

## Exploring the size dependence of cyclic and acyclic $\pi$ -systems on cation $-\pi$ binding ‡

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### **Supporting Information**

(22 pages including this page)

**Table S1:** The MP2(FULL) interaction energy (IE) and the charges on the metal ions of the various acyclic conjugated  $\pi$  systems with  $\text{Li}^+$  and  $\text{Mg}^{2+}$  cations calculated in conjugation with 6-31G\* basis sets.

**Table S2:** The MP2(FULL) interaction energy (IE) and the charges on the metal ions of the various cyclic conjugated  $\pi$  systems with  $\text{Li}^+$  and  $\text{Mg}^{2+}$  cations calculated in conjugation with 6-31G\* basis sets.

**Table S3:** The MP2(FULL)/6-31G\* optimized cartesian coordinates of the acyclic  $\text{Li}^+$  complexes considered in the study.

**Table S4:** The MP2(FULL)/6-31G\* optimized cartesian coordinates of the cyclic  $\text{Li}^+$  complexes considered in the study.

**Table S5:** The MP2(FULL)/6-31G\* optimized cartesian coordinates of the acyclic  $\text{Mg}^{2+}$  complexes considered in the study.

**Table S6:** The MP2(FULL)/6-31G\* optimized cartesian coordinates of the cyclic  $\text{Mg}^{2+}$  complexes considered in the study.

**Table S7:** The total energy of the  $\text{Li}^+$  and  $\text{Mg}^{2+}$  complexes of the acyclic systems at the MP2(FULL)/6-311++G\*\* level.

**Table S8:** The total energy of the  $\text{Li}^+$  and  $\text{Mg}^{2+}$  complexes of the cyclic systems at the MP2(FULL)/6-311++G\*\* level.

**Table S9:** The MP2(FULL)/cc-pVDZ //MP2(FULL)/6-31G\* charges (in au) on the  $\text{Li}^+$  and  $\text{Mg}^{2+}$  ions in the various acyclic complexes considered in the study.

**Table S10:** The MP2(FULL)/cc-pVDZ //MP2(FULL)/6-31G\* charges (in au) on the  $\text{Li}^+$  and  $\text{Mg}^{2+}$  ions in the various cyclic complexes considered in the study.

**Table S1:** The MP2(FULL) interaction energy (IE) and the charges on the metal ions of the various acyclic conjugated  $\pi$  systems with  $\text{Li}^+$  and  $\text{Mg}^{2+}$  cations calculated in conjugation with 6-31G\* basis sets.

$\pi$ -system	IE(kcal/mol)		Charges (amu)	
	$\text{Li}^+$	$\text{Mg}^{2+}$	$\text{Li}^+$	$\text{Mg}^{2+}$
<b>1</b>	-21.12	-71.73	0.728	1.369
<b>2</b>	-28.56	-95.58	0.623	1.162
<b>3a</b>	-28.74	-103.00	0.664	1.199
<b>3b</b>	-31.54	-111.54	0.609	1.134
<b>4a</b>	-33.59	-120.24	0.604	1.126
<b>4b</b>	-33.83	-126.87	0.596	1.072
<b>5</b>	-28.91	-96.00	0.590	1.137
<b>6</b>	-31.94	-110.41	0.589	1.128
<b>7a</b>	-33.19	-117.36	0.580	1.087
<b>7b</b>	-33.17	-123.88	0.573	1.077
<b>8a</b>	-31.30	-109.31	0.613	1.145
<b>9a</b>	-33.51	-119.12	0.606	1.126
<b>9b</b>	-33.52	-125.14	0.599	1.075
<b>10a</b>	-33.43	-117.83	0.608	1.135
<b>8b</b>	-32.30	-112.49	0.584	1.124
<b>9c</b>	-34.83	-128.16	0.570	1.077

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<b>10b</b>	-34.52	-126.50	0.573	1.079
<b>11</b>	-38.80	-129.06	0.505	1.016
<b>12a</b>	-39.96	-140.04	0.490	0.934
<b>13</b>	-41.90	-132.08	0.464	1.119
<b>12b</b>	-33.23	-118.50	0.602	1.100
<b>14</b>	-49.03	-153.33	0.374	0.710

**Table S2:** The MP2(FULL) interaction energy (IE) and the charges on the metal ions of the various cyclic conjugated  $\pi$  systems with  $\text{Li}^+$  and  $\text{Mg}^{2+}$  cations calculated in conjugation with 6-31G\* basis sets.

