text{-3'}$			
6	-1.116177	-0.548012	0.675208
1	-1.203565	-1.514217	1.173513
6	-1.116177	-0.548012	-0.675208
1	-1.203565	-1.514217	-1.173513
6	-1.116177	0.648653	-1.586562
1	-0.402113	0.531649	-2.410287
1	-2.099612	0.755187	-2.055887
1	-0.907278	1.587373	-1.067475
6	-1.116177	0.648653	1.586562
1	-2.099612	0.755187	2.055887
1	-0.402113	0.531649	2.410287
1	-0.907278	1.587373	1.067475
19	1.895441	-0.206720	0.000000
Zero-point correction = 0.111234			
Thermal correction to Energy = 0.119026			
Thermal correction to Enthalpy = 0.119970			
Thermal correction to Gibbs free Energy = 0.077326			
Total energy = -755.632041			
Nuclear repulsion energy = 211.977435			
$\text{K}^+\text{-3''}$			
6	-1.017866	0.665542	-0.400798
1	-1.113425	0.528263	-1.481075
6	-1.182028	-0.405609	0.400331
1	-1.165660	-0.253763	1.483259
6	-0.826275	2.075300	0.084269
1	-1.692179	2.687103	-0.187089
1	0.043004	2.563900	-0.373007
1	-0.723111	2.114110	1.172980
6	-1.507948	-1.791616	-0.078673
1	-0.828431	-2.546738	0.333201
1	-1.483742	-1.853014	-1.170443
1	-2.513306	-2.074127	0.248687
19	1.930608	-0.233023	-0.003015
Zero-point correction = 0.111093			
Thermal correction to Energy = 0.118866			
Thermal correction to Enthalpy = 0.119810			
Thermal correction to Gibbs free Energy = 0.076493			
Total energy = -755.633932			
Nuclear repulsion energy = 207.799003			
$\text{K}^+\text{-4}$			
6	1.118098	-0.097433	-0.027787
6	0.553193	0.960948	-0.653289
1	0.672924	1.019620	-1.736739
6	1.875642	-1.139739	-0.810871

1	2.933445	-1.124960	-0.527182
1	1.513041	-2.152627	-0.597423
1	1.813757	-0.964665	-1.887960
6	-0.126075	2.150054	-0.027547
1	-1.046386	2.419087	-0.560943
1	-0.359776	2.014099	1.031965
1	0.522621	3.029735	-0.095004
6	1.142519	-0.297236	1.467604
1	2.167882	-0.184834	1.836363
1	0.526141	0.414837	2.021682
1	0.840147	-1.317532	1.737307
19	-1.945476	-0.663807	-0.047933

Zero-point correction = 0.139872
Thermal correction to Energy = 0.149068
Thermal correction to Enthalpy = 0.150012
Thermal correction to Gibbs free Energy = 0.104369
Total energy = -794.804505
Nuclear repulsion energy = 290.323272

K⁺-5

6	-0.794537	-0.673345	0.162994
6	-0.777297	0.686622	0.165074
6	-1.472510	1.538982	-0.870039
1	-1.847358	0.981081	-1.726756
1	-2.328237	2.044548	-0.408141
1	-0.810694	2.332063	-1.238338
6	-0.240574	-1.529728	1.281617
1	0.281902	-0.980444	2.066742
1	-1.063612	-2.063930	1.769592
1	0.423302	-2.315173	0.893781
6	-1.496486	-1.503957	-0.887405
1	-2.475752	-1.826082	-0.515417
1	-1.658461	-0.982838	-1.830860
1	-0.929486	-2.417220	-1.099250
6	-0.178412	1.527225	1.273392
1	-0.978270	1.996794	1.856904
1	0.442435	0.978244	1.984997
1	0.409291	2.358089	0.860352
19	2.120728	-0.019996	-0.493021

Zero-point correction = 0.168348
Thermal correction to Energy = 0.179293
Thermal correction to Enthalpy = 0.180237
Thermal correction to Gibbs free Energy = 0.130092
Total energy = -833.971943
Nuclear repulsion energy = 378.517396

K⁺-6

6	-0.268747	-1.450204	0.655029
6	-0.268747	-1.450204	-0.655029
6	1.087553	-1.337672	0.000000
1	1.756385	-2.196426	0.000000
1	1.637256	-0.390779	0.000000
1	-0.793900	-1.665746	1.575564

1	-0.793900	-1.665746	-1.575564
19	-0.268747	1.649852	0.000000

Zero-point correction = 0.057876
Thermal correction to Energy = 0.063348
Thermal correction to Enthalpy = 0.064292
Thermal correction to Gibbs free Energy = 0.027974
Total energy = -715.207921
Nuclear repulsion energy = 131.328090

K⁺-7

6	-1.171766	-0.603205	0.677370
6	-1.171766	-0.603205	-0.677370
6	-1.171766	0.911326	-0.782568
6	-1.171766	0.911326	0.782568
1	-2.076586	1.334781	-1.227171
1	-0.314677	1.394416	-1.272223
1	-2.076586	1.334781	1.227171
1	-0.314677	1.394416	1.272223
1	-1.276083	-1.389780	1.422402
1	-1.276083	-1.389780	-1.422402
19	1.866161	-0.335594	0.000000

Zero-point correction = 0.088850
Thermal correction to Energy = 0.094864
Thermal correction to Enthalpy = 0.095808
Thermal correction to Gibbs free Energy = 0.057765
Total energy = -754.416492
Nuclear repulsion energy = 203.885505

K⁺-8

6	-0.653960	1.594638	0.000000
6	-1.073856	0.752710	1.222235
6	-1.073856	-0.656647	0.674754
6	-1.073856	-0.656647	-0.674754
6	-1.073856	0.752710	-1.222235
1	0.437023	1.741745	0.000000
1	-2.089986	1.010839	1.546769
1	-0.428136	0.899764	2.095597
1	-1.204481	-1.541551	1.295629
1	-1.204481	-1.541551	-1.295629
1	-2.089986	1.010839	-1.546769
1	-0.428136	0.899764	-2.095597
1	-1.094231	2.594053	0.000000
19	1.989406	-0.831289	0.000000

Zero-point correction = 0.120015
Thermal correction to Energy = 0.126808
Thermal correction to Enthalpy = 0.127752
Thermal correction to Gibbs free Energy = 0.087189
Total energy = -793.627540
Nuclear repulsion energy = 280.421777

K⁺-9

6	-0.108334	-1.526625	0.774916
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6	-0.108334	-1.526625	-0.774916
6	-1.143787	-0.561283	-1.385670
6	-1.143787	0.764359	-0.675294
6	-1.143787	0.764359	0.675294
6	-1.143787	-0.561283	1.385670
1	-0.293242	-2.535268	1.154746
1	0.887696	-1.262953	-1.161107
1	-0.967562	-0.446624	-2.459180
1	-1.244907	1.690313	-1.242599
1	-1.244907	1.690313	1.242599
1	-2.143004	-1.006369	1.285680
1	0.887696	-1.262953	1.161107
1	-0.293242	-2.535268	-1.154746
1	-2.143004	-1.006369	-1.285680
1	-0.967562	-0.446624	2.459180
19	1.909102	1.210758	0.000000

Zero-point correction = 0.149943
Thermal correction to Energy = 0.157846
Thermal correction to Enthalpy = 0.158790
Thermal correction to Gibbs free Energy = 0.115758
Total energy = -832.793329
Nuclear repulsion energy = 367.480073

K⁺-10

6	-0.103108	1.458872	0.675608
6	-0.103108	1.458872	-0.675608
6	-0.980186	0.616474	-1.567610
6	-0.980186	0.616474	1.567610
6	-0.980186	-0.892689	-1.296460
6	-0.980186	-0.892689	1.296460
6	-1.661692	-1.327049	0.000000
1	0.511922	2.212041	1.173785
1	0.511922	2.212041	-1.173785
1	-2.013987	0.981126	-1.483862
1	-0.689247	0.788819	2.609160
1	-1.486401	-1.385922	-2.133784
1	0.053753	-1.279155	1.319132
1	-2.690167	-0.943824	0.000000
1	-1.745418	-2.420144	0.000000
1	-1.486401	-1.385922	2.133784
1	-2.013987	0.981126	1.483862
1	0.053753	-1.279155	-1.319132
1	-0.689247	0.788819	-2.609160
19	2.442916	-0.289445	0.000000

Zero-point correction = 0.179731
Thermal correction to Energy = 0.188590
Thermal correction to Enthalpy = 0.189534
Thermal correction to Gibbs free Energy = 0.144567
Total energy = -871.962747
Nuclear repulsion energy = 453.603020

K⁺-11

6	-0.243790	0.880553	1.365604
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6	-0.160492	-0.449742	1.582370
6	1.711602	0.365350	-1.285691
6	1.049516	-1.271766	1.251492
6	0.822870	-0.890542	-1.302981
6	1.027466	-1.885318	-0.155966
1	1.943871	-0.648584	1.352589
1	2.643994	0.155761	-0.746701
1	0.982744	-1.436275	-2.239634
1	2.011625	0.587208	-2.315637
1	1.151645	-2.078661	1.984928
1	-0.227356	-0.565237	-1.341601
1	1.982021	-2.400929	-0.311686
1	0.254541	-2.664727	-0.210255
6	0.859939	1.734615	0.792985
1	1.805770	1.492923	1.293302
1	0.646969	2.778679	1.044977
6	1.075163	1.646823	-0.728527
1	0.119318	1.825426	-1.247673
1	1.718943	2.487874	-1.010956
1	-1.134454	1.409300	1.719980
1	-0.989453	-0.958567	2.083196
19	-2.619148	-0.040212	-0.482660

Zero-point correction = 0.209512
Thermal correction to Energy = 0.219355
Thermal correction to Enthalpy = 0.220299
Thermal correction to Gibbs free Energy = 0.173083
Total energy = -911.1228095
Nuclear repulsion energy = 548.9180591003

K⁺-6'

6	-0.820837	0.398071	0.657614
6	-0.820837	0.398071	-0.657614
6	-1.294362	-0.879787	0.000000
1	-2.358511	-1.123655	0.000000
1	-0.678402	-1.789855	0.000000
6	-0.820837	1.133576	1.945845
1	-0.245901	0.611443	2.717537
1	-0.427249	2.146009	1.826304
1	-1.850203	1.204925	2.313581
6	-0.820837	1.133576	-1.945845
1	-0.427249	2.146009	-1.826304
1	-0.245901	0.611443	-2.717537
1	-1.850203	1.204925	-2.313581
19	1.871046	-0.953278	0.000000

Zero-point correction = 0.116225
Thermal correction to Energy = 0.124768
Thermal correction to Enthalpy = 0.125713
Thermal correction to Gibbs free Energy = 0.081436
Total energy = -793.564418
Nuclear repulsion energy = 269.100576

K⁺-7'

6	0.786520	-0.306707	0.681039
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6	0.786520	-0.306707	-0.681039
6	0.990043	1.197259	-0.780987
6	0.990043	1.197259	0.780987
1	0.206413	1.793828	-1.274179
1	1.943460	1.500138	-1.225390
1	0.206413	1.793828	1.274179
1	1.943460	1.500138	1.225390
6	0.786520	-1.366545	1.731912
1	0.044097	-1.171197	2.515083
1	0.593678	-2.354931	1.304663
1	1.761602	-1.401055	2.229924
6	0.786520	-1.366545	-1.731912
1	1.761602	-1.401055	-2.229924
1	0.593678	-2.354931	-1.304663
1	0.044097	-1.171197	-2.515083
19	-2.097657	0.472545	0.000000

Zero-point correction = 0.146051
Thermal correction to Energy = 0.155276
Thermal correction to Enthalpy = 0.156220
Thermal correction to Gibbs free Energy = 0.110751
Total energy = -832.769007
Nuclear repulsion energy = 362.431505

K⁺-8'

6	0.629060	-1.983150	0.000000
6	0.938352	-1.089046	1.212816
6	0.739934	0.315772	0.678567
6	0.739934	0.315772	-0.678567
6	0.938352	-1.089046	-1.212816
1	-0.434041	-2.269420	0.000000
1	1.982298	-1.209118	1.533663
1	0.323416	-1.316395	2.093585
1	1.982298	-1.209118	-1.533663
1	0.323416	-1.316395	-2.093585
1	1.194464	-2.918063	0.000000
6	0.739934	1.492207	-1.609097
1	0.548618	2.439267	-1.097591
1	1.715588	1.577550	-2.100987
1	0.005253	1.372875	-2.415683
6	0.739934	1.492207	1.609097
1	1.715588	1.577550	2.100987
1	0.548618	2.439267	1.097591
1	0.005253	1.372875	2.415683
19	-2.247567	0.143728	0.000000

Zero-point correction = 0.177006
Thermal correction to Energy = 0.187090
Thermal correction to Enthalpy = 0.188034
Thermal correction to Gibbs free Energy = 0.139440
Total energy = -871.974995
Nuclear repulsion energy = 457.891523

K⁺-9'

6	0.212891	-1.991105	0.773266
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6	0.212891	-1.991105	-0.773266
6	-0.865670	-1.061503	-1.356360
6	-0.865670	0.289700	-0.679072
6	-0.865670	0.289700	0.679072
6	-0.865670	-1.061503	1.356360
1	0.064839	-3.004310	1.158409
1	1.194293	-1.681249	-1.162800
1	-0.722835	-0.956355	-2.437521
1	-1.850725	-1.529384	1.222922
1	1.194293	-1.681249	1.162800
1	0.064839	-3.004310	-1.158409
1	-1.850725	-1.529384	-1.222922
1	-0.722835	-0.956355	2.437521
6	-0.976010	1.499252	-1.571018
1	-1.942808	1.492724	-2.087181
1	-0.906903	2.450188	-1.036733
1	-0.217035	1.483265	-2.365359
6	-0.976010	1.499252	1.571018
1	-0.217035	1.483265	2.365359
1	-0.906903	2.450188	1.036733
1	-1.942808	1.492724	2.087181
19	2.036624	0.981795	0.000000

Zero-point correction = 0.206802

Thermal correction to Energy = 0.217952
Thermal correction to Enthalpy = 0.218896
Thermal correction to Gibbs free Energy = 0.168514

Total energy = -911.137755

Nuclear repulsion energy = 562.238564

K⁺-10'

6	-0.975210	0.310811	0.678546
6	-0.975210	0.310811	-0.678546
6	-0.828278	-0.980063	-1.459946
6	-0.828278	-0.980063	1.459946
6	0.531203	-1.677481	-1.297901
6	0.531203	-1.677481	1.297901
6	0.684002	-2.469652	0.000000
1	-1.620357	-1.683637	-1.169538
1	-0.993457	-0.766275	2.521712
1	0.678551	-2.366638	-2.137345
1	1.342643	-0.934385	1.388448
1	-0.070186	-3.266848	0.000000
1	1.657608	-2.974411	0.000000
1	0.678551	-2.366638	2.137345
1	-1.620357	-1.683637	1.169538
1	1.342643	-0.934385	-1.388448
1	-0.993457	-0.766275	-2.521712
6	-1.175609	1.532822	1.544989
1	-2.123645	1.448292	2.088070
1	-0.400711	1.600097	2.322486
1	-1.211909	2.478636	0.998689
6	-1.175609	1.532822	-1.544989
1	-2.123645	1.448292	-2.088070

1 -1.211909 2.478636 -0.998689
 1 -0.400711 1.600097 -2.322486
 19 1.702161 1.645996 0.000000

Zero-point correction = 0.236919

Thermal correction to Energy = 0.248680

Thermal correction to Enthalpy = 0.249625

Thermal correction to Gibbs free Energy = 0.198912

Total energy = -950.304171

Nuclear repulsion energy = 666.401453

K⁺-11'

6 0.465926 0.900771 -0.890360
 6 0.438324 -0.427485 -1.172784
 6 -2.434299 0.392150 0.755300
 6 -0.865765 -1.152170 -1.399515
 6 -1.675840 -0.911914 1.049164
 6 -1.432930 -1.835862 -0.147919
 1 -1.617694 -0.466155 -1.797138
 1 -3.110383 0.244447 -0.096435
 1 -2.223817 -1.488824 1.802953
 1 -3.082526 0.611556 1.611010
 1 -0.716753 -1.916185 -2.172657
 1 -0.723212 -0.648744 1.533083
 1 -2.387465 -2.300060 -0.422484
 1 -0.779209 -2.664680 0.158512
 6 -0.797062 1.737276 -0.802968
 1 -1.473291 1.505499 -1.633405
 1 -0.510793 2.785966 -0.945825
 6 -1.579212 1.644699 0.518657
 1 -0.883950 1.767471 1.365762
 1 -2.246896 2.513252 0.564671
 6 1.727514 1.719035 -0.720679
 1 1.813839 2.437716 -1.542934
 1 1.686250 2.330534 0.193083
 1 2.656725 1.141438 -0.725084
 6 1.655089 -1.307461 -1.352120
 1 1.724065 -1.631673 -2.396377
 1 2.610927 -0.827116 -1.122243
 1 1.568684 -2.232563 -0.764497
 19 1.825529 -0.300848 1.651018