$\pi$ -system	IE(kcal/mol)		Charges (amu)	
	$\text{Li}^+$	$\text{Mg}^{2+}$	$\text{Li}^+$	$\text{Mg}^{2+}$
<b>15</b>	-30.03	-95.24	0.611	1.207
<b>16</b>	-37.46	-114.20	0.487	0.971
<b>17</b>	-23.62	-113.19	0.551	0.905
<b>18</b>	-40.25	-130.30	0.507	0.953
<b>19a</b>	-42.52	-142.26	0.506	0.933
<b>19b</b>	-42.01	-141.20	0.525	0.946
<b>20a</b>	-42.76	-139.98	0.500	0.922
<b>20b</b>	-41.82	-141.99	0.541	0.965
<b>21a</b>	-44.14	-150.52	0.504	0.919
<b>21b</b>	-43.81	-150.63	0.524	0.930

**Table S3:** The MP2(FULL)/6-31G\* optimized cartesian coordinates of the acyclic Li<sup>+</sup> complexes considered in the study.

<b>1</b>				<b>3</b>			
6	0.000000	0.674449	-0.353735	1	-0.614947	-3.959242	0.033041
1	-0.927274	1.241674	-0.401175	3	0.000000	0.000000	1.942528
1	0.927274	1.241674	-0.401175	<hr/>			
6	0.000000	-0.674449	-0.353735	<b>3b</b>			
1	0.927274	-1.241674	-0.401175	6	2.986287	-0.125480	-0.126830
1	-0.927274	-1.241674	-0.401175	1	3.893725	0.468766	-0.112079
3	0.000000	0.000000	1.949839	1	3.108121	-1.208321	-0.129579
<hr/>				6	1.766956	0.452836	-0.245785
<b>2</b>				1	1.696651	1.541069	-0.302278
6	0.000000	1.846576	-0.090687	3	1.324563	-0.216791	1.831642
1	-0.681246	2.691025	-0.085936	6	0.514151	-0.301460	-0.262851
1	1.061661	2.071043	0.000796	1	0.572553	-1.375407	-0.462743
6	-0.444696	0.585464	-0.286512	6	-0.705708	0.277977	-0.077506
1	-1.511433	0.405206	-0.433832	1	-0.756295	1.361745	0.061347
6	0.444696	-0.585464	-0.286512	6	-1.965169	-0.432658	-0.103474
1	1.511433	-0.405206	-0.433832	1	-1.941513	-1.505658	-0.285263
6	0.000000	-1.846576	-0.090687	6	-3.141588	0.200513	0.063199
1	0.681246	-2.691025	-0.085936	1	-3.193085	1.272899	0.230435
1	-1.061661	-2.071043	0.000796	1	-4.083424	-0.335095	0.024712
3	0.000000	0.000000	1.854776	<hr/>			
<hr/>				<b>4a</b>			
<b>3a</b>				6	-0.508567	-1.794555	-0.090662
6	0.000000	3.067020	-0.003477	1	-1.595171	-1.676956	-0.032503
1	-1.075252	3.207859	0.073016	6	0.266548	-0.677490	-0.220402
1	0.614947	3.959242	0.033041	1	1.348063	-0.794786	-0.336891
6	0.544261	1.845420	-0.175911	6	-0.266548	0.677490	-0.220402
1	1.623827	1.742980	-0.289058	1	-1.348063	0.794786	-0.336891
6	-0.257836	0.632050	-0.231734	6	0.508567	1.794555	-0.090662
1	-1.345643	0.757045	-0.264056	1	1.595171	1.676956	-0.032503
6	0.257836	-0.632050	-0.231734	6	0.000000	3.149142	-0.090731
1	1.345643	-0.757045	-0.264056	1	-1.074831	3.286956	-0.197771
6	-0.544261	-1.845420	-0.175911	6	0.810321	4.219551	0.011684
1	-1.623827	-1.742980	-0.289058	1	1.887876	4.112724	0.101982
6	0.000000	-3.067020	-0.003477	1	0.418119	5.230073	-0.005934
1	1.075252	-3.207859	0.073016	6	0.000000	-3.149142	-0.090731
<hr/>				1	1.074831	-3.286956	-0.197771

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6	-0.810321	-4.219551	0.011684
1	-1.887876	-4.112724	0.101982
1	-0.418119	-5.230073	-0.005934
3	0.000000	0.000000	1.874522

**4b**

6	-1.706960	-0.302379	-0.231975
1	-1.769552	-1.384751	-0.380677
6	-2.951891	0.456994	-0.251233
1	-2.872185	1.542171	-0.344687
3	-2.568747	-0.186336	1.828466
6	-4.180010	-0.102230	-0.111776
1	-4.314676	-1.183392	-0.078366
6	-0.477885	0.284574	-0.098119
1	-0.432472	1.374577	-0.015403
6	0.772739	-0.413403	-0.105390
1	0.760220	-1.496436	-0.227441
6	1.961064	0.239228	0.002620
1	1.957045	1.325923	0.109595
6	3.249459	-0.407961	-0.027514
1	3.271477	-1.490366	-0.139703
6	4.402128	0.281950	0.072086
1	4.409388	1.362903	0.180906
1	-5.080530	0.502159	-0.126266
1	5.365662	-0.214419	0.044449

**5**

6	-1.530796	-0.412616	-0.283893
1	-2.611186	-0.320459	-0.262534
1	-1.140274	-1.374979	-0.618613
6	-0.739358	0.649220	-0.008888
1	-1.214651	1.593172	0.249247
6	0.741042	0.646379	0.000280
1	1.216815	1.583666	0.281149
6	1.531646	-0.412509	-0.288367
1	2.612026	-0.324766	-0.251362
1	1.141324	-1.364903	-0.649613
3	-0.006418	-0.871525	1.578980

**6**

6	-2.595810	-0.315442	-0.325620
1	-3.652722	-0.127913	-0.477950
1	-2.271844	-1.350607	-0.462788
6	-1.731186	0.699605	-0.089162
1	-2.134770	1.707254	-0.006765
6	-0.281409	0.567999	0.138758
1	0.213002	1.411619	0.620744
6	0.477554	-0.498843	-0.238591
1	0.000631	-1.329035	-0.767560
3	-1.327336	-0.766299	1.629198
6	1.922215	-0.604406	-0.052002
6	2.753620	0.452451	-0.047431
1	3.822311	0.320681	0.078123

1	2.401669	1.467167	-0.208248
1	2.333819	-1.608442	0.021136

**7a**

6	0.546896	0.023443	1.549603
1	1.541637	-0.106926	1.108543
6	-0.542453	0.135092	0.733758
1	-1.516311	0.261616	1.205763
6	-0.542453	0.135092	-0.733758
1	-1.516311	0.261616	-1.205763
6	0.546896	0.023443	-1.549603
1	1.541637	-0.106926	-1.108543
3	0.530765	1.970536	0.000000
6	0.494824	-0.002725	3.008727
6	0.494824	-0.002725	-3.008727
6	-0.542453	-0.493479	3.710125
1	-0.530689	-0.497975	4.794109
6	-0.542453	-0.493479	-3.710125
1	-0.530689	-0.497975	-4.794109
1	1.378663	0.346806	3.537709
1	-1.410333	-0.933315	3.227915
1	-1.410333	-0.933315	-3.227915
1	1.378663	0.346806	-3.537709

**7b**

6	3.655843	0.423925	0.137772
1	4.732480	0.376818	0.020185
1	3.282699	1.245100	0.756933
6	2.837482	-0.414635	-0.545399
1	3.298767	-1.175162	-1.172728
6	1.370185	-0.437235	-0.483580
1	0.880397	-1.317598	-0.896093
6	0.598898	0.587243	-0.004563
1	1.096419	1.530785	0.238992
3	2.156204	-0.567883	1.633914
6	-0.843259	0.588748	0.129117
6	-1.616317	-0.526366	0.195454
6	-3.070464	-0.521167	0.251240
1	-3.546007	-1.355680	0.761444
6	-3.837656	0.420272	-0.327946
1	-4.918951	0.384202	-0.257971
1	-3.410402	1.232037	-0.909145
1	-1.320141	1.562764	0.209423
1	-1.132144	-1.504326	0.234650

**8a**

6	0.703197	-0.709776	-0.259843
1	0.492921	-1.676347	-0.725720
6	-0.335440	0.147662	-0.058140
1	-0.145819	1.117650	0.410632
6	-1.712629	-0.158916	-0.446103
1	-1.870264	-1.010393	-1.110871