Zero-point correction = 0.266985

Thermal correction to Energy = 0.279644

Thermal correction to Enthalpy = 0.280588

Thermal correction to Gibbs free Energy = 0.228219

Total energy = -989.465758

Nuclear repulsion energy = 779.000818

Table S4. The MP2/6-31G* optimized coordinates of Mg²⁺-A (in Å)

Mg²⁺-1			
6	0.000000	0.687862	-0.983309
1	-0.934220	1.250381	-1.071143
1	0.934220	1.250381	-1.071143
6	0.000000	-0.687862	-0.983309
1	0.934220	-1.250381	-1.071143
1	-0.934220	-1.250381	-1.071143
12	0.000000	0.000000	1.340356
Zero-point correction = 0.053478			
Thermal correction to Energy = 0.057977			
Thermal correction to Enthalpy = 0.058921			
Thermal correction to Gibbs free Energy = 0.027359			
Total energy = -277.217150			
Nuclear repulsion energy = 72.969878			
Mg²⁺-2			
6	-0.864722	0.297524	-0.439389
1	-0.949563	0.494406	-1.512634
6	0.187628	0.906348	0.248516
1	0.133727	0.934542	1.344255
1	0.661786	1.772675	-0.234082
6	-1.930942	-0.504010	0.166399
1	-2.836024	0.131076	0.103188
1	-2.181590	-1.382653	-0.439859
1	-1.767037	-0.763187	1.213225
12	1.882243	-0.448836	-0.027271
Zero-point correction = 0.082063			
Thermal correction to Energy = 0.087598			
Thermal correction to Enthalpy = 0.088543			
Thermal correction to Gibbs free Energy = 0.053487			
Total energy = -316.409241			
Nuclear repulsion energy = 122.099817			
Mg²⁺-3			
6	-0.099982	0.721803	0.000000
6	-0.924146	-0.429718	0.000000
1	-1.488536	-0.614840	0.924072
1	-1.488536	-0.614840	-0.924072
6	0.288305	1.374818	1.269346
1	1.330983	1.709097	1.253179
1	-0.309898	2.299592	1.338523
1	0.080172	0.780062	2.160162
6	0.288305	1.374818	-1.269346
1	-0.309898	2.299592	-1.338523
1	1.330983	1.709097	-1.253179
1	0.080172	0.780062	-2.160162
12	0.288305	-2.216513	0.000000
Zero-point correction = 0.110390			
Thermal correction to Energy = 0.117382			

Thermal correction to Enthalpy = 0.118326
Thermal correction to Gibbs free Energy = 0.079403
Total energy = -355.598990
Nuclear repulsion energy = 183.729026

Mg²⁺-3'

6	-0.569114	-0.293133	0.698427
1	-0.822569	-1.250685	1.178307
6	-0.569114	-0.293133	-0.698427
1	-0.822569	-1.250685	-1.178307
6	-0.569114	0.912015	-1.585259
1	-0.109805	0.717299	-2.557639
1	-1.628553	1.132068	-1.793220
1	-0.136328	1.805073	-1.131270
6	-0.569114	0.912015	1.585259
1	-1.628553	1.132068	1.793220
1	-0.109805	0.717299	2.557639
1	-0.136328	1.805073	1.131270
12	1.587770	-1.019508	0.000000

Zero-point correction = 0.110933

Thermal correction to Energy = 0.118077
Thermal correction to Enthalpy = 0.119021
Thermal correction to Gibbs free Energy = 0.079864

Total energy = -355.586981

Nuclear repulsion energy = 186.558855

Mg²⁺-3''

6	0.000000	0.696529	-0.516372
1	0.977675	1.193515	-0.594658
6	0.000000	-0.696529	-0.516372
1	-0.977675	-1.193515	-0.594658
6	-1.216458	1.554070	-0.721930
1	-1.185319	1.871104	-1.775473
1	-1.200925	2.480137	-0.140104
1	-2.157583	1.017828	-0.571455
6	1.216458	-1.554070	-0.721930
1	1.200925	-2.480137	-0.140104
1	2.157583	-1.017828	-0.571455
1	1.185319	-1.871104	-1.775473
12	0.000000	0.000000	1.751917

Zero-point correction = 0.110885

Thermal correction to Energy = 0.118078
Thermal correction to Enthalpy = 0.119022
Thermal correction to Gibbs free Energy = 0.080428

Total energy = -355.586958

Nuclear repulsion energy = 185.887068

Mg²⁺-4

6	0.773650	0.079810	-0.078544
6	-0.512310	0.250044	-0.632986
1	-0.653227	-0.266631	-1.598001
6	1.732223	-0.901316	-0.671795

1	2.508847	-0.311742	-1.183626
1	2.264374	-1.477323	0.092041
1	1.286679	-1.565668	-1.417677
6	-1.392709	1.473547	-0.414741
1	-2.410934	1.314606	-0.778508
1	-1.430081	1.821496	0.619981
1	-0.973667	2.289783	-1.017078
6	1.304639	0.988958	0.972394
1	1.855618	1.781779	0.437718
1	0.542394	1.487967	1.572436
1	2.035382	0.491538	1.615099
12	-1.371528	-1.409339	0.550970

Zero-point correction = 0.139354

Thermal correction to Energy = 0.147938
Thermal correction to Enthalpy = 0.148882
Thermal correction to Gibbs free Energy = 0.106343

Total energy = -394.770866

Nuclear repulsion energy = 257.123426

Mg²⁺-5

6	0.000000	0.708664	-0.308669
6	0.000000	-0.708664	-0.308669
6	-1.270129	-1.507572	-0.509306
1	-2.189073	-1.032808	-0.160555
1	-1.382508	-1.644603	-1.595565
1	-1.189864	-2.509894	-0.081798
6	1.270129	1.507572	-0.509306
1	2.189073	1.032808	-0.160555
1	1.382508	1.644603	-1.595565
1	1.189864	2.509894	-0.081798
6	-1.270129	1.507572	-0.509306
1	-1.382508	1.644603	-1.595565
1	-2.189073	1.032808	-0.160555
1	-1.189864	2.509894	-0.081798
6	1.270129	-1.507572	-0.509306
1	1.382508	-1.644603	-1.595565
1	2.189073	-1.032808	-0.160555
1	1.189864	-2.509894	-0.081798
12	0.000000	0.000000	1.939920

Zero-point correction = 0.167971

Thermal correction to Energy = 0.178182
Thermal correction to Enthalpy = 0.179126
Thermal correction to Gibbs free Energy = 0.133522

Total energy = -433.945579

Nuclear repulsion energy = 342.089522

Mg²⁺-6

6	-1.271566	0.516893	-0.000176
6	0.087830	0.809717	0.000060
6	-1.749601	-0.790651	0.000024
1	-2.817924	-1.005319	0.000446
1	-1.081341	-1.650630	-0.000146
1	-1.994863	1.332722	0.000012

1 0.298431 1.886812 0.000288
12 1.932977 -0.314945 -0.000004
Zero-point correction = 0.058723
Thermal correction to Energy = 0.063738
Thermal correction to Enthalpy = 0.064682
Thermal correction to Gibbs free Energy = 0.030873
Total energy = -315.166592
Nuclear repulsion energy = 104.893701

Mg²⁺-7

6 0.589987 0.775871 0.690648
6 0.589987 0.775871 -0.690648
6 0.589987 -0.761352 -0.786565
6 0.589987 -0.761352 0.786565
1 1.518437 -1.152070 -1.223284
1 -0.201492 -1.302029 -1.349477
1 1.518437 -1.152070 1.223284
1 -0.201492 -1.302029 1.349477
1 0.772483 1.562120 1.425347
1 0.772483 1.562120 -1.425347
12 -1.528212 0.134144 0.000000

Zero-point correction = 0.088098
Thermal correction to Energy = 0.093549
Thermal correction to Enthalpy = 0.094493
Thermal correction to Gibbs free Energy = 0.059406
Total energy = -354.361942
Nuclear repulsion energy = 188.827580

Mg²⁺-8

6 -0.091503 1.329705 0.000000
6 -0.608868 0.532131 1.211076
6 -0.608868 -0.894725 0.691857
6 -0.608868 -0.894725 -0.691857
6 -0.608868 0.532131 -1.211076
1 1.051243 1.402016 0.000000
1 -1.663288 0.803117 1.391353
1 -0.091972 0.702495 2.161297
1 -0.795447 -1.778361 1.306053
1 -0.795447 -1.778361 -1.306053
1 -1.663288 0.803117 -1.391353
1 -0.091972 0.702495 -2.161297
1 -0.357261 2.391051 0.000000
12 1.630773 -0.572890 0.000000

Zero-point correction = 0.119128
Thermal correction to Energy = 0.125097
Thermal correction to Enthalpy = 0.126041
Thermal correction to Gibbs free Energy = 0.089298
Total energy = -393.593606
Nuclear repulsion energy = 261.572576

Mg²⁺-9

6 0.296004 -1.206355 0.787794
6 0.296004 -1.206355 -0.787794

6 -0.744894 -0.238301 -1.401367
6 -0.744894 1.094845 -0.689628
6 -0.744894 1.094845 0.689628
6 -0.744894 -0.238301 1.401367
1 0.137609 -2.224581 1.155459
1 1.308264 -1.003264 -1.239212
1 -0.585868 -0.130588 -2.477436
1 -0.895581 2.024397 -1.244281
1 -0.895581 2.024397 1.244281
1 -1.747031 -0.676208 1.277454
1 1.308264 -1.003264 1.239212
1 0.137609 -2.224581 -1.155459
1 -1.747031 -0.676208 -1.277454
1 -0.585868 -0.130588 2.477436
12 1.490886 0.684851 0.000000

Zero-point correction = 0.149452
Thermal correction to Energy = 0.156277
Thermal correction to Enthalpy = 0.157221
Thermal correction to Gibbs free Energy = 0.118820
Total energy = -432.776448
Nuclear repulsion energy = 347.111355

Mg²⁺-10

6 -0.407865 -1.505230 0.687804
6 -0.407865 -1.505230 -0.687804
6 0.442843 -0.623053 -1.590495
6 0.442843 -0.623053 1.590495
6 0.442843 0.902559 -1.330461
6 0.442843 0.902559 1.330461
6 1.060979 1.385952 0.000000
1 -0.989382 -2.288658 1.179324
1 -0.989382 -2.288658 -1.179324
1 1.483210 -0.968908 -1.495448
1 0.153714 -0.804711 2.629379
1 0.998470 1.382581 -2.144885
1 -0.570995 1.369988 1.553139
1 2.102215 1.045008 0.000000
1 1.096012 2.480786 0.000000
1 0.998470 1.382581 2.144885
1 1.483210 -0.968908 1.495448
1 -0.570995 1.369988 -1.553139
1 0.153714 -0.804711 -2.629379
12 -1.454000 0.457216 0.000000

Zero-point correction = 0.179047
Thermal correction to Energy = 0.186930
Thermal correction to Enthalpy = 0.187874
Thermal correction to Gibbs free Energy = 0.146974
Total energy = -471.960212
Nuclear repulsion energy = 435.849971

Mg²⁺-11

6 -1.448999 1.187657 0.117844
6 -0.218708 1.801239 0.107916

6	0.357733	-1.674389	-0.558147
6	0.919365	1.388230	-0.790234
6	1.514052	-0.987792	0.239205
6	1.977686	0.441482	-0.180958
1	0.518204	0.943545	-1.706422
1	0.544695	-1.472964	-1.617803
1	2.382608	-1.646138	0.119327
1	0.482132	-2.753505	-0.422675
1	1.444224	2.301674	-1.090218
1	1.447344	-1.139080	1.365984
1	2.737505	0.298067	-0.954999
1	2.502234	0.926373	0.652269
6	-1.797871	-0.036243	-0.721990
1	-1.522882	0.149072	-1.767341
1	-2.883525	-0.163330	-0.699641
6	-1.160611	-1.394849	-0.299656
1	-1.477623	-1.684160	0.748188
1	-1.693599	-2.180167	-0.847659
1	-2.253014	1.654972	0.695741
1	-0.095183	2.704939	0.711712
12	-0.249084	-0.190942	1.444138

Zero-point correction = 0.208936

Thermal correction to Energy = 0.217845

Thermal correction to Enthalpy = 0.218789

Thermal correction to Gibbs free Energy = 0.175632

Total energy = -511.130972

Nuclear repulsion energy = 531.074496

Mg²⁺-6'

6	-0.862390	-0.396725	0.003750
6	0.325140	0.369376	-0.007841
6	-0.742206	-1.777021	-0.009655
1	-1.610847	-2.433985	-0.019082
1	0.225487	-2.279118	-0.014269
6	-2.225347	0.255495	0.010411
1	-3.012201	-0.497704	0.072248
1	-2.329778	0.929606	0.865240
1	-2.380122	0.835957	-0.904384
6	0.235535	1.845848	-0.012109
1	-0.258546	2.168061	0.923477
1	1.181617	2.380594	-0.100064
1	-0.441009	2.181788	-0.814964
12	2.353417	-0.422253	0.007039

Zero-point correction = 0.114747

Thermal correction to Energy = 0.123015

Thermal correction to Enthalpy = 0.123959

Thermal correction to Gibbs free Energy = 0.081185

Total energy = -393.535415

Nuclear repulsion energy = 232.383821

Mg²⁺-7'

6	0.220296	-0.329468	0.701145
6	0.220296	-0.329468	-0.701145

6	0.700232	1.144192	-0.783159
6	0.700232	1.144192	0.783159
1	0.122451	1.908271	-1.346452
1	1.707165	1.221997	-1.212158
1	0.122451	1.908271	1.346452
1	1.707165	1.221997	1.212158
6	0.220296	-1.411910	1.720782
1	-0.219272	-1.095136	2.670364
1	-0.284142	-2.312054	1.359865
1	1.267057	-1.677694	1.925811
6	0.220296	-1.411910	-1.720782
1	1.267057	-1.677694	-1.925811
1	-0.284142	-2.312054	-1.359865
1	-0.219272	-1.095136	-2.670364
12	-1.573034	0.922955	0.000000

Zero-point correction = 0.145021

Thermal correction to Energy = 0.153628

Thermal correction to Enthalpy = 0.154573

Thermal correction to Gibbs free Energy = 0.112289

Total energy = -432.738061

Nuclear repulsion energy = 332.988788

Mg²⁺-8'

6	-0.155364	-1.869864	0.000000
6	0.354344	-1.059928	1.202428
6	0.354344	0.383455	0.701877
6	0.354344	0.383455	-0.701877
6	0.354344	-1.059928	-1.202428
1	-1.290667	-1.977241	0.000000
1	1.409141	-1.329509	1.379455
1	-0.159320	-1.232099	2.155115
1	1.409141	-1.329509	-1.379455
1	-0.159320	-1.232099	-2.155115
1	0.141971	-2.922886	0.000000
6	0.698652	1.533344	-1.595458
1	0.470999	2.505296	-1.152433
1	1.784086	1.499932	-1.767278
1	0.221796	1.453849	-2.575569
6	0.698652	1.533344	1.595458
1	1.784086	1.499932	1.767278
1	0.470999	2.505296	1.152433
1	0.221796	1.453849	2.575569
12	-1.855050	0.003493	0.000000

Zero-point correction = 0.176091

Thermal correction to Energy = 0.185200

Thermal correction to Enthalpy = 0.186144

Thermal correction to Gibbs free Energy = 0.142672

Total energy = -471.961771

Nuclear repulsion energy = 423.957421

Mg²⁺-9'

6	0.903445	1.600770	0.785313
6	0.903445	1.600770	-0.785313

6	0.903445	0.174672	-1.375632
6	-0.090715	-0.763310	-0.699509
6	-0.090715	-0.763310	0.699509
6	0.903445	0.174672	1.375632
1	1.759551	2.171202	1.157751
1	0.064871	2.199461	-1.237848
1	0.733910	0.213941	-2.455564
1	1.905076	-0.259301	1.235185
1	0.064871	2.199461	1.237848
1	1.759551	2.171202	-1.157751
1	1.905076	-0.259301	-1.235185
1	0.733910	0.213941	2.455564
6	-0.739566	-1.819984	-1.549701
1	0.020990	-2.585852	-1.757875
1	-1.579375	-2.320383	-1.066098
1	-1.060310	-1.424551	-2.516814
6	-0.739566	-1.819984	1.549701
1	-1.060310	-1.424551	2.516814
1	-1.579375	-2.320383	1.066098
1	0.020990	-2.585852	1.757875
12	-1.284061	1.142099	0.000000

Zero-point correction = 0.206296
 Thermal correction to Energy = 0.216301
 Thermal correction to Enthalpy = 0.217246
 Thermal correction to Gibbs free Energy = 0.171944
 Total energy = -511.138820
 Nuclear repulsion energy = 524.049570

Mg²⁺-10'