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6	-2.783803	0.534389	0.007964
1	-3.793318	0.274736	-0.292499
1	-2.668371	1.427923	0.620856
3	-1.364479	-0.886990	1.640685
6	2.097053	-0.426122	0.064214
6	2.633136	0.806323	0.013733
1	3.678633	0.971235	0.248511
1	2.730772	-1.278120	0.298644
1	2.059807	1.672922	-0.302561

**8b**

6	-2.441424	-0.804012	-0.162639
1	-3.493682	-1.002753	-0.331912
1	-1.813186	-1.682629	0.009236
6	-1.936353	0.448354	-0.273784
1	-2.626637	1.262895	-0.485605
6	-0.529392	0.829013	-0.073506
1	-0.329023	1.886468	0.101131
6	0.529882	-0.027665	-0.152214
1	0.360162	-1.067921	-0.445568
3	-1.211443	-0.262070	1.781028
6	1.908996	0.361852	0.049698
1	2.113257	1.401906	0.297359
6	2.922099	-0.514994	-0.085721
1	3.954232	-0.212499	0.050588
1	2.746358	-1.554543	-0.349317

**9a**

6	-1.710444	0.246590	0.030176
1	-1.609014	1.211947	0.535876
6	-0.578939	-0.420810	-0.343101
1	-0.675203	-1.355837	-0.902221
6	0.765576	0.052114	-0.042326
1	0.869861	1.077995	0.322851
6	1.884878	-0.717338	-0.175257
1	1.768289	-1.744018	-0.534915
3	-0.006636	-1.035962	1.719313
6	3.247641	-0.259889	0.076506
6	3.653778	1.009238	-0.106987
1	4.679496	1.301700	0.087153
6	-3.056899	-0.199011	-0.256133
1	-3.176639	-1.134091	-0.800916
6	-4.139747	0.514078	0.106971
1	-5.143479	0.177920	-0.127156
1	-4.049329	1.458782	0.636167
1	3.970964	-1.014141	0.378083
1	2.989901	1.777801	-0.491956

**9b**

6	-0.897097	0.046552	0.079535
1	-1.023166	1.086927	0.377182
6	0.429749	-0.432247	-0.177799

1	0.524771	-1.476417	-0.490065
6	1.565356	0.326599	-0.103966
1	1.483768	1.389489	0.143189
6	2.893476	-0.199944	-0.399695
1	2.945947	-1.182264	-0.874048
3	2.535526	-0.404567	1.774683
6	-1.983922	-0.757987	-0.051880
1	-1.819678	-1.806993	-0.304018
6	-3.364279	-0.335930	0.130264
1	-4.073339	-1.103369	0.431891
6	-3.806935	0.913339	-0.101152
1	-3.153943	1.696250	-0.475496
6	4.046585	0.437005	-0.076990
1	4.045554	1.444061	0.339917
1	5.014038	0.005762	-0.310525
1	-4.848132	1.175940	0.048019

**9c**

6	3.498752	0.996053	-0.108436
1	4.526520	1.305971	-0.259340
1	2.786575	1.798076	0.104551
6	3.118776	-0.292879	-0.296831
1	3.889934	-1.019782	-0.546344
6	1.762520	-0.826076	-0.127943
1	1.668189	-1.908399	-0.038686
6	0.618617	-0.071537	-0.147409
1	0.692497	0.998733	-0.365406
3	2.338698	0.203819	1.776162
6	-0.706336	-0.591863	0.020841
1	-0.822481	-1.660774	0.199178
6	-1.808243	0.201486	-0.068745
1	-1.675942	1.267714	-0.265289
6	-3.162991	-0.272961	0.065030
1	-3.313390	-1.334390	0.252910
6	-4.225057	0.549189	-0.041830
1	-5.240252	0.181200	0.055390
1	-4.103973	1.611724	-0.233515

**10a**

6	0.501285	1.794428	0.138034
1	1.583784	1.668455	0.234440
6	-0.270641	0.676394	0.011265
1	-1.354411	0.789051	-0.082206
6	0.270641	-0.676394	0.011265
1	1.354411	-0.789051	-0.082206
6	-0.501285	-1.794428	0.138034
1	-1.583784	-1.668455	0.234440
3	0.000000	0.000000	2.106935
6	0.000000	-3.164416	0.102010
6	0.000000	3.164416	0.102010
6	1.079645	-3.544397	-0.604483
1	1.411656	-4.576434	-0.606654

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6	-1.079645	3.544397	-0.604483
1	-1.411656	4.576434	-0.606654
1	1.635515	-2.849935	-1.227684
1	-0.577001	-3.912630	0.640742
1	0.577001	3.912630	0.640742
1	-1.635515	2.849935	-1.227684

**10b**

6	-1.567110	0.832189	0.006214
1	-1.302390	1.857978	0.263175
6	-0.559720	-0.085130	-0.134623
1	-0.798836	-1.082594	-0.516736
6	0.828314	0.182522	0.111445
1	1.106379	1.170189	0.477291
6	1.787032	-0.754635	-0.113139
1	1.469907	-1.748074	-0.435674
6	3.216760	-0.546456	0.053497
6	-2.988268	0.558772	-0.238372
6	3.826890	0.644300	-0.090691
1	4.898190	0.744599	0.041763
6	-3.574093	-0.664720	-0.250636
1	-4.634853	-0.777430	-0.443617
1	3.816832	-1.428255	0.265410
1	3.283627	1.540582	-0.375303
1	-3.004594	-1.594465	-0.166416
1	-3.626467	1.430850	-0.370436
3	-2.342210	-0.371479	1.732790

**11**

6	0.525795	1.108508	0.682827
6	-0.086443	0.193724	1.653752
6	-0.086443	-1.161398	1.663333
6	-0.086443	-1.161398	-1.663333
6	-0.086443	0.193724	-1.653752
6	0.525795	1.108508	-0.682827
1	0.949662	2.000631	1.141259
1	-0.560444	0.693895	2.501003
1	-0.574879	-1.697949	2.471584
1	-0.574879	-1.697949	-2.471584
1	-0.560444	0.693895	-2.501003
1	0.949662	2.000631	-1.141259
1	0.497615	-1.753337	-0.971426
1	0.497615	-1.753337	0.971426
3	-1.619605	-0.058830	0.000000

**12a**

6	1.132583	-1.453952	-0.267458
6	-0.253011	-1.266471	0.159399
6	-1.113640	-0.273143	-0.212737
6	1.426132	1.849636	-0.007614
6	2.316912	0.827215	0.047498
6	2.182973	-0.578055	-0.349984

1	1.391710	-2.494275	-0.462548
1	-0.667624	-2.084870	0.754526
1	1.710252	2.827487	0.369659
1	3.302547	1.067697	0.449497
1	3.132159	-1.034565	-0.623697
1	0.473626	1.787807	-0.514126
1	-0.803532	0.444832	-0.969087
3	0.828895	0.065185	1.587797
6	-2.492708	-0.197515	0.224260
6	-3.332676	0.750192	-0.232342
1	-4.368566	0.789405	0.085147
1	-2.846893	-0.950162	0.926828
1	-3.009755	1.503651	-0.945717

**12b**

6	1.261364	-1.442369	-0.131570
6	-0.115295	-1.129035	-0.489638
6	-0.889788	-0.109567	-0.019777
6	1.846457	1.691823	-0.507571
6	2.201429	0.847833	0.474389
6	2.228156	-0.612545	0.331576
1	1.535079	-2.486945	-0.265798
1	-0.577546	-1.817355	-1.203706
1	1.918149	2.766374	-0.378549
1	2.608139	1.250001	1.401683
1	3.172496	-1.085115	0.603461
1	1.510898	1.330928	-1.475248
1	-0.461900	0.621665	0.668267
6	-2.281354	0.070442	-0.424005
3	-2.218860	-1.230994	1.378033
6	-3.151602	0.872550	0.237074
1	-4.182701	0.974049	-0.084240
1	-2.827896	1.509826	1.059576
1	-2.634344	-0.505240	-1.282414

**13**

6	-1.102759	-1.558378	-0.000789
6	0.317297	-1.218782	-0.109736
6	0.980012	-0.412907	0.759292
6	-1.517055	1.738083	0.397413
6	-2.049658	0.771449	-0.385825
6	-2.119641	-0.673992	-0.112872
1	-1.353917	-2.616004	0.059187
1	0.873012	-1.675559	-0.933210
1	-1.628735	2.786790	0.128913
1	-2.577320	1.090994	-1.287732
1	-3.131082	-1.078723	-0.129349
1	-1.108258	1.518356	1.379864
1	0.486602	-0.126308	1.686763
6	2.327404	0.123327	0.516925
6	2.811120	0.394242	-0.716023
1	3.807934	0.794231	-0.864481