6	-0.258834	-0.992801	0.696624
6	-0.258834	-0.992801	-0.696624
6	0.740987	-0.138575	-1.496966
6	0.740987	-0.138575	1.496966
6	0.740987	1.402566	-1.326926
6	0.740987	1.402566	1.326926
6	1.323168	1.939375	0.000000
1	1.753512	-0.488862	-1.249423
1	0.588148	-0.356707	2.557173
1	1.332996	1.837461	-2.140645
1	-0.262002	1.854923	1.608655
1	2.380423	1.654211	0.000000
1	1.302061	3.034897	0.000000
1	1.332996	1.837461	2.140645
1	1.753512	-0.488862	1.249423
1	-0.262002	1.854923	-1.608655
1	0.588148	-0.356707	-2.557173
6	-1.022306	-1.993737	1.527746
1	-0.321284	-2.791219	1.810495
1	-1.385883	-1.550634	2.458796
1	-1.856977	-2.461360	1.007358
6	-1.022306	-1.993737	-1.527746
1	-0.321284	-2.791219	-1.810495
1	-1.856977	-2.461360	-1.007358

1	-1.385883	-1.550634	-2.458796
12	-1.144043	1.021500	0.000000

Zero-point correction = 0.235952
 Thermal correction to Energy = 0.246970
 Thermal correction to Enthalpy = 0.247914
 Thermal correction to Gibbs free Energy = 0.200250
 Total energy = -550.316731
 Nuclear repulsion energy = 626.874435

Mg²⁺-11'

6	-1.311869	-0.604865	-0.223659
6	-1.100795	0.769329	-0.266120
6	2.230556	-0.748709	-0.266300
6	0.094825	1.352539	-1.014975
6	2.188519	0.632539	0.454647
6	1.335649	1.770718	-0.193121
1	0.406868	0.681105	-1.819350
1	2.375528	-0.550216	-1.332975
1	3.222907	0.992216	0.491593
1	3.135306	-1.258345	0.079991
1	-0.269830	2.262132	-1.506118
1	2.073843	0.540426	1.581599
1	2.005034	2.280987	-0.892200
1	1.075321	2.528482	0.558324
6	-0.295369	-1.583835	-0.844404
1	-0.097250	-1.302353	-1.885221
1	-0.778517	-2.564374	-0.878405
6	1.081271	-1.802014	-0.140812
1	0.939091	-2.142658	0.928290
1	1.497947	-2.727480	-0.553864
6	-2.607833	-1.239064	0.226161
1	-3.165004	-1.512914	-0.680187
1	-2.443847	-2.167984	0.780913
1	-3.245079	-0.578105	0.812702
6	-2.116801	1.784613	0.199058
1	-2.751174	2.042913	-0.659328
1	-2.773565	1.433760	0.996081
1	-1.631116	2.709498	0.522366
12	0.286219	-0.221217	1.322745

Zero-point correction = 0.265830
 Thermal correction to Energy = 0.277858
 Thermal correction to Enthalpy = 0.278803
 Thermal correction to Gibbs free Energy = 0.229004
 Total energy = -589.487186
 Nuclear repulsion energy = 737.038123

Table S5. The MP2/6-31G* optimized coordinates of $\text{Ca}^{2+}\text{-A}$ (in Å)

$\text{Ca}^{2+}\text{-1}$			
6	0.000000	0.679119	-1.538390
1	-0.929941	1.242414	-1.629448
1	0.929941	1.242414	-1.629448
6	0.000000	-0.679119	-1.538390
1	0.929941	-1.242414	-1.629448
1	-0.929941	-1.242414	-1.629448
20	0.000000	0.000000	1.248924
Zero-point correction = 0.053360			
Thermal correction to Energy = 0.058030			
Thermal correction to Enthalpy = 0.058975			
Thermal correction to Gibbs free Energy = 0.026296			
Total energy = -754.459217			
Nuclear repulsion energy = 90.161487			
$\text{Ca}^{2+}\text{-2}$			
6	-1.336322	0.295589	-0.452288
1	-1.416051	0.413216	-1.536741
6	-0.531038	1.162805	0.230224
1	-0.591480	1.211216	1.321697
1	-0.138717	2.046602	-0.281457
6	-2.220264	-0.729334	0.168037
1	-3.255349	-0.386671	0.032459
1	-2.163470	-1.694975	-0.343653
1	-2.048837	-0.851689	1.240102
20	1.706982	-0.255603	-0.005413
Zero-point correction = 0.082351			
Thermal correction to Energy = 0.088205			
Thermal correction to Enthalpy = 0.089150			
Thermal correction to Gibbs free Energy = 0.052337			
Total energy = -793.640728			
Nuclear repulsion energy = 147.884382			
$\text{Ca}^{2+}\text{-3}$			
6	0.911140	-0.746891	0.000000
6	0.948582	0.628455	0.000000
1	1.222764	1.139428	0.929141
1	1.222764	1.139428	-0.929141
6	0.948582	-1.531527	1.272878
1	0.200335	-2.330314	1.280680
1	1.923090	-2.034414	1.325328
1	0.849916	-0.911447	2.166907
6	0.948582	-1.531527	-1.272878
1	1.923090	-2.034414	-1.325328
1	0.200335	-2.330314	-1.280680
1	0.849916	-0.911447	-2.166907
20	-1.546676	1.368122	0.000000
Zero-point correction = 0.110974			
Thermal correction to Energy = 0.118164			

Thermal correction to Enthalpy = 0.119108
 Thermal correction to Gibbs free Energy = 0.078908

Total energy = -832.822218

Nuclear repulsion energy = 216.479076

$\text{Ca}^{2+}\text{-3'}$			
6	0.902352	0.848445	0.679717
1	1.004745	1.810511	1.181636
6	0.902352	0.848445	-0.679717
1	1.004745	1.810511	-1.181636
6	0.902352	-0.356445	-1.595241
1	0.214339	-0.251242	-2.446660
1	1.891194	-0.438798	-2.065042
1	0.770105	-1.331691	-1.100688
6	0.902352	-0.356445	1.595241
1	1.891194	-0.438798	2.065042
1	0.214339	-0.251242	2.446660
1	0.770105	-1.331691	1.100688
20	-1.470860	-0.274078	0.000000
Zero-point correction = 0.110944			
Thermal correction to Energy = 0.118076			
Thermal correction to Enthalpy = 0.119020			
Thermal correction to Gibbs free Energy = 0.079699			
Total energy = -832.819112			
Nuclear repulsion energy = 234.024116			
$\text{Ca}^{2+}\text{-3''}$			
6	0.426222	0.533347	-0.972221
1	1.501021	0.328015	-1.057988
6	-0.426222	-0.533347	-0.972221
1	-1.501021	-0.328015	-1.057988
6	0.000000	1.971621	-1.108987
1	0.252273	2.303007	-2.123643
1	0.537605	2.654675	-0.441702
1	-1.080032	2.102696	-0.989703
6	0.000000	-1.971621	-1.108987
1	-0.537605	-2.654675	-0.441702
1	1.080032	-2.102696	-0.989703
1	-0.252273	-2.303007	-2.123643
20	0.000000	0.000000	1.710029
Zero-point correction = 0.110871			
Thermal correction to Energy = 0.118147			
Thermal correction to Enthalpy = 0.119091			
Thermal correction to Gibbs free Energy = 0.079207			
Total energy = -832.818826			
Nuclear repulsion energy = 223.549844			
$\text{Ca}^{2+}\text{-4}$			
6	1.071234	0.096734	0.033545
6	0.302232	1.135755	-0.403777
1	0.617767	1.639467	-1.318283
6	2.315642	-0.312031	-0.708086

1	3.188853	0.001894	-0.124549
1	2.392716	-1.397305	-0.827632
1	2.381880	0.162636	-1.689223
6	-0.845292	1.815739	0.320398
1	-1.701943	2.039771	-0.334090
1	-1.182392	1.330828	1.249967
1	-0.510623	2.805157	0.656733
6	0.841096	-0.645296	1.339320
1	1.658125	-0.404273	2.031606
1	-0.062610	-0.369542	1.906390
1	0.908427	-1.736933	1.218676
20	-1.489984	-0.830856	-0.312900

Zero-point correction = 0.139465

Thermal correction to Energy = 0.148051

Thermal correction to Enthalpy = 0.148995

Thermal correction to Gibbs free Energy = 0.106412

Total energy = -871.997581

Nuclear repulsion energy = 312.307800

Ca²⁺-5

6	-0.543019	-0.453665	0.686389
6	-0.543019	-0.453665	-0.686389
6	-0.543019	-1.722962	-1.503885
1	-0.011464	-2.548003	-1.029178
1	-1.580422	-2.046388	-1.652063
1	-0.114498	-1.560381	-2.496531
6	-0.758127	0.790649	1.544342
1	-0.833144	1.755131	1.019723
1	-1.729423	0.702060	2.047590
1	-0.041908	0.858100	2.379416
6	-0.543019	-1.722962	1.503885
1	-1.580422	-2.046388	1.652063
1	-0.011464	-2.548003	1.029178
1	-0.114498	-1.560381	2.496531
6	-0.758127	0.790649	-1.544342
1	-1.729423	0.702060	-2.047590
1	-0.833144	1.755131	-1.019723
1	-0.041908	0.858100	-2.379416
20	1.537585	1.115535	0.000000

Zero-point correction = 0.168048

Thermal correction to Energy = 0.178194

Thermal correction to Enthalpy = 0.179138

Thermal correction to Gibbs free Energy = 0.132977

Total energy = -911.171328

Nuclear repulsion energy = 401.352766

Ca²⁺-6

6	0.964338	-0.704848	0.336786
6	1.918773	-0.247661	-0.443247
6	1.160999	0.850557	0.215531
1	1.648508	1.444832	0.988329
1	0.489297	1.458499	-0.414051
1	0.852473	-1.521691	1.051665

1	2.861116	-0.447247	-0.939802
20	-1.505803	-0.016134	-0.067028

Zero-point correction = 0.057924

Thermal correction to Energy = 0.062959

Thermal correction to Enthalpy = 0.063903

Thermal correction to Gibbs free Energy = 0.029243

Total energy = -792.383080

Nuclear repulsion energy = 141.501629

Ca²⁺-7

6	1.022489	0.766669	0.683534
6	1.022489	0.766669	-0.683534
6	1.022489	-0.757931	-0.784390
6	1.022489	-0.757931	0.784390
1	1.945837	-1.162630	-1.212289
1	0.220183	-1.289741	-1.333849
1	1.945837	-1.162630	1.212289
1	0.220183	-1.289741	1.333849
1	1.209348	1.548974	1.419113
1	1.209348	1.548974	-1.419113
20	-1.564523	0.085097	0.000000

Zero-point correction = 0.088779

Thermal correction to Energy = 0.094256

Thermal correction to Enthalpy = 0.095200

Thermal correction to Gibbs free Energy = 0.059404

Total energy = -831.600065

Nuclear repulsion energy = 222.680460

Ca²⁺-8

6	0.980989	-0.932618	-0.719737
6	0.814304	-1.045714	0.815428
6	0.493352	0.381603	1.243504
6	0.797504	1.258344	0.246503
6	1.368116	0.542806	-0.959085
1	0.055595	-1.208113	-1.283732
1	1.770901	-1.327759	1.275975
1	0.115492	-1.825719	1.156553
1	0.275532	0.672336	2.272485
1	0.812829	2.341754	0.364855
1	2.460841	0.654514	-0.917610
1	1.070448	0.946057	-1.933075
1	1.710427	-1.641424	-1.117939
20	-1.749883	0.008092	-0.178859

Zero-point correction = 0.119666

Thermal correction to Energy = 0.126049

Thermal correction to Enthalpy = 0.126994

Thermal correction to Gibbs free Energy = 0.087909

Total energy = -870.819134

Nuclear repulsion energy = 303.881696

Ca²⁺-9			
6	-0.056784	-1.390745	0.780148
6	-0.056784	-1.390745	-0.780148
6	-1.051278	-0.382638	-1.399482
6	-1.051278	0.944064	-0.682207
6	-1.051278	0.944064	0.682207
6	-1.051278	-0.382638	1.399482
1	-0.286118	-2.393942	1.148736
1	0.957875	-1.234291	-1.214727
1	-0.871944	-0.274280	-2.472717
1	-1.227780	1.868116	-1.237632
1	-1.227780	1.868116	1.237632
1	-2.064732	-0.798851	1.306345
1	0.957875	-1.234291	1.214727
1	-0.286118	-2.393942	-1.148736
1	-2.064732	-0.798851	-1.306345
1	-0.871944	-0.274280	2.472717
20	1.644873	0.780916	0.000000
Zero-point correction = 0.149832			
Thermal correction to Energy = 0.157103			
Thermal correction to Enthalpy = 0.158047			
Thermal correction to Gibbs free Energy = 0.117375			
Total energy = -909.994392			
Nuclear repulsion energy = 395.253087			
Ca²⁺-10			
6	-0.978426	1.192718	0.682771
6	-0.978426	1.192718	-0.682771
6	-0.978426	-0.000420	-1.613938
6	-0.978426	-0.000420	1.613938
6	-0.067602	-1.197906	-1.302759
6	-0.067602	-1.197906	1.302759
6	-0.339066	-1.950514	0.000000
1	-1.162247	2.158397	1.161407
1	-1.162247	2.158397	-1.161407
1	-2.012881	-0.375723	-1.635164
1	-0.782386	0.345557	2.634448
1	-0.163960	-1.901746	-2.136479
1	1.019987	-0.930088	1.381715
1	-1.392014	-2.256657	0.000000
1	0.243782	-2.877731	0.000000
1	-0.163960	-1.901746	2.136479
1	-2.012881	-0.375723	1.635164
1	1.019987	-0.930088	-1.381715
1	-0.782386	0.345557	-2.634448
20	1.683952	0.915599	0.000000
Zero-point correction = 0.179348			
Thermal correction to Energy = 0.187704			
Thermal correction to Enthalpy = 0.188648			
Thermal correction to Gibbs free Energy = 0.145622			
Total energy = -949.169210			
Nuclear repulsion energy = 486.055156			

Ca²⁺-11			
6	-1.671897	-0.802602	0.452137
6	-0.602893	-1.340813	1.101513
6	0.366000	1.954452	-0.017945
6	0.490099	-0.545545	1.769933
6	1.585093	1.017387	-0.103213
6	1.711004	-0.193372	0.889611
1	0.075378	0.374882	2.191969
1	0.234918	2.279354	1.019241
1	2.466348	1.641374	0.071537
1	0.652974	2.857596	-0.566915
1	0.858269	-1.133984	2.615694
1	1.769655	0.755125	-1.173135
1	2.531862	0.048252	1.569638
1	2.096996	-1.110993	0.395100
6	-1.952180	0.676293	0.311782
1	-1.963281	1.130215	1.311187
1	-2.966565	0.789111	-0.080110
6	-1.006893	1.521614	-0.574284
1	-0.911932	1.083352	-1.599817
1	-1.550217	2.445837	-0.797678
1	-2.455593	-1.489316	0.117673
1	-0.586431	-2.426372	1.243996
20	0.311881	-1.048446	-1.464780
Zero-point correction = 0.209014			
Thermal correction to Energy = 0.218408			
Thermal correction to Enthalpy = 0.219352			
Thermal correction to Gibbs free Energy = 0.174476			
Total energy = -988.331987			
Nuclear repulsion energy = 594.663394			
Ca²⁺-6'			
6	-0.528433	0.536491	0.666669
6	-0.528433	0.536491	-0.666669
6	-1.298256	-0.600269	0.000000
1	-2.389902	-0.586752	0.000000
1	-0.972169	-1.661673	0.000000
6	-0.528433	1.362208	1.902103
1	-0.235588	0.800237	2.792408
1	0.103348	2.246372	1.789968
1	-1.561175	1.698923	2.064635
6	-0.528433	1.362208	-1.902103
1	0.103348	2.246372	-1.789968
1	-0.235588	0.800237	-2.792408
1	-1.561175	1.698923	-2.064635
20	1.361041	-1.321271	0.000000
Zero-point correction = 0.115865			
Thermal correction to Energy = 0.124029			
Thermal correction to Enthalpy = 0.124973			
Thermal correction to Gibbs free Energy = 0.080238			
Total energy = -870.754771			
Nuclear repulsion energy = 285.037158			

Ca²⁺-7'			
6	0.561416	-0.488282	0.689961
6	0.561416	-0.488282	-0.689961
6	0.981390	0.985657	-0.781603
6	0.981390	0.985657	0.781603
1	0.358858	1.723186	-1.333233
1	1.979672	1.123688	-1.210575
1	0.358858	1.723186	1.333233
1	1.979672	1.123688	1.210575
6	0.561416	-1.563103	1.724062
1	0.024311	-1.276306	2.633554
1	0.144822	-2.496876	1.337173
1	1.598192	-1.762485	2.021976
6	0.561416	-1.563103	-1.724062
1	1.598192	-1.762485	-2.021976
1	0.144822	-2.496876	-1.337173
1	0.024311	-1.276306	-2.633554
20	-1.673119	0.908316	0.000000
Zero-point correction = 0.145768			
Thermal correction to Energy = 0.154436			
Thermal correction to Enthalpy = 0.155380			
Thermal correction to Gibbs free Energy = 0.112264			
Total energy = -909.965925			
Nuclear repulsion energy = 383.272895			
Ca²⁺-8'			
6	0.840029	1.497376	0.842867
6	0.418029	0.204196	1.577662
6	-0.566260	-0.479396	0.624166
6	-0.970456	0.405024	-0.345612
6	-0.323188	1.766052	-0.131842
1	1.818042	1.411877	0.308859
1	-0.123392	0.460478	2.498639
1	1.250351	-0.428271	1.934862
1	-1.069195	2.411945	0.352305
1	-0.039728	2.291162	-1.052219
1	1.031287	2.326838	1.527564
6	-2.104657	0.243520	-1.310781
1	-2.386396	-0.799410	-1.471133
1	-2.982947	0.758986	-0.902270
1	-1.891587	0.712588	-2.275911
6	-1.187775	-1.802678	0.977712
1	-1.893799	-1.646115	1.802722
1	-1.751305	-2.240750	0.150813
1	-0.455955	-2.532963	1.340323
20	1.593014	-0.686547	-0.880979
Zero-point correction = 0.176603			
Thermal correction to Energy = 0.186234			
Thermal correction to Enthalpy = 0.187178			
Thermal correction to Gibbs free Energy = 0.140914			
Total energy = -949.177601			
Nuclear repulsion energy = 483.064865			

Ca²⁺-9'			
6	1.143383	1.474455	0.778475
6	1.143383	1.474455	-0.778475
6	1.143383	0.051783	-1.372391
6	0.180700	-0.905807	-0.688392
6	0.180700	-0.905807	0.688392
6	1.143383	0.051783	1.372391
1	2.013127	2.022757	1.150253
1	0.312785	2.073948	-1.219105
1	0.959505	0.094708	-2.450732
1	2.154431	-0.365052	1.258485
1	0.312785	2.073948	1.219105
1	2.013127	2.022757	-1.150253
1	2.154431	-0.365052	-1.258485
1	0.959505	0.094708	2.450732
6	-0.464205	-1.957958	-1.556893
1	0.308734	-2.678406	-1.853717
1	-1.250738	-2.525723	-1.056496
1	-0.859425	-1.538328	-2.487876
6	-0.464205	-1.957958	1.556893
1	-0.859425	-1.538328	2.487876
1	-1.250738	-2.525723	1.056496
1	0.308734	-2.678406	1.853717
20	-1.565798	1.094126	0.000000
Zero-point correction = 0.206696			
Thermal correction to Energy = 0.217213			
Thermal correction to Enthalpy = 0.218157			
Thermal correction to Gibbs free Energy = 0.170276			
Total energy = -988.348346			
Nuclear repulsion energy = 589.877998			
Ca²⁺-10'			
6	0.012363	-1.082580	0.687274
6	0.012363	-1.082580	-0.687274
6	1.048144	-0.290028	-1.477602
6	1.048144	-0.290028	1.477602
6	1.048144	1.241061	-1.317864
6	1.048144	1.241061	1.317864
6	1.623371	1.773930	0.000000
1	2.049429	-0.650032	-1.202239
1	0.927226	-0.526456	2.539152
1	1.642482	1.671576	-2.131326
1	0.039963	1.671086	1.557952
1	2.686164	1.506666	0.000000
1	1.599738	2.870008	0.000000
1	1.642482	1.671576	2.131326
1	2.049429	-0.650032	1.202239
1	0.039963	1.671086	-1.557952
1	0.927226	-0.526456	-2.539152
6	-0.843999	-2.000204	1.536237
1	-0.206585	-2.809520	1.914756
1	-1.231345	-1.491921	2.427579
1	-1.671243	-2.475509	1.007049

6 -0.843999 -2.000204 -1.536237
 1 -0.206585 -2.809520 -1.914756
 1 -1.671243 -2.475509 -1.007049
 1 -1.231345 -1.491921 -2.427579
 20 -1.615090 0.989116 0.000000

Zero-point correction = 0.236125

Thermal correction to Energy = 0.247719

Thermal correction to Enthalpy = 0.248663

Thermal correction to Gibbs free Energy = 0.198302

Total energy = -1027.518032

Nuclear repulsion energy = 698.004508

Ca²⁺-11'

6 -0.874123 -0.451686 -0.950020
 6 -0.599368 0.879256 -0.807589
 6 2.288988 -0.913011 0.162958
 6 0.751396 1.443492 -1.170092
 6 1.998006 0.412998 0.883386
 6 1.696499 1.648437 0.023510
 1 1.239053 0.808713 -1.912328
 1 2.852105 -0.695758 -0.752737
 1 2.858127 0.664666 1.513860
 1 2.971012 -1.491174 0.795238
 1 0.600159 2.414360 -1.657100
 1 1.214187 0.244474 1.671050
 1 2.653865 1.998170 -0.378072
 1 1.344106 2.466562 0.665817
 6 0.179550 -1.465544 -1.346528
 1 0.777157 -1.113677 -2.192763
 1 -0.326044 -2.370894 -1.698877
 6 1.122433 -1.851591 -0.188231
 1 0.526084 -2.060066 0.737514
 1 1.553060 -2.832535 -0.417710
 6 -2.246707 -1.067307 -0.710978
 1 -2.651513 -1.406686 -1.672423
 1 -2.204455 -1.995308 -0.112075
 1 -3.018109 -0.391797 -0.317639
 6 -1.603369 1.923480 -0.347623
 1 -2.029568 2.437912 -1.218214
 1 -2.487753 1.551398 0.196216
 1 -1.118541 2.706038 0.248819
 20 -1.051638 -0.214278 1.660434

Zero-point correction = 0.265312

Thermal correction to Energy = 0.277693

Thermal correction to Enthalpy = 0.278637

Thermal correction to Gibbs free Energy = 0.227409

Total energy = -1066.6848334

Nuclear repulsion energy = 817.7356097384

Table S6. The MP2/6-31G* optimized coordinates of Cu⁺-A (in Å)

Cu⁺-1			
6	0.000000	0.701760	-1.119589
1	-0.922834	1.248646	-1.310041
1	0.922834	1.248646	-1.310041
6	0.000000	-0.701760	-1.119589
1	0.922834	-1.248646	-1.310041
1	-0.922834	-1.248646	-1.310041
29	0.000000	0.000000	0.643974
Zero-point correction = 0.055181			
Thermal correction to Energy = 0.058824			
Thermal correction to Enthalpy = 0.059768			
Thermal correction to Gibbs free Energy = 0.029586			
Total energy = -1717.007322			
Nuclear repulsion energy = 154.049172			
Cu⁺-2			
6	0.868832	0.294055	0.487355
1	0.903651	0.341643	1.579121
6	0.141327	1.295481	-0.179924
1	0.358679	1.516105	-1.225689
1	-0.319673	2.102601	0.388554
6	1.953801	-0.509672	-0.171860
1	2.913821	-0.038709	0.065363
1	1.999425	-1.535206	0.203848
1	1.850213	-0.530282	-1.259823
29	-0.878961	-0.287425	-0.019476
Zero-point correction = 0.084141			
Thermal correction to Energy = 0.089195			
Thermal correction to Enthalpy = 0.090140			
Thermal correction to Gibbs free Energy = 0.055607			
Total energy = -1756.1854456			
Nuclear repulsion energy = 231.426232			
Cu⁺-3			
6	0.713277	-0.392675	0.000000
6	0.870066	1.009006	0.000000
1	1.139235	1.522868	0.923111
1	1.139235	1.522868	-0.923111
6	0.870066	-1.174401	1.279668
1	0.202031	-2.039926	1.316194
1	1.895450	-1.559394	1.316661
1	0.710333	-0.561230	2.170605
6	0.870066	-1.174401	-1.279668
1	1.895450	-1.559394	-1.316661
1	0.202031	-2.039926	-1.316194
1	0.710333	-0.561230	-2.170605
29	-0.959826	0.540351	0.000000
Zero-point correction = 0.112674			
Thermal correction to Energy = 0.119158			

Thermal correction to Enthalpy = 0.120103
Thermal correction to Gibbs free Energy = 0.082302

Total energy = -1795.364140

Nuclear repulsion energy = 321.257803

Cu⁺-3'

6	-0.791250	-0.139152	0.707067
1	-1.198119	-1.035278	1.184281
6	-0.791250	-0.139152	-0.707067
1	-1.198119	-1.035278	-1.184281
6	-0.791250	1.096499	-1.564519
1	-0.373485	0.898672	-2.554334
1	-1.831343	1.411150	-1.706917
1	-0.251878	1.933751	-1.117599
6	-0.791250	1.096499	1.564519
1	-1.831343	1.411150	1.706917
1	-0.373485	0.898672	2.554334
1	-0.251878	1.933751	1.117599
29	0.906885	-0.617405	0.000000

Zero-point correction = 0.113030

Thermal correction to Energy = 0.119648

Thermal correction to Enthalpy = 0.120592

Thermal correction to Gibbs free Energy = 0.082295

Total energy = -1795.361157

Nuclear repulsion energy = 317.639588

Cu⁺-3''

6	0.000000	0.705059	-0.735868
1	0.960683	1.199846	-0.910643
6	0.000000	-0.705059	-0.735868
1	-0.960683	-1.199846	-0.910643
6	-1.227377	1.523273	-1.034187
1	-1.216100	1.777112	-2.099458
1	-1.248115	2.464135	-0.478675
1	-2.149102	0.971241	-0.831836
6	1.227377	-1.523273	-1.034187
1	1.248115	-2.464135	-0.478675
1	2.149102	-0.971241	-0.831836
1	1.216100	-1.777112	-2.099458
29	0.000000	0.000000	1.030410

Zero-point correction = 0.113062

Thermal correction to Energy = 0.119630

Thermal correction to Enthalpy = 0.120574

Thermal correction to Gibbs free Energy = 0.083104

Total energy = -1795.362421

Nuclear repulsion energy = 316.570978

Cu⁺-4

6	0.724430	0.400017	-0.086857
6	-0.522721	0.577750	-0.740212
1	-0.535386	0.330119	-1.806322
6	1.908301	-0.080040	-0.893761
1	2.489338	0.798060	-1.198378

1	2.575802	-0.719014	-0.308523
1	1.611159	-0.614219	-1.800710
6	-1.596385	1.539401	-0.304988
1	-2.573421	1.250821	-0.698792
1	-1.676977	1.641845	0.778639
1	-1.356791	2.527929	-0.713372
6	1.070189	1.134465	1.184113
1	1.499612	2.105257	0.908395
1	0.211231	1.326435	1.830171
1	1.827476	0.595782	1.759901
29	-0.468101	-1.057675	0.217214

Zero-point correction = 0.141548

Thermal correction to Energy = 0.149631

Thermal correction to Enthalpy = 0.150575

Thermal correction to Gibbs free Energy = 0.109159

Total energy = -1834.538745

Nuclear repulsion energy = 415.621926

Cu⁺-5

6	0.000000	0.715536	-0.509003
6	0.000000	-0.715536	-0.509003
6	-1.262886	-1.495452	-0.803363
1	-2.176576	-1.035366	-0.424671
1	-1.364536	-1.580323	-1.892439
1	-1.198131	-2.509802	-0.401871
6	1.262886	1.495452	-0.803363
1	2.176576	1.035366	-0.424671
1	1.364536	1.580323	-1.892439
1	1.198131	2.509802	-0.401871
6	-1.262886	1.495452	-0.803363
1	-1.364536	1.580323	-1.892439
1	-2.176576	1.035366	-0.424671
1	-1.198131	2.509802	-0.401871
6	1.262886	-1.495452	-0.803363
1	1.364536	-1.580323	-1.892439
1	2.176576	-1.035366	-0.424671
1	1.198131	-2.509802	-0.401871
29	0.000000	0.000000	1.250506

Zero-point correction = 0.170021

Thermal correction to Energy = 0.179676

Thermal correction to Enthalpy = 0.180620

Thermal correction to Gibbs free Energy = 0.136452

Total energy = -1873.712070

Nuclear repulsion energy = 523.259312

Cu⁺-6

6	-0.193313	-0.896274	0.694258
6	-0.193313	-0.896274	-0.694258
6	1.063252	-1.373799	0.000000
1	1.233082	-2.448442	0.000000
1	1.975571	-0.786765	0.000000
1	-0.831173	-1.207947	1.514941
1	-0.831173	-1.207947	-1.514941

29 -0.193313 0.849972 0.000000
Zero-point correction = 0.060222
Thermal correction to Energy = 0.064404
Thermal correction to Enthalpy = 0.065349
Thermal correction to Gibbs free Energy = 0.032784
Total energy = -1754.933794
Nuclear repulsion energy = 218.377516

Cu⁺⁷

6 -0.815327 -0.178923 0.710428
6 -0.815327 -0.178923 -0.710428
6 -0.815327 1.343873 -0.779991
6 -0.815327 1.343873 0.779991
1 -1.753789 1.716496 -1.200756
1 0.008863 1.848902 -1.291965
1 -1.753789 1.716496 1.200756
1 0.008863 1.848902 1.291965
1 -1.201760 -0.910933 1.421521
1 -1.201760 -0.910933 -1.421521
29 0.877973 -0.665115 0.000000

Zero-point correction = 0.090537
Thermal correction to Energy = 0.095549
Thermal correction to Enthalpy = 0.096494
Thermal correction to Gibbs free Energy = 0.061526
Total energy = -1794.144711
Nuclear repulsion energy = 306.778930

Cu⁺⁸

6 -0.269336 1.729476 0.000000
6 -0.808508 0.947989 1.208783
6 -0.808508 -0.477998 0.705766
6 -0.808508 -0.477998 -0.705766
6 -0.808508 0.947989 -1.208783
1 0.834742 1.711612 0.000000
1 -1.852311 1.227542 1.407770
1 -0.250646 1.109032 2.135750
1 -1.171716 -1.318126 1.298652
1 -1.171716 -1.318126 -1.298652
1 -1.852311 1.227542 -1.407770
1 -0.250646 1.109032 -2.135750
1 -0.562606 2.780542 0.000000
29 0.941290 -0.777441 0.000000

Zero-point correction = 0.121515
Thermal correction to Energy = 0.127240
Thermal correction to Enthalpy = 0.128184
Thermal correction to Gibbs free Energy = 0.091338
Total energy = -1833.362308
Nuclear repulsion energy = 407.937243

Cu⁺⁹

6 1.186401 0.954859 -0.702149
6 1.522109 -0.553425 -0.815959
6 1.080435 -1.386558 0.406943

6 -0.205809 -0.873130 0.999630
6 -0.313305 0.509415 1.215070
6 0.814510 1.380626 0.728087
1 2.012894 1.560623 -1.081600
1 1.076491 -0.972758 -1.727998
1 1.003520 -2.443532 0.139212
1 -0.839844 -1.548991 1.575173
1 -1.027012 0.889545 1.947711
1 1.681092 1.250769 1.391539
1 0.344030 1.225488 -1.373357
1 2.599395 -0.678038 -0.947499
1 1.842954 -1.318951 1.194700
1 0.543530 2.439472 0.761294
29 -1.163555 -0.020495 -0.443755

Zero-point correction = 0.151073
Thermal correction to Energy = 0.158163
Thermal correction to Enthalpy = 0.159107
Thermal correction to Gibbs free Energy = 0.118650
Total energy = -1872.532574

Nuclear repulsion energy = 518.520087

Cu⁺¹⁰

6 -0.942912 0.946363 0.700769
6 -0.942912 0.946363 -0.700769
6 -0.942912 -0.283256 -1.578236
6 -0.942912 -0.283256 1.578236
6 0.195772 -1.273336 -1.289356
6 0.195772 -1.273336 1.289356
6 0.069890 -2.079698 0.000000
1 -1.234369 1.885088 1.175232
1 -1.234369 1.885088 -1.175232
1 -1.906564 -0.800658 -1.473159
1 -0.878694 0.039569 2.621723
1 0.272417 -1.966483 -2.132764
1 1.174963 -0.743457 1.295536
1 -0.894159 -2.602151 0.000000
1 0.842396 -2.856216 0.000000
1 0.272417 -1.966483 2.132764
1 -1.906564 -0.800658 1.473159
1 1.174963 -0.743457 -1.295536
1 -0.878694 0.039569 -2.621723
29 0.864053 0.980386 0.000000

Zero-point correction = 0.180296
Thermal correction to Energy = 0.188399
Thermal correction to Enthalpy = 0.189343
Thermal correction to Gibbs free Energy = 0.146987
Total energy = -1911.705125

Nuclear repulsion energy = 627.136968

Cu⁺¹¹

6 -0.588284 -1.557144 0.364806
6 0.748932 -1.337009 0.702055
6 -0.911742 1.784797 0.196204

6	1.209312	-0.120266	1.470240
6	0.495709	1.592250	-0.402545
6	1.595406	1.058131	0.552793
1	0.422992	0.200310	2.161443
1	-0.801327	2.031601	1.258551
1	0.865403	2.563948	-0.746048
1	-1.353387	2.669205	-0.273543
1	2.077317	-0.383168	2.081509
1	0.429606	1.121694	-1.448716
1	1.880121	1.901315	1.190858
1	2.500457	0.812000	-0.019056
6	-1.732098	-0.664699	0.817301
1	-1.614932	-0.430336	1.882597
1	-2.654983	-1.244867	0.729212
6	-1.932396	0.645384	0.027021
1	-2.054248	0.421778	-1.046445
1	-2.904993	1.048154	0.329292
1	-0.848502	-2.557675	0.015772
1	1.450187	-2.164457	0.580763
29	0.320595	-0.496488	-1.002188