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1	2.931891	0.371068	1.387170
1	2.253456	0.151254	-1.625904
3	0.522034	1.268548	-0.630512

**14**

6	-2.852156	0.957042	-0.513002
6	2.069219	1.257840	0.731745
6	2.171853	0.631656	-0.465745
6	-2.042492	-0.112594	-0.358316
6	1.634375	-0.687021	-0.839986
6	-1.354559	-0.417043	0.907903
6	-0.125255	-0.986550	0.960151

1	-3.350988	1.155080	-1.456165
1	2.526536	2.231722	0.876854
1	2.726055	1.141425	-1.253450
1	-1.879145	-0.784441	-1.202399
1	-1.848853	-0.126552	1.834257
1	2.073467	-1.121539	-1.735476
1	0.328622	-1.176479	1.933146
6	0.632538	-1.388561	-0.248592
1	0.358626	-2.342837	-0.700463
1	-3.073680	1.629960	0.312909
1	1.621904	0.796206	1.606714
3	-0.094560	1.022946	-0.420288

**Table S4:** The MP2(FULL)/6-31G\* optimized cartesian coordinates of the cyclic Li<sup>+</sup> complexes.

**15**

6	-0.790363	0.677070	-0.182247
6	-0.790363	-0.677070	-0.182247
6	0.790363	-0.677070	-0.182247
6	0.790363	0.677070	-0.182247
1	-1.546657	1.439482	-0.337197
1	1.546657	1.439482	-0.337197
1	-1.546657	-1.439482	-0.337197
1	1.546657	-1.439482	-0.337197
3	0.000000	0.000000	1.907570

**16**

6	0.000000	1.404878	-0.125055
6	1.216660	0.702439	-0.125055
6	1.216660	-0.702439	-0.125055
6	0.000000	-1.404878	-0.125055
6	-1.216660	-0.702439	-0.125055
6	-1.216660	0.702439	-0.125055
1	0.000000	2.491599	-0.142048
1	2.157788	1.245800	-0.142048
1	2.157788	-1.245800	-0.142048
1	0.000000	-2.491599	-0.142048
1	-2.157788	-1.245800	-0.142048
1	-2.157788	1.245800	-0.142048
3	0.000000	0.000000	1.784756

**17**

6	-0.659730	0.256518	1.577451
6	0.696629	0.336328	1.549614
6	1.585181	-0.442669	0.671870
6	-1.508119	-0.541723	0.677436
6	1.585181	-0.442669	-0.671870
6	-1.508119	-0.541723	-0.677436
6	-0.659730	0.256518	-1.577451
1	-1.175367	0.749360	2.405520
1	1.181495	0.903245	2.346741
1	2.344005	-1.026451	1.191173

1	-2.281705	-1.124380	1.175873
1	-2.281705	-1.124380	-1.175873
1	2.344005	-1.026451	-1.191173
1	-1.175367	0.749360	-2.405520
6	0.696629	0.336328	-1.549614
1	1.181495	0.903245	-2.346741
3	-0.501464	1.898331	0.000000

**18**

6	0.012276	2.486314	0.707613
6	0.031841	1.302646	1.412409
6	0.068704	0.063100	0.721142
6	0.068704	0.063100	-0.721142
6	0.031841	1.302646	-1.412409
6	0.012276	2.486314	-0.707613
1	0.127648	-1.189379	2.496830
1	0.000573	3.431838	1.242526
1	0.041678	1.304587	2.500184
6	0.111285	-1.186999	1.408267
6	0.111285	-1.186999	-1.408267
1	0.041678	1.304587	-2.500184
1	0.000573	3.431838	-1.242526
6	0.155227	-2.386648	-0.710959
6	0.155227	-2.386648	0.710959
1	0.127648	-1.189379	-2.496830
1	0.206686	-3.328344	-1.251259
1	0.206686	-3.328344	1.251259
3	-1.768386	-1.259453	0.000000

**19a**

6	-0.008393	3.729295	0.710405
6	0.003684	2.548997	1.412322
6	0.019217	1.304157	0.723046
6	0.019217	1.304157	-0.723046
6	0.003684	2.548997	-1.412322
6	-0.008393	3.729295	-0.710405
6	0.034999	0.085981	1.412240
6	0.034999	0.085981	-1.412240