Zero-point correction = 0.210250

Thermal correction to Energy = 0.219028

Thermal correction to Enthalpy = 0.219972

Thermal correction to Gibbs free Energy = 0.176687

Total energy = -1950.880579

Nuclear repulsion energy = 763.752240

Cu⁺-6'

6	-0.496525	0.243134	0.697184
6	-0.496525	0.243134	-0.697184
6	-1.535173	-0.615935	0.000000
1	-2.550917	-0.213454	0.000000
1	-1.504371	-1.701777	0.000000
6	-0.496525	1.194928	1.838349
1	-0.428210	0.682085	2.800306
1	0.303843	1.935121	1.760162
1	-1.458731	1.723156	1.811966
6	-0.496525	1.194928	-1.838349
1	0.303843	1.935121	-1.760162
1	-0.428210	0.682085	-2.800306
1	-1.458731	1.723156	-1.811966
29	0.977556	-0.700919	0.000000

Zero-point correction = 0.117771

Thermal correction to Energy = 0.125151

Thermal correction to Enthalpy = 0.126095

Thermal correction to Gibbs free Energy = 0.086043

Total energy = -1833.301536

Nuclear repulsion energy = 391.992126

Cu⁺-7'

6	-0.511620	-0.055851	0.716961
6	-0.511620	-0.055851	-0.716961
6	-0.511620	-1.584545	-0.778181

6	-0.511620	-1.584545	0.778181
1	0.305555	-2.095139	-1.297014
1	-1.454839	-1.954739	-1.193871
1	0.305555	-2.095139	1.297014
1	-1.454839	-1.954739	1.193871
6	-1.076481	0.911761	1.707362
1	-0.597628	0.823245	2.686511
1	-0.999079	1.948649	1.367848
1	-2.140400	0.680112	1.838331
6	-1.076481	0.911761	-1.707362
1	-2.140400	0.680112	-1.838331
1	-0.999079	1.948649	-1.367848
1	-0.597628	0.823245	-2.686511
29	1.205843	0.342736	0.000000

Zero-point correction = 0.147475

Thermal correction to Energy = 0.155742

Thermal correction to Enthalpy = 0.156687

Thermal correction to Gibbs free Energy = 0.114637

Total energy = -1872.506745

Nuclear repulsion energy = 502.856568

Cu⁺-8'

6	-0.007228	-2.061729	0.000000
6	0.533192	-1.272465	1.198799
6	0.533192	0.164972	0.713122
6	0.533192	0.164972	-0.713122
6	0.533192	-1.272465	-1.198799
1	-1.110553	-2.055813	0.000000
1	1.581647	-1.548832	1.385506
1	-0.011077	-1.433861	2.134974
1	1.581647	-1.548832	-1.385506
1	-0.011077	-1.433861	-2.134974
1	0.296843	-3.110276	0.000000
6	1.075086	1.266140	-1.578178
1	0.922752	2.260507	-1.151752
1	2.155738	1.113029	-1.687879
1	0.637203	1.244997	-2.579545
6	1.075086	1.266140	1.578178
1	2.155738	1.113029	1.687879
1	0.922752	2.260507	1.151752
1	0.637203	1.244997	2.579545
29	-1.221141	0.426242	0.000000

Zero-point correction = 0.178351

Thermal correction to Energy = 0.187293

Thermal correction to Enthalpy = 0.188237

Thermal correction to Gibbs free Energy = 0.144714

Total energy = -1911.719400

Nuclear repulsion energy = 620.982370

Cu⁺-9'

6	1.178367	1.571928	0.775185
6	1.178367	1.571928	-0.775185
6	1.178367	0.154885	-1.367266

6	0.138777	-0.729625	-0.710570
6	0.138777	-0.729625	0.710570
6	1.178367	0.154885	1.367266
1	2.040612	2.124621	1.156873
1	0.308487	2.123847	-1.168918
1	1.017074	0.199625	-2.448899
1	2.162262	-0.312515	1.215226
1	0.308487	2.123847	1.168918
1	2.040612	2.124621	-1.156873
1	2.162262	-0.312515	-1.215226
1	1.017074	0.199625	2.448899
6	-0.402247	-1.873847	-1.527420
1	0.391623	-2.623774	-1.634990
1	-1.263315	-2.367383	-1.073622
1	-0.681461	-1.546001	-2.532085
6	-0.402247	-1.873847	1.527420
1	-0.681461	-1.546001	2.532085
1	-1.263315	-2.367383	1.073622
1	0.391623	-2.623774	1.634990
29	-1.140336	0.528382	0.000000

Zero-point correction = 0.207891
Thermal correction to Energy = 0.218195
Thermal correction to Enthalpy = 0.219139
Thermal correction to Gibbs free Energy = 0.171914
Total energy = -1950.886163
Nuclear repulsion energy = 745.255730

Cu⁺-10'

6	-0.728845	0.575381	0.709346
6	-0.728845	0.575381	-0.709346
6	-0.728845	-0.731995	-1.490461
6	-0.728845	-0.731995	1.490461
6	0.500686	-1.633950	-1.284718
6	0.500686	-1.633950	1.284718
6	0.503215	-2.453172	0.000000
1	-1.636200	-1.300375	-1.240778
1	-0.803261	-0.486392	2.554126
1	0.578797	-2.317914	-2.136091
1	1.432815	-1.030569	1.346573
1	-0.378002	-3.105420	0.000000
1	1.376980	-3.114320	0.000000
1	0.578797	-2.317914	2.136091
1	-1.636200	-1.300375	1.240778
1	1.432815	-1.030569	-1.346573
1	-0.803261	-0.486392	-2.554126
6	-1.211798	1.769310	1.500257
1	-2.294472	1.668702	1.648616
1	-0.748807	1.798369	2.490010
1	-1.032629	2.728412	1.014118
6	-1.211798	1.769310	-1.500257
1	-2.294472	1.668702	-1.648616
1	-1.032629	2.728412	-1.014118
1	-0.748807	1.798369	-2.490010

29	1.069478	0.657702	0.000000
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Zero-point correction = 0.237093
Thermal correction to Energy = 0.248370
Thermal correction to Enthalpy = 0.249314
Thermal correction to Gibbs free Energy = 0.200427
Total energy = -1990.053348
Nuclear repulsion energy = 866.809624

Cu⁺-11'

6	-1.095151	0.765482	0.315482
6	-1.071537	-0.631911	0.511510
6	2.321277	0.624655	0.360689
6	0.063203	-1.275465	1.297929
6	1.976351	-0.670902	-0.397597
6	1.228673	-1.760728	0.413400
1	0.451338	-0.586046	2.052674
1	2.514182	0.363979	1.407939
1	2.907154	-1.141752	-0.731071
1	3.270113	1.000377	-0.035537
1	-0.333015	-2.137463	1.845210
1	1.582376	-0.434594	-1.450868
1	1.978444	-2.223566	1.064508
1	0.892485	-2.564705	-0.255802
6	-0.050159	1.671034	0.979245
1	0.092299	1.379800	2.026810
1	-0.477241	2.678754	1.005556
6	1.324078	1.794699	0.287944
1	1.185023	2.087956	-0.766837
1	1.826587	2.656729	0.740999
6	-2.345069	1.491374	-0.127468
1	-2.889893	1.819198	0.766303
1	-2.094155	2.387980	-0.701421
1	-3.022469	0.883428	-0.727742
6	-2.266656	-1.524777	0.277125
1	-2.823808	-1.604013	1.218755
1	-2.952936	-1.159949	-0.487553
1	-1.953095	-2.535301	-0.000984
29	-0.022878	-0.130055	-1.051051

Zero-point correction = 0.267100
Thermal correction to Energy = 0.279016
Thermal correction to Enthalpy = 0.279960
Thermal correction to Gibbs free Energy = 0.230253
Total energy = -2029.228968
Nuclear repulsion energy = 1018.740595

Table S7. The MP2/6-31G* optimized coordinates of $\text{Zn}^{2+}\text{-A}$ (in Å)

$\text{Zn}^{2+}\text{-1}$			
6	0.000000	0.697101	-1.354171
1	-0.938013	1.254208	-1.454733
1	0.938013	1.254208	-1.454733
6	0.000000	-0.697101	-1.354171
1	0.938013	-1.254208	-1.454733
1	-0.938013	-1.254208	-1.454733
30	0.000000	0.000000	0.735633
Zero-point correction = 0.053688			
Thermal correction to Energy = 0.058022			
Thermal correction to Enthalpy = 0.058966			
Thermal correction to Gibbs free Energy = 0.026920			
Total energy = -1855.276592			
Nuclear repulsion energy = 142.496956			
$\text{Zn}^{2+}\text{-2}$			
6	-1.482648	0.276259	-0.441690
1	-1.572475	0.468376	-1.515749
6	-0.395871	0.904306	0.247152
1	-0.508501	0.953289	1.337325
1	-0.076610	1.850440	-0.215495
6	-2.525992	-0.504640	0.173015
1	-3.397026	0.198179	0.137119
1	-2.871176	-1.329949	-0.465090
1	-2.363037	-0.793965	1.211356
30	1.240530	-0.180064	-0.012011
Zero-point correction = 0.081693			
Thermal correction to Energy = 0.087217			
Thermal correction to Enthalpy = 0.088162			
Thermal correction to Gibbs free Energy = 0.052086			
Total energy = -1894.480140			
Nuclear repulsion energy = 206.432375			
$\text{Zn}^{2+}\text{-3}$			
6	0.807607	-1.046408	0.000000
6	0.855688	0.405819	0.000000
1	1.294884	0.825741	0.914720
1	1.294884	0.825741	-0.914720
6	0.855688	-1.781881	1.266770
1	0.280736	-2.712960	1.233077
1	1.912506	-2.104346	1.371085
1	0.616916	-1.187007	2.149810
6	0.855688	-1.781881	-1.266770
1	1.912506	-2.104346	-1.371085
1	0.280736	-2.712960	-1.233077
1	0.616916	-1.187007	-2.149810
30	-0.948604	1.186108	0.000000
Zero-point correction = 0.109990			
Thermal correction to Energy = 0.117102			

Thermal correction to Enthalpy = 0.118046
 Thermal correction to Gibbs free Energy = 0.077293

Total energy = -1933.676864

Nuclear repulsion energy = 288.857104

$\text{Zn}^{2+}\text{-3'}$			
6	-0.932499	-0.040728	0.711346
1	-1.227468	-0.990197	1.182926
6	-0.932499	-0.040728	-0.711346
1	-1.227468	-0.990197	-1.182926
6	-0.932499	1.165104	-1.579589
1	-0.520248	0.968833	-2.572585
1	-2.004105	1.386489	-1.739302
1	-0.478608	2.053900	-1.138667
6	-0.932499	1.165104	1.579589
1	-2.004105	1.386489	1.739302
1	-0.520248	0.968833	2.572585
1	-0.478608	2.053900	1.138667
30	1.028028	-0.677685	0.000000
Zero-point correction = 0.110686			
Thermal correction to Energy = 0.117740			
Thermal correction to Enthalpy = 0.118684			
Thermal correction to Gibbs free Energy = 0.078978			
Total energy = -1933.661593			
Nuclear repulsion energy = 303.940474			
$\text{Zn}^{2+}\text{-3''}$			
6	0.000000	0.709835	-0.904615
1	0.982096	1.197910	-0.985603
6	0.000000	-0.709835	-0.904615
1	-0.982096	-1.197910	-0.985603
6	-1.207009	1.547468	-1.162584
1	-1.144146	1.790225	-2.238047
1	-1.187371	2.509641	-0.643972
1	-2.155267	1.029921	-0.996838
6	1.207009	-1.547468	-1.162584
1	1.187371	-2.509641	-0.643972
1	2.155267	-1.029921	-0.996838
1	1.144146	-1.790225	-2.238047
30	0.000000	0.000000	1.151177
Zero-point correction = 0.110788			
Thermal correction to Energy = 0.117824			
Thermal correction to Enthalpy = 0.118768			
Thermal correction to Gibbs free Energy = 0.079906			
Total energy = -1933.661716			
Nuclear repulsion energy = 304.335137			
$\text{Zn}^{2+}\text{-4}$			
6	1.211133	-0.168083	-0.064587
6	0.115669	0.563748	-0.669629
1	-0.063464	0.237365	-1.707217
6	1.682795	-1.426909	-0.673019

1	2.662877	-1.188859	-1.127578
1	1.908119	-2.190457	0.080367
1	1.041258	-1.824407	-1.462238
6	-0.069815	2.058942	-0.442493
1	-0.974179	2.425935	-0.932481
1	-0.087703	2.357381	0.607253
1	0.776963	2.566240	-0.921666
6	1.981833	0.405063	1.048203
1	2.753595	1.034185	0.557801
1	1.421461	1.079116	1.698947
1	2.520246	-0.350816	1.624081
30	-1.382962	-0.424742	0.213063

Zero-point correction = 0.139026

Thermal correction to Energy = 0.147518

Thermal correction to Enthalpy = 0.148462

Thermal correction to Gibbs free Energy = 0.105283

Total energy = -1972.853207

Nuclear repulsion energy = 391.668854

Zn²⁺-5

6	0.000000	0.725308	-0.662355
6	0.000000	-0.725308	-0.662355
6	-1.269720	-1.499439	-0.889652
1	-2.185745	-1.037239	-0.519511
1	-1.372446	-1.576319	-1.984846
1	-1.192282	-2.520645	-0.510678
6	1.269720	1.499439	-0.889652
1	2.185745	1.037239	-0.519511
1	1.372446	1.576319	-1.984846
1	1.192282	2.520645	-0.510678
6	-1.269720	1.499439	-0.889652
1	-1.372446	1.576319	-1.984846
1	-2.185745	1.037239	-0.519511
1	-1.192282	2.520645	-0.510678
6	1.269720	-1.499439	-0.889652
1	1.372446	-1.576319	-1.984846
1	2.185745	-1.037239	-0.519511
1	1.192282	-2.520645	-0.510678
30	0.000000	0.000000	1.378668

Zero-point correction = 0.167668

Thermal correction to Energy = 0.177714

Thermal correction to Enthalpy = 0.178658

Thermal correction to Gibbs free Energy = 0.133150

Total energy = -2012.032905

Nuclear repulsion energy = 510.565911

Zn²⁺-6

6	-0.500410	0.892086	0.000030
6	-1.828825	0.517851	0.000007
6	-2.251304	-0.816385	-0.000019
1	-3.311601	-1.071971	-0.000097
1	-1.549430	-1.650514	0.000366
1	-0.292036	1.967086	0.000258

1	-2.584814	1.305016	-0.000257
30	1.174037	-0.137031	-0.000012

Zero-point correction = 0.059042

Thermal correction to Energy = 0.063984

Thermal correction to Enthalpy = 0.064928

Thermal correction to Gibbs free Energy = 0.030290

Total energy = -1893.248332

Nuclear repulsion energy = 183.813520

Zn²⁺-7

6	-0.967082	-0.120407	0.711638
6	-0.967082	-0.120407	-0.711638
6	-0.967082	1.393836	-0.778282
6	-0.967082	1.393836	0.778282
1	-1.926280	1.713849	-1.215399
1	-0.179348	1.927922	-1.319251
1	-1.926280	1.713849	1.215399
1	-0.179348	1.927922	1.319251
1	-1.248625	-0.906181	1.425936
1	-1.248625	-0.906181	-1.425936
30	0.997282	-0.691744	0.000000

Zero-point correction = 0.088106

Thermal correction to Energy = 0.093749

Thermal correction to Enthalpy = 0.094693

Thermal correction to Gibbs free Energy = 0.057816

Total energy = -1932.435101

Nuclear repulsion energy = 294.041612

Zn²⁺-8

6	-0.419659	1.527543	0.000000
6	-0.967704	0.750833	1.204340
6	-0.967704	-0.670568	0.704149
6	-0.967704	-0.670568	-0.704149
6	-0.967704	0.750833	-1.204340
1	0.725845	1.505051	0.000000
1	-2.030711	1.022292	1.349558
1	-0.477600	0.921600	2.167856
1	-1.163015	-1.559000	1.311181
1	-1.163015	-1.559000	-1.311181
1	-2.030711	1.022292	-1.349558
1	-0.477600	0.921600	-2.167856
1	-0.627846	2.601321	0.000000
30	1.099583	-0.500153	0.000000

Zero-point correction = 0.118662

Thermal correction to Energy = 0.124603

Thermal correction to Enthalpy = 0.125547

Thermal correction to Gibbs free Energy = 0.088218

Total energy = -1971.668927

Nuclear repulsion energy = 408.393933

Zn²⁺-9

6	0.030684	-1.393940	0.786378
6	0.030684	-1.393940	-0.786378

6	-1.038459	-0.464505	-1.402818
6	-1.038459	0.864361	-0.700097
6	-1.038459	0.864361	0.700097
6	-1.038459	-0.464505	1.402818
1	-0.089605	-2.415731	1.159955
1	1.029369	-1.139282	-1.235294
1	-0.889280	-0.354972	-2.480056
1	-1.206997	1.800008	-1.241993
1	-1.206997	1.800008	1.241993
1	-2.038099	-0.907806	1.265707
1	1.029369	-1.139282	1.235294
1	-0.089605	-2.415731	-1.159955
1	-2.038099	-0.907806	-1.265707
1	-0.889280	-0.354972	2.480056
30	1.031468	0.598819	0.000000

Zero-point correction = 0.148436
 Thermal correction to Energy = 0.155699
 Thermal correction to Enthalpy = 0.156643
 Thermal correction to Gibbs free Energy = 0.116337
 Total energy = -2010.849715
 Nuclear repulsion energy = 525.794606

Zn²⁺-10

6	-1.027908	1.113132	0.696668
6	-1.027908	1.113132	-0.696668
6	-1.027908	-0.103941	-1.593074
6	-1.027908	-0.103941	1.593074
6	0.068063	-1.145191	-1.299551
6	0.068063	-1.145191	1.299551
6	-0.032930	-1.946070	0.000000
1	-1.163877	2.087936	1.173968
1	-1.163877	2.087936	-1.173968
1	-2.010554	-0.592953	-1.502479
1	-0.944971	0.228652	2.631628
1	0.127540	-1.841891	-2.144478
1	1.105717	-0.666903	1.410080
1	-0.990186	-2.480829	0.000000
1	0.745091	-2.717235	0.000000
1	0.127540	-1.841891	2.144478
1	-2.010554	-0.592953	1.502479
1	1.105717	-0.666903	-1.410080
1	-0.944971	0.228652	-2.631628
30	1.002267	0.669227	0.000000

Zero-point correction = 0.177719
 Thermal correction to Energy = 0.185835
 Thermal correction to Enthalpy = 0.186779
 Thermal correction to Gibbs free Energy = 0.144648
 Total energy = -2050.035049
 Nuclear repulsion energy = 639.048954

Zn²⁺-11

6	-1.369255	-1.151717	0.291913
6	-0.109733	-1.744205	0.305765

6	0.340893	1.785468	0.671798
6	1.034985	-1.241270	1.145856
6	1.430645	1.036945	-0.139612
6	2.015527	-0.288260	0.423262
1	0.641098	-0.751924	2.041874
1	0.601345	1.705172	1.732874
1	2.288129	1.712330	-0.267860
1	0.424065	2.847003	0.418449
1	1.607081	-2.112745	1.481010
1	1.212775	1.045347	-1.280721
1	2.769107	0.003258	1.161291
1	2.568738	-0.819228	-0.362454
6	-1.731898	0.102677	1.067841
1	-1.416075	-0.000663	2.113229
1	-2.821872	0.186027	1.073779
6	-1.155442	1.420743	0.483171
1	-1.454731	1.525587	-0.599009
1	-1.730116	2.245700	0.919653
1	-2.171400	-1.692275	-0.222005
1	0.008305	-2.690129	-0.232686
30	-0.175359	-0.090858	-1.115913

Zero-point correction = 0.207428
 Thermal correction to Energy = 0.216625
 Thermal correction to Enthalpy = 0.217569
 Thermal correction to Gibbs free Energy = 0.173196
 Total energy = -2089.211607
 Nuclear repulsion energy = 768.843727

Zn²⁺-6'

6	0.268240	0.475995	-0.009140
6	1.342856	-0.425592	0.002226
6	1.064589	-1.788192	-0.004967
1	1.853606	-2.539712	-0.010356
1	0.045401	-2.177189	-0.007314
6	0.460696	1.933499	-0.008577
1	-0.440456	2.532978	-0.132901
1	0.936506	2.215193	0.951221
1	1.193997	2.210141	-0.784190
6	2.768662	0.076997	0.005947
1	2.938075	0.755907	0.846357
1	3.465877	-0.757758	0.092214
1	2.987461	0.613155	-0.923025
30	-1.613691	-0.149632	0.001835

Zero-point correction = 0.114871
 Thermal correction to Energy = 0.123082
 Thermal correction to Enthalpy = 0.124026
 Thermal correction to Gibbs free Energy = 0.080941
 Total energy = -1971.627710
 Nuclear repulsion energy = 356.546289

Zn²⁺-7'

6	0.622357	-0.235037	0.726171
6	0.622357	-0.235037	-0.726171

6	1.252011	1.158242	-0.775988
6	1.252011	1.158242	0.775988
1	0.759053	1.970340	-1.319852
1	2.261128	1.063447	-1.202141
1	0.759053	1.970340	1.319852
1	2.261128	1.063447	1.202141
6	0.622357	-1.343549	1.712241
1	0.286230	-1.024913	2.702964
1	0.073257	-2.230829	1.384352
1	1.681156	-1.635979	1.818693
6	0.622357	-1.343549	-1.712241
1	1.681156	-1.635979	-1.818693
1	0.073257	-2.230829	-1.384352
1	0.286230	-1.024913	-2.702964
30	-1.336079	0.292000	0.000000

Zero-point correction = 0.145024

Thermal correction to Energy = 0.153712

Thermal correction to Enthalpy = 0.154657

Thermal correction to Gibbs free Energy = 0.111286

Total energy = -2010.823460

Nuclear repulsion energy = 491.324913

Zn²⁺-8'

6	-0.742415	1.781325	0.000000
6	-1.010482	0.862620	1.194969
6	-0.561977	-0.503920	0.718797
6	-0.561977	-0.503920	-0.718797
6	-1.010482	0.862620	-1.194969
1	0.328599	2.151139	0.000000
1	-2.104429	0.781325	1.333144
1	-0.604286	1.179435	2.160864
1	-2.104429	0.781325	-1.333144
1	-0.604286	1.179435	-2.160864
1	-1.317987	2.711165	0.000000
6	-0.561977	-1.713293	-1.587555
1	-0.017418	-2.560398	-1.164437
1	-1.615763	-2.020513	-1.684659
1	-0.198424	-1.499064	-2.595220
6	-0.561977	-1.713293	1.587555
1	-1.615763	-2.020513	1.684659
1	-0.017418	-2.560398	1.164437
1	-0.198424	-1.499064	2.595220
30	1.337925	0.298110	0.000000

Zero-point correction = 0.175442

Thermal correction to Energy = 0.184603

Thermal correction to Enthalpy = 0.185547

Thermal correction to Gibbs free Energy = 0.141352

Total energy = -2050.048722

Nuclear repulsion energy = 616.225945

Zn²⁺-9'

6	1.160862	1.424441	0.782136
6	1.160862	1.424441	-0.782136

6	1.160862	0.005359	-1.377155
6	0.146810	-0.904873	-0.714730
6	0.146810	-0.904873	0.714730
6	1.160862	0.005359	1.377155
1	2.017662	1.990913	1.159883
1	0.314096	2.006200	-1.227101
1	1.000722	0.042608	-2.458325
1	2.148909	-0.458084	1.222751
1	0.314096	2.006200	1.227101
1	2.017662	1.990913	-1.159883
1	2.148909	-0.458084	-1.222751
1	1.000722	0.042608	2.458325
6	-0.494835	-1.979218	-1.534408
1	0.264581	-2.767927	-1.656292
1	-1.368328	-2.439572	-1.071035
1	-0.751983	-1.627803	-2.536105
6	-0.494835	-1.979218	1.534408
1	-0.751983	-1.627803	2.536105
1	-1.368328	-2.439572	1.071035
1	0.264581	-2.767927	1.656292
30	-1.031191	0.798627	0.000000

Zero-point correction = 0.205172

Thermal correction to Energy = 0.215660

Thermal correction to Enthalpy = 0.216604

Thermal correction to Gibbs free Energy = 0.169271

Total energy = -2089.222871

Nuclear repulsion energy = 746.877223

Zn²⁺-10'

6	-0.035350	-1.093960	0.709108
6	-0.035350	-1.093960	-0.709108
6	0.982990	-0.277749	-1.503871
6	0.982990	-0.277749	1.503871
6	0.982990	1.250557	-1.293366
6	0.982990	1.250557	1.293366
6	1.605430	1.773468	0.000000
1	1.987306	-0.659311	-1.265770
1	0.816982	-0.482010	2.564740
1	1.485727	1.726263	-2.143927
1	-0.066382	1.669451	1.455822
1	2.666288	1.498709	0.000000
1	1.576948	2.868739	0.000000
1	1.485727	1.726263	2.143927
1	1.987306	-0.659311	1.265770
1	-0.066382	1.669451	-1.455822
1	0.816982	-0.482010	-2.564740
6	-0.798851	-2.111052	1.510777
1	-0.101965	-2.940202	1.706164
1	-1.100732	-1.714845	2.483012
1	-1.670100	-2.528503	1.007904
6	-0.798851	-2.111052	-1.510777
1	-0.101965	-2.940202	-1.706164
1	-1.670100	-2.528503	-1.007904

1 -1.100732 -1.714845 -2.483012
30 -1.005295 0.721217 0.000000

Zero-point correction = 0.234432

Thermal correction to Energy = 0.245799

Thermal correction to Enthalpy = 0.246743

Thermal correction to Gibbs free Energy =
0.197582

Total energy = -2128.3999912

Nuclear repulsion energy = 875.2808978352

Zn²⁺-11'

6 1.275039 -0.644385 0.399395
6 1.107871 0.758979 0.458839
6 -2.227725 -0.714992 0.487587
6 -0.048406 1.358526 1.251026
6 -2.082959 0.629675 -0.262170
6 -1.294277 1.771925 0.436758
1 -0.350217 0.681533 2.053865
1 -2.402747 -0.493852 1.546152
1 -3.083824 1.032416 -0.468721
1 -3.140880 -1.195849 0.123009
1 0.338748 2.261839 1.735169
1 -1.857479 0.471594 -1.385890
1 -1.994755 2.230583 1.141657
1 -1.049261 2.562828 -0.284998
6 0.266429 -1.593386 1.064488
1 0.106452 -1.298536 2.108511
1 0.738203 -2.579442 1.094372
6 -1.106215 -1.776641 0.360727
1 -0.948391 -2.047000 -0.719210
1 -1.530717 -2.713013 0.740585
6 2.560364 -1.286424 -0.050694
1 3.125331 -1.513731 0.865234
1 2.386457 -2.239208 -0.557531
1 3.188842 -0.653138 -0.675757
6 2.167496 1.730984 0.009238
1 2.832229 1.897194 0.868831
1 2.784586 1.384343 -0.820426
1 1.732060 2.698885 -0.251292
30 -0.152678 -0.063100 -1.068158

Zero-point correction = 0.264349

Thermal correction to Energy = 0.276638

Thermal correction to Enthalpy = 0.277582

Thermal correction to Gibbs free Energy =
0.226814

Total energy = -2167.575609

Nuclear repulsion energy = 1022.032158

Table S15. The complexation energies (in kcal/mol) of Li⁺, Na⁺ and K⁺ ion complexes of alkenes in various levels of theories.

A	Li ⁺ -A				Na ⁺ -A				K ⁺ -A			
	P	Q	R	S	P	Q	R	S	P	Q	R	S
1	-22.97	-24.30	-20.87	-20.70	-15.70	-16.80	-12.96	-12.97	-9.17	-10.49	-7.21	-8.81
2	-25.41	-27.08	-23.73	-23.53	-17.16	-18.60	-14.84	-14.87	-9.87	-11.71	-8.43	-10.55
3	-27.72	-29.40	-26.42	-26.00	-18.53	-20.03	-16.58	-16.51	-10.51	-12.68	-9.52	-12.06
3'	-26.49	-29.14	-25.32	-25.74	-17.76	-19.96	-15.86	-16.39	-9.79	-12.77	-8.91	-12.21
3''	-26.03	-28.53	-24.94	-25.31	-17.36	-19.40	-15.55	-16.02	-9.81	-12.42	-8.96	-11.90
4	-26.84	-30.62	-26.60	-27.90	-18.10	-20.61	-16.69	-17.42	-9.89	-13.38	-9.54	-13.43
5	-27.65	-32.55	-28.29	-30.30	-18.10	-21.31	-17.17	-18.34	-9.97	-14.22	-10.11	-14.77
6	-19.97	-22.82	-19.72	-20.74	-12.94	-14.07	-11.33	-11.22	-6.98	-9.07	-6.31	-8.67
7	-23.45	-26.39	-22.87	-23.66	-16.04	-17.76	-14.22	-14.50	-8.57	-11.35	-7.73	-10.88
8	-26.75	-30.10	-25.65	-26.40	-18.16	-20.72	-16.26	-16.91	-10.24	-13.29	-9.37	-12.84
9	-29.09	-33.31	-28.38	-29.21	-19.57	-22.44	-17.72	-18.03	-11.00	-14.30	-10.11	-13.68
10	-30.58	-34.74	-30.13	-30.39	-20.71	-23.39	-18.85	-18.67	-11.72	-14.79	-10.77	-13.91
11	-29.65	-34.16	-29.85	-29.65	-18.79	-21.37	-17.32	-16.98	-9.82	-12.93	-9.28	-12.45
6'	-25.24	-28.41	-26.03	-26.79	-15.66	-18.18	-14.99	-15.79	-8.70	-12.19	-8.90	-12.78
7'	-26.82	-30.92	-27.43	-28.99	-16.89	-19.76	-16.02	-17.05	-9.21	-13.27	-9.38	-13.87
8'	-28.69	-33.07	-28.76	-30.07	-18.79	-22.27	-17.88	-19.05	-10.30	-14.56	-10.44	-15.19
9'	-30.77	-35.92	-31.20	-32.37	-19.96	-23.66	-19.14	-19.80	-10.83	-15.57	-10.98	-15.98
10'	-31.44	-36.65	-32.22	-32.82	-20.22	-23.69	-19.42	-19.70	-11.02	-15.81	-11.11	-16.06
11'	-31.25	-36.66	-32.43	-32.58	-19.47	-22.73	-18.87	-18.84	-10.23	-14.67	-10.54	-15.06

P, Q, R and **S** are the calculated complexation energies at HF/6-31G*, MP2/6-31G*, HF/6-311++G** and MP2/6-311++G** level of theories respectively.

Table S16. The complexation energies (kcal/mol) of Mg²⁺ and Ca²⁺ ion alkene complexes in various level of theories.

A	Mg ²⁺ -A				Ca ²⁺ -A			
	P	Q	R	S	P	Q	R	S
1	-74.94	-75.31	-72.27	-69.89	-37.24	-38.85	-36.74	-38.47
2	-89.16	-88.85	-87.19	-83.29	-44.00	-45.75	-45.11	-46.85
3	-100.54	-100.11	-99.11	-94.53	-50.40	-51.83	-52.81	-54.22
3'	-91.00	-95.01	-89.77	-89.64	-45.53	-52.31	-49.78	-56.51
3''	-89.80	-93.45	-88.63	-88.33	-45.16	-49.68	-47.74	-52.13
4	-99.61	-102.79	-99.01	-97.67	-49.33	-56.69	-54.93	-62.28
5	-101.59	-108.19	-101.64	-103.17	-52.94	-61.49	-59.67	-68.15
6	-105.22	-93.65	-103.03	-87.52	-38.28	-41.14	-41.21	-44.22
7	-82.51	-87.63	-81.39	-82.55	-43.32	-48.70	-46.93	-52.37
8	-95.96	-102.50	-95.07	-96.79	-49.42	-55.67	-52.84	-58.97
9	-106.03	-114.22	-105.87	-107.83	-55.48	-62.62	-59.54	-66.23
10	-113.61	-123.71	-114.16	-116.60	-59.40	-66.50	-63.67	-69.95
11	-117.81	-128.57	-118.79	-120.93	-58.04	-66.35	-64.06	-71.41
6'	-108.57	-104.51	-108.12	-99.62	-47.52	-53.80	-53.77	-60.28
7'	-96.18	-104.36	-96.65	-100.00	-51.19	-58.99	-57.91	-65.92
8'	-107.46	-116.77	-108.09	-111.65	-55.41	-63.85	-61.67	-69.97
9'	-116.22	-126.75	-117.52	-120.85	-60.43	-69.87	-67.06	-75.71
10'	-122.33	-134.21	-124.27	-127.60	-62.82	-72.17	-69.94	-78.25
11'	-126.27	-138.62	-128.52	-131.38	-64.67	-74.29	-72.93	-81.84

P, Q, R and **S** are the calculated complexation energies at HF/6-31G*, MP2/6-31G*, HF/6-311++G** and MP2/6-311++G** level of theories respectively.

Table S17. The complexation energies (in kcal/mol) of Cu⁺, Zn²⁺ ion alkene complexes in various levels of theories

A	Cu ⁺ -A				Zn ²⁺ -A			
	P	Q	R	S	P	Q	R	S
1	-34.02	-79.07	-1.68	-38.49	-99.29	-111.25	-97.26	-110.58
2	-37.34	-83.85	-4.53	-42.13	-120.09	-131.98	-118.15	-131.33
3	-40.10	-88.18	-6.65	-45.30	-134.53	-147.62	-132.94	-146.99
3'	-39.93	-88.73	-6.54	-45.80	-121.35	-140.47	-119.68	-139.12
3''	-39.58	-87.99	-6.17	-45.01	-120.06	-139.01	-118.33	-137.60
4	-41.81	-92.56	-7.64	-48.24	-135.46	-153.10	-134.23	-152.37
5	-43.46	-97.09	-8.28	-51.01	-136.87	-161.63	-135.42	-159.61
6	-31.86	-83.00	4.28	-36.00	-139.86	-143.58	-137.04	-141.48
7	-37.99	-86.75	-3.46	-42.11	-114.65	-132.18	-111.73	-129.38
8	-42.62	-92.79	-7.39	-46.97	-124.96	-148.41	-121.59	-144.28
9	-46.62	-96.61	-9.66	-48.06	-132.74	-158.83	-128.92	-152.91
10	-48.62	-99.07	-11.86	-50.50	-141.43	-169.31	-139.52	-165.14
11	-46.61	-106.88	-5.19	-52.09	-145.90	-177.81	-143.84	-172.96
6'	-37.72	-93.18	-0.93	-44.84	-146.97	-161.06	-145.27	-159.57
7'	-41.31	-94.64	-5.84	-48.31	-131.83	-156.59	-129.51	-153.76
8'	-45.45	-100.11	-9.21	-52.34	-141.25	-169.97	-138.66	-166.09
9'	-49.11	-103.63	-11.00	-52.83	-147.50	-178.13	-144.29	-172.13
10'	-49.84	-104.36	-12.06	-53.81	-153.49	-185.09	-152.02	-180.59
11'	-48.55	-112.02	-6.33	-55.52	-157.39	-192.75	-155.45	-187.08

P, Q, R and **S** are the calculated complexation energies at HF/6-31G*, MP2/6-31G*, HF/6-311++G** and MP2/6-311++G** level of theories respectively.

Table S18. Comparison of complexation energies of metal ion complexes at MP2/6-311++G**, MP2(FULL)/6-311++G** and B3LYP/6-311++G** level of theories.

Str.No	^a Li ⁺ -A	^b Li ⁺ -A	^c Li ⁺ -A	^a Cu ⁺ -A	^b Cu ⁺ -A	^d Cu ⁺ -A
1	-19.41	-19.67	-25.52	-34.07	-35.53	-31.51
2	-22.17	-22.47	-29.10	-37.51	-38.98	-35.15
3	-24.53	-24.87	-32.07	-40.29	-41.77	-38.26
3'	-24.19	-24.53	-31.87	-40.87	-42.38	-38.20
3''	-23.78	-24.12	-31.65	-40.17	-41.65	-37.43
4	-26.02	-26.49	-36.52	-42.98	-44.50	-40.27
5	-28.05	-28.64	-40.76	-45.40	-46.97	-42.42
6	-19.62	-19.97	-26.49	-32.04	-33.57	-29.65
7	-21.96	-22.47	-33.84	-37.40	-38.91	-34.86
8	-24.69	-25.14	-35.45	-41.92	-43.44	-39.44
9	-27.07	-27.67	-42.01	-42.57	-43.93	-44.61
10	-28.35	-28.94	-44.25	-44.93	-46.22	-41.99
11	-27.37	-28.08	-44.46	-45.11	-46.33	-40.75
6'	-25.44	-25.93	-35.59	-40.22	-41.85	-37.41
7'	-26.98	-27.61	-39.69	-42.91	-44.49	-39.90
8'	-28.06	-28.59	-40.69	-46.50	-48.08	-43.72
9'	-29.92	-30.68	-46.14	-46.51	-48.05	-43.98
10'	-30.47	-31.20	-48.36	-47.63	-48.97	-44.23
11'	-29.97	-30.81	-47.91	-47.72	-48.95	-44.67

^aComplexation energies were calculated at MP2/6-311++G**//MP2/6-31G* level of theory.

^bComplexation energies were calculated at MP2(FULL)/6-311++G**//MP2/6-31G* level of theory.

^cComplexation energies were calculated at B3LYP-D/6-311++G**//MP2/6-31G* level of theory.

^dComplexation energies were calculated at MP2/gen//MP2/6-31G* level of theory. In the calculation 6-311++G** basis set was used for C and H, and LANL2DZ used as a basis set and ECP for Cu⁺ in the complex.

Table S19. The MP2/6-311++G** HOMO-LUMO energy gap (in eV) values of metal ion complexes

Str. No	A	Li ⁺ -A	Na ⁺ -A	K ⁺ -A	Mg ²⁺ -A	Ca ²⁺ -A	Cu ⁺ -A	Zn ²⁺ -A
M-1	11.15	11.65	10.97	10.72	10.49	10.17	12.01	11.36
M-2	10.49	11.01	10.36	10.19	9.73	9.44	11.32	10.72
M-3	10.13	10.62	9.96	9.83	9.59	9.11	10.88	10.68
M-3'	10.00	10.42	9.80	9.78	8.85	9.33	10.74	9.53
M-3''	10.03	10.44	9.83	9.77	8.81	8.99	10.71	9.47
M-4	9.70	10.15	9.44	9.45	8.56	8.85	10.31	9.48
M-5	9.44	9.71	9.14	9.16	8.08	8.23	9.90	8.86
M-6	10.52	10.65	10.11	10.24	9.61	9.53	11.07	9.88
M-7	10.31	10.97	9.98	10.04	9.55	9.63	10.93	10.00
M-8	10.00	10.51	9.81	9.67	9.35	9.18	10.78	9.85
M-9	10.03	10.74	9.96	9.72	9.74	9.38	10.85	10.09
M-10	9.95	10.82	9.95	9.67	10.23	9.46	10.94	10.38
M-11	9.92	11.01	9.81	9.54	10.54	9.73	11.48	10.95
M-6'	9.58	10.28	9.45	9.43	7.90	8.81	10.20	8.89
M-7'	9.50	10.04	9.22	9.30	8.36	8.52	9.98	8.97
M-8'	9.37	9.75	9.09	9.03	8.43	8.33	9.95	8.98
M-9'	9.33	9.94	9.19	9.10	8.75	8.46	10.02	9.12
M-10'	9.27	10.12	9.20	9.10	9.28	8.60	10.09	9.41
M-11'	9.30	10.31	9.25	9.10	9.64	8.77	10.70	10.03

Table S20. The π -bond orbital energies (in eV) of metal ion **A** at MP2/6-311++G** level of theory

	A	Li⁺-A	Na⁺-A	K⁺-A	Mg²⁺-A	Ca²⁺-A	Cu⁺-A	Zn²⁺-A
M-1	-10.22	-15.44	-15.04	-16.64	-20.51	-19.41	-17.44	-21.29
M-2	-9.94	-15.05	-14.46	-14.04	-19.95	-18.95	-17.16	x
M-3	-9.69	-14.73	-14.12	-13.59	-19.57	-18.56	-16.90	x
M-3'	-9.69	-14.79	-14.14	-13.64	-19.53	-18.82	-16.88	-20.17
M-3''	-9.66	-14.82	-14.16	-13.61	-19.62	-18.74	-16.90	-20.24
M-4	-9.45	-14.50	-13.90	-13.37	-19.10	-18.46	-16.66	x
M-5	-9.27	-14.26	-13.67	-13.16	-18.76	-18.15	-16.43	-19.33
M-6	-9.87	-14.50	-14.33	-13.86	-16.93	-18.92	-16.84	-18.21
M-7	-9.63	-14.67	-14.07	-13.62	-20.03	-18.80	-16.70	-20.36
M-8	-9.66	-14.60	-14.03	-13.57	-19.61	-18.59	-16.64	-20.18
M-9	-9.68	-14.45	-13.92	-13.52	-19.33	-18.35	-16.56	-19.94
M-10	-9.66	-14.53	-13.90	-13.45	-19.44	-18.29	-16.68	-19.95
M-11	-9.63	-14.56	-13.83	-13.35	-19.37	-18.17	-16.65	-20.03
M-6'	-9.32	-14.43	-13.78	-13.30	-16.42	-18.55	-16.21	-16.78
M-7'	-9.13	-14.08	-13.56	-13.08	-19.21	-18.14	-16.15	-19.39
M-8'	-9.18	-14.10	-13.52	-13.05	-18.79	-17.99	-16.20	-19.27
M-9'	-9.21	-14.04	-13.45	-13.03	-18.62	-17.84	-16.17	-19.20
M-10'	-9.24	-14.20	-13.53	-13.00	-18.84	-17.84	-16.33	-19.40
M-11'	-9.23	-14.18	-13.42	-12.85	-18.88	-17.81	-16.25	-19.63

x – C=C bond was not observed.

Table S21. The MP2/6-311++G** natural bond orbital occupation number of π -bond in complex.

	A	Li⁺-A	Na⁺-A	K⁺-A	Mg²⁺-A	Ca²⁺-A	Cu⁺-A	Zn²⁺-A
M-1	1.9993	1.9642	1.9762	1.9896	1.7933	1.9201	1.8584	1.6482
M-2	1.9820	1.9565	1.9654	1.9759	1.7886	1.9131	1.8500	-
M-3	1.9631	1.9483	1.9539	1.9621	1.7751	1.9054	1.8447	-
M-3'	1.9661	1.9472	1.9534	1.9629	1.7489	1.9204	1.8356	1.5863
M-3''	1.9631	1.9473	1.9536	1.9614	1.7560	1.9065	1.8366	1.5886
M-4	1.9455	1.9332	1.9409	1.9467	1.7368	1.9097	1.8259	-
M-5	1.9281	1.9220	1.9271	1.9323	1.7080	1.8983	1.8085	1.5295
M-6	1.9288	1.9312	1.9194	1.9203	1.5823	1.8847	1.8005	1.6393
M-7	1.9472	1.9174	1.9374	1.9419	1.8350	1.8905	1.8250	1.5943
M-8	1.9569	1.9335	1.9431	1.9526	1.7979	1.9002	1.8344	1.6550
M-9	1.9633	1.9327	1.9465	1.9571	1.8137	1.8993	1.8542	1.6921
M-10	1.9696	1.9393	1.9531	1.9631	1.8387	1.9056	1.8718	1.7365
M-11	1.9674	1.9398	1.9591	1.9658	1.8426	1.9111	1.8674	1.7493
M-6'	1.8991	1.8790	1.8919	1.8959	1.5940	1.8459	1.7751	1.5333
M-7'	1.9124	1.8952	1.9114	1.9139	1.8050	1.8701	1.7985	1.5340
M-8'	1.9204	1.9124	1.9175	1.9234	1.7629	1.8805	1.8074	1.5921
M-9'	1.9308	1.9168	1.9258	1.9316	1.7873	1.8834	1.8295	1.6414
M-10'	1.9363	1.9260	1.9348	1.9381	1.8233	1.8989	1.8549	1.7097
M-11'	1.9328	1.9266	1.9344	1.9360	1.8360	1.9115	1.8585	1.7360

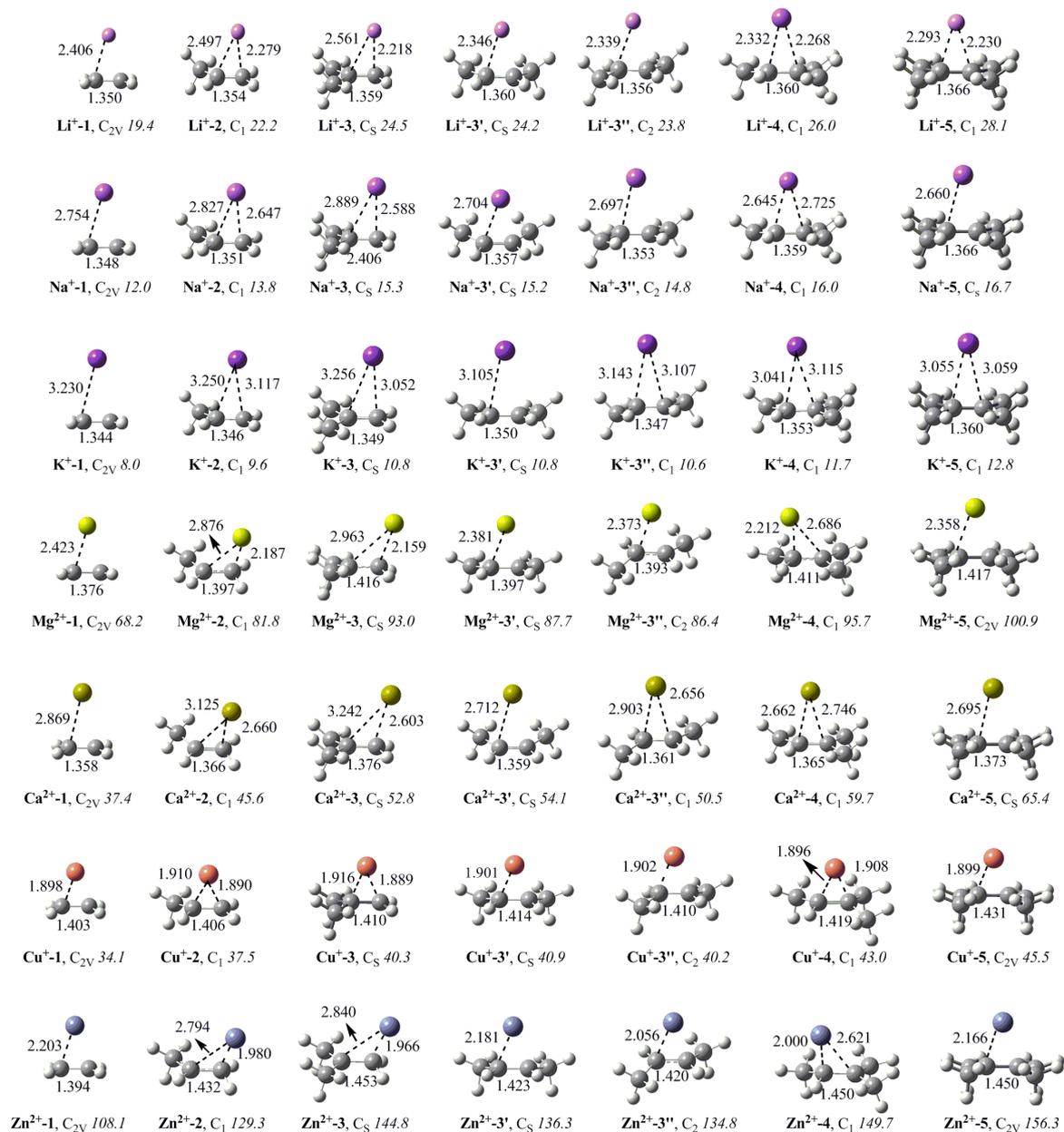


Fig. S1 The MP2/6-31G* structure and geometries (Å) of the various metal ion complexes of ethylene and methyl substituted ethylene. Along with structure name point group and complexation energy (in kcal/mol) are also given.

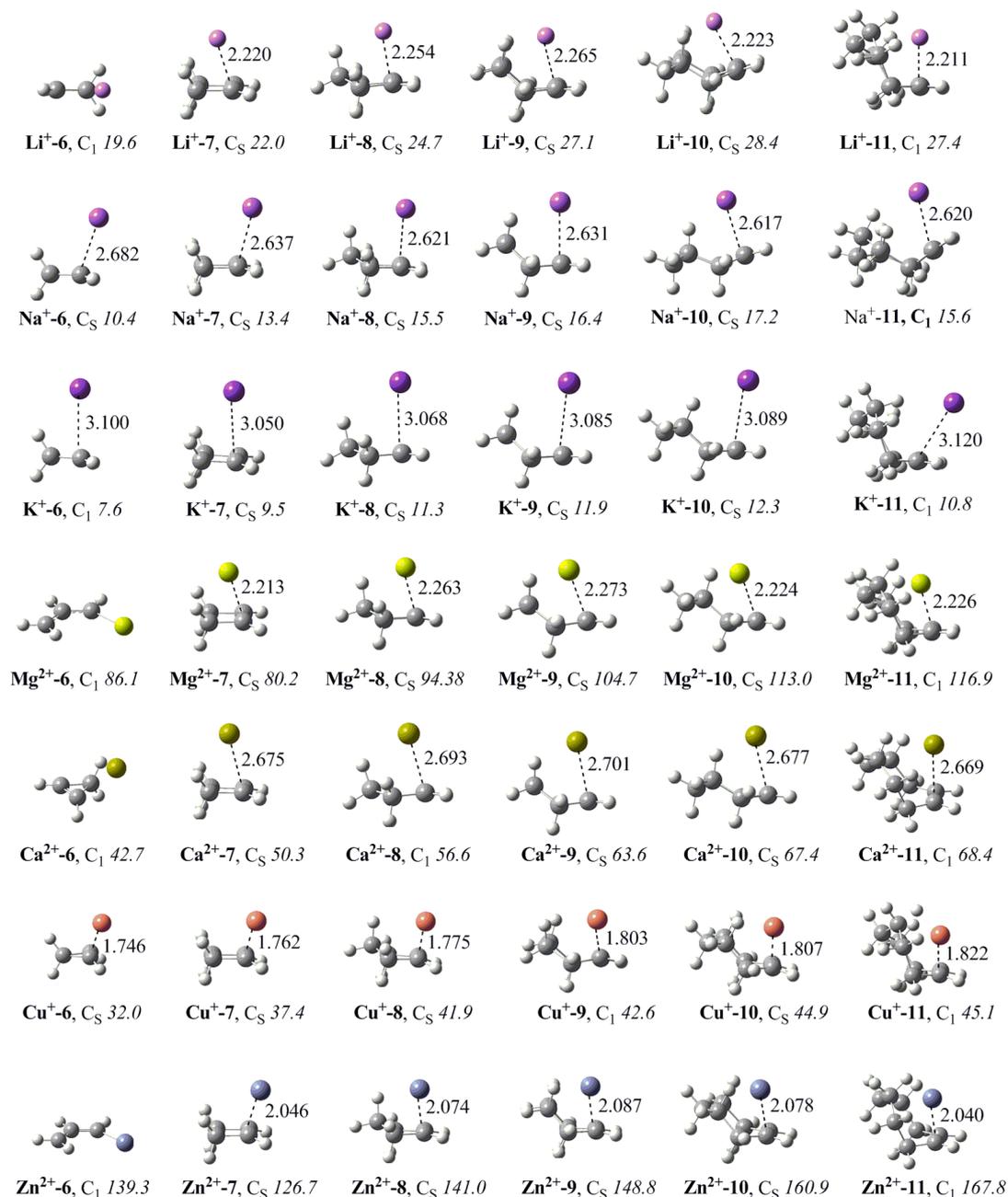


Fig. S2 The MP2/6-31G* structure and geometries (Å) of the various metal ion complexes of cycloalkenes. Along with structure name point group and complexation energy (in kcal/mol) are also given.

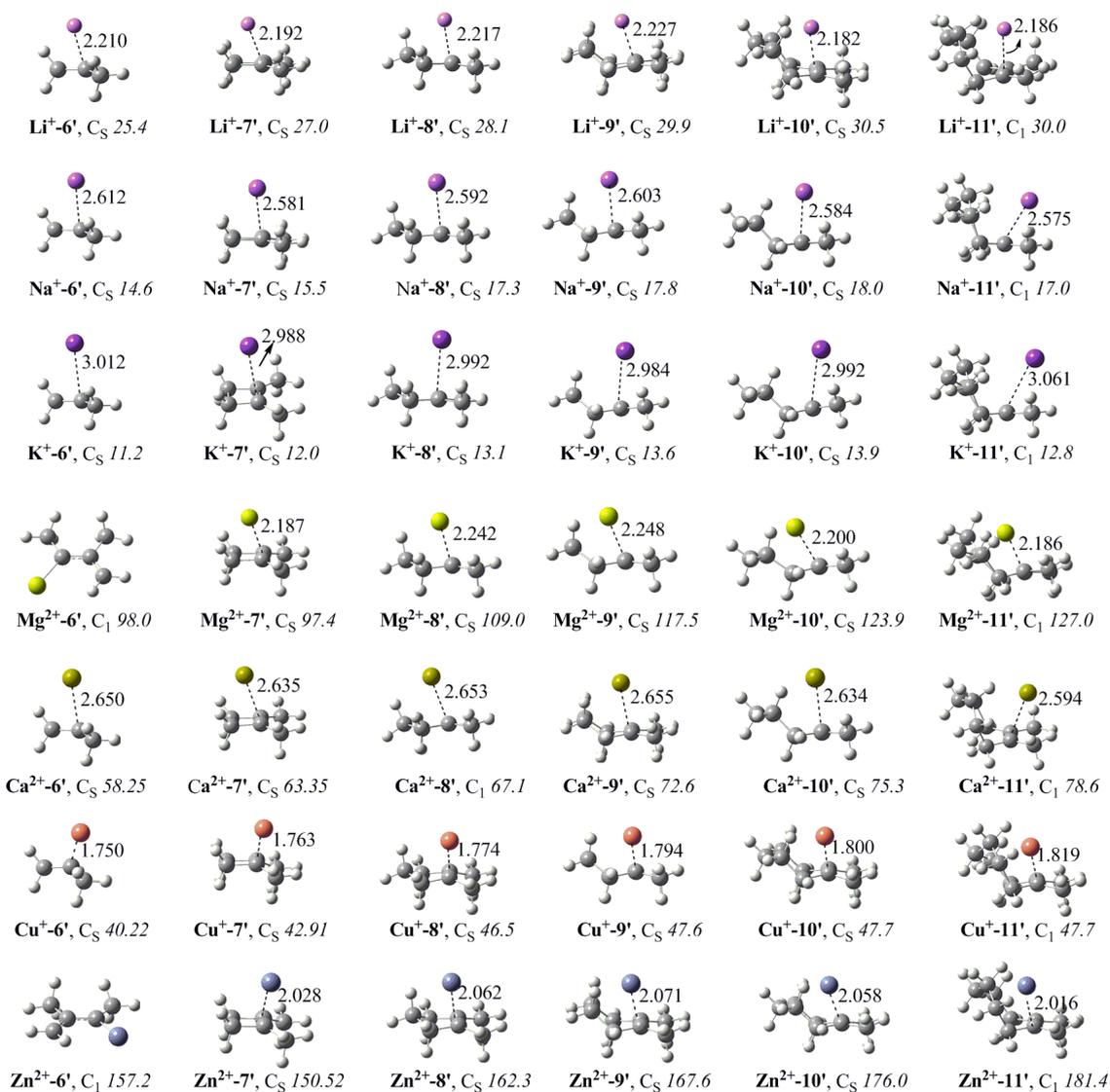


Fig. S3 The MP2/6-31G* structure and geometries (Å) of various metal ion complexes of methylsubstituted analogues of cycloalkenes. Along with structure name point group and complexation energy (in kcal/mol) are also given.

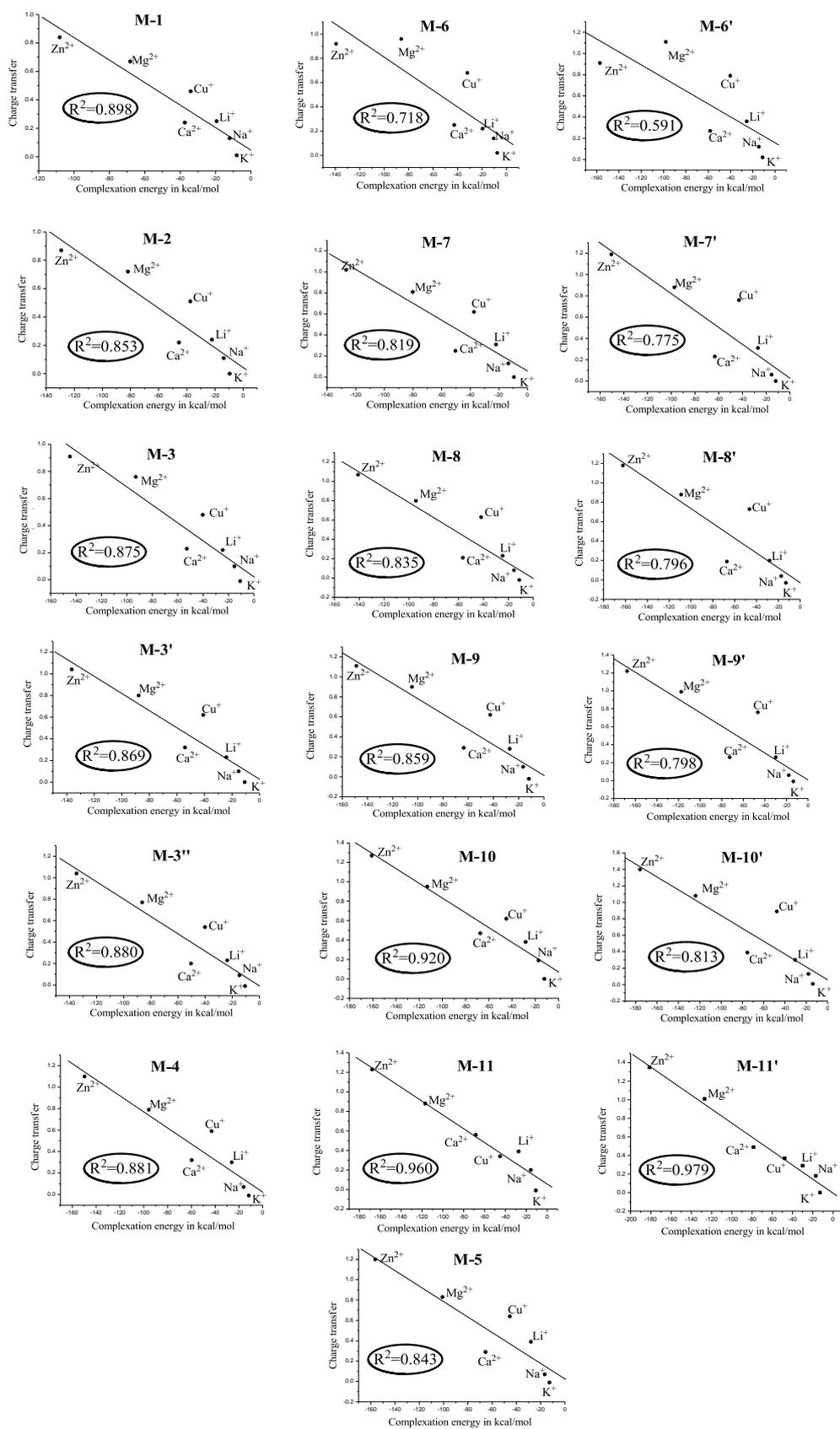


Fig. S4 Correlation graphs of charge transfer (in amu) and the complexation energy (in kcal/mol) of the various metal ion alkene complexes.

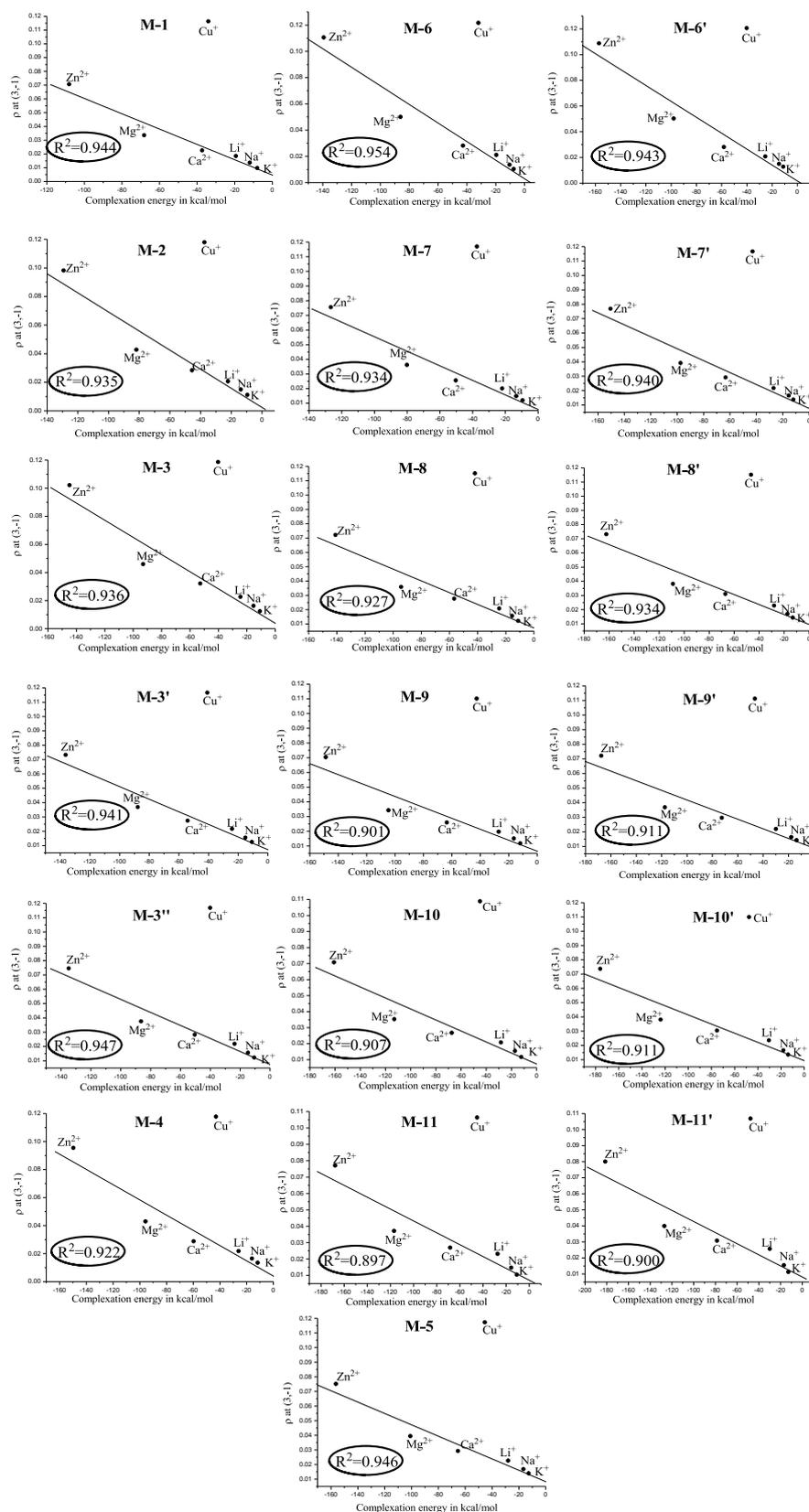


Fig. S5 Correlation graphs of electron density (in au) at (3,-1) intermolecular bond critical point and the complexation energy (in kcal/mol) of the various metal ion alkene complexes.

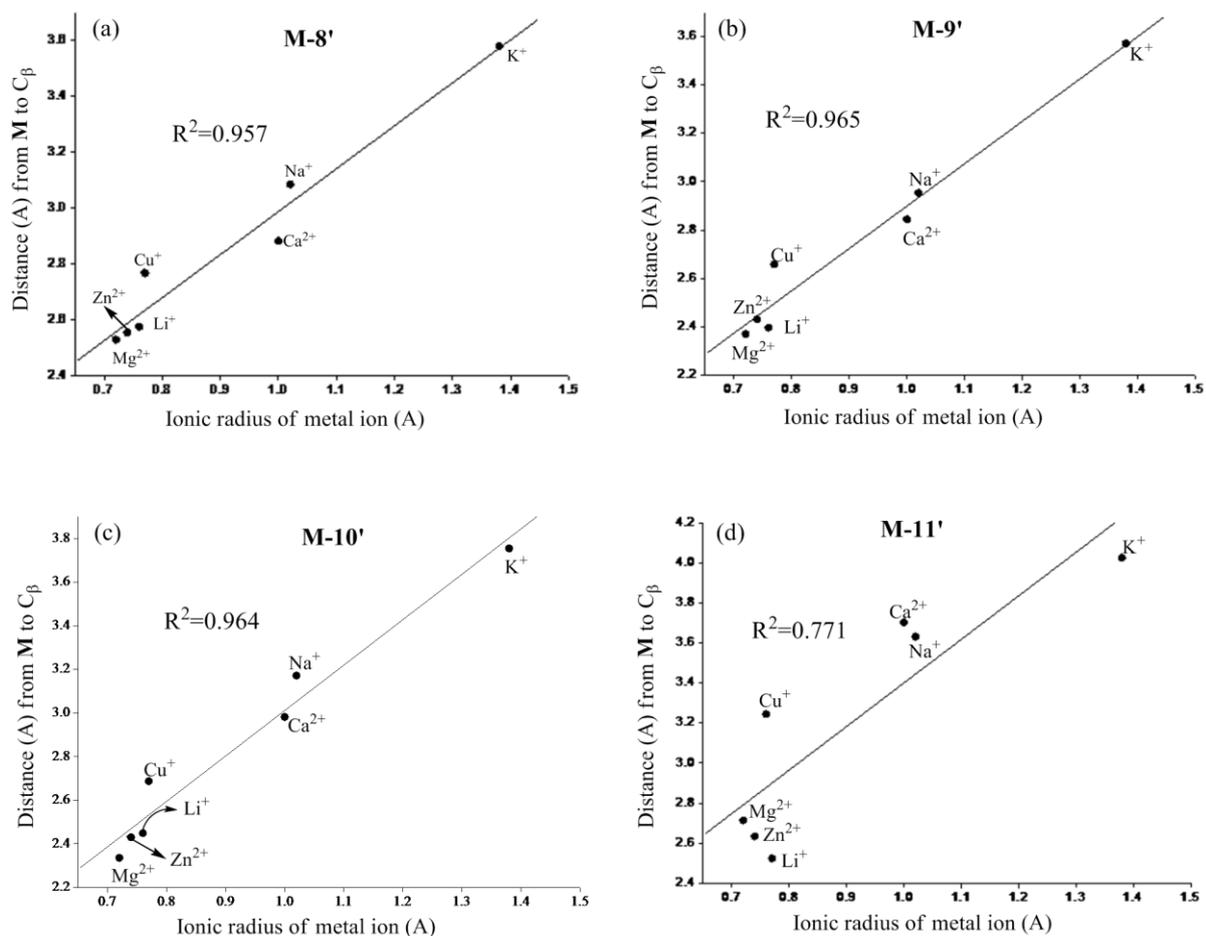


Fig. S6 Effective Ionic radius of metal ion versus M-C_β distance of metal ion dimethyl substituted alkenes (8'-11').