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6	0.073038	-1.136715	-0.726802
6	0.073038	-1.136715	0.726802
6	0.111574	-2.394995	1.411604
1	0.128613	-2.398808	2.500461
6	0.145550	-3.590131	0.714524
6	0.145550	-3.590131	-0.714524
6	0.111574	-2.394995	-1.411604
1	0.043846	0.086854	2.502301
1	-0.016180	4.675863	1.243930
1	0.007483	2.551201	2.500201
1	0.007483	2.551201	-2.500201
1	-0.016180	4.675863	-1.243930
1	0.043846	0.086854	-2.502301
1	0.190815	-4.533218	1.252979
1	0.190815	-4.533218	-1.252979
1	0.128613	-2.398808	-2.500461
3	-1.755062	-2.440951	0.000000

**19b**

6	-3.661687	0.711087	-0.074941
6	-2.483461	1.415267	-0.054410
6	-1.234209	0.725612	-0.048601
6	-1.234209	-0.725612	-0.048601
6	-2.483461	-1.415267	-0.054410
6	-3.661687	-0.711087	-0.074941
6	0.000000	1.408134	-0.036463
6	0.000000	-1.408134	-0.036463
6	1.234209	-0.725612	-0.048601
6	1.234209	0.725612	-0.048601
6	2.483461	1.415267	-0.054410
1	2.485676	2.503130	-0.066040
6	3.661687	0.711087	-0.074941
6	3.661687	-0.711087	-0.074941
6	2.483461	-1.415267	-0.054410
1	0.000000	2.498571	-0.048816
1	-4.607822	1.244785	-0.096082
1	-2.485676	2.503130	-0.066040
1	-2.485676	-2.503130	-0.066040
1	-4.607822	-1.244785	-0.096082
1	0.000000	-2.498571	-0.048816
1	4.607822	1.244785	-0.096082
1	4.607822	-1.244785	-0.096082
1	2.485676	-2.503130	-0.066040
3	0.000000	0.000000	1.818180

**20a**

6	3.618484	-0.307174	0.026043
6	2.905068	0.875325	0.016843
6	1.493839	0.863187	0.009017
6	0.800882	-0.381200	-0.059382
6	1.554324	-1.575182	-0.033109
6	2.937117	-1.536311	-0.016834
6	0.765430	2.093127	-0.026488

6	-0.648578	-0.364197	-0.053825
6	-1.339193	0.897039	-0.092446
6	-0.598130	2.118975	-0.040310
6	-2.761490	0.914901	-0.114518
1	-3.270742	1.876775	-0.140154
6	-3.501468	-0.262458	-0.145430
6	-2.827725	-1.505932	-0.133341
6	-1.435384	-1.549674	-0.101886
1	1.324149	3.026782	-0.003551
1	4.704652	-0.289267	0.038400
1	3.423291	1.831226	0.045736
1	1.067521	-2.544162	-0.085688
1	3.499456	-2.466011	-0.015398
1	-1.137129	3.063034	-0.076697
1	-4.587049	-0.227625	-0.185675
1	-3.394737	-2.432380	-0.175196
1	-0.952200	-2.521742	-0.101658
3	-2.152088	-0.333062	1.764624

**20b**

6	-0.322730	-0.050805	3.561686
6	0.856855	-0.073099	2.845985
6	0.838192	-0.080278	1.430474
6	-0.414293	-0.047523	0.730468
6	-1.602919	-0.009276	1.499412
6	-1.554637	-0.018437	2.881387
6	2.068991	-0.112671	0.686509
6	-0.414293	-0.047523	-0.730468
6	0.838192	-0.080278	-1.430474
6	2.068991	-0.112671	-0.686509
6	0.856855	-0.073099	-2.845985
1	1.815346	-0.108174	-3.359816
6	-0.322730	-0.050805	-3.561686
6	-1.554637	-0.018437	-2.881387
6	-1.602919	-0.009276	-1.499412
1	3.009542	-0.152752	1.233445
1	-0.301665	-0.061079	4.647739
1	1.815346	-0.108174	3.359816
1	-2.572330	0.005398	1.012452
1	-2.482097	-0.003897	3.447318
1	3.009542	-0.152752	-1.233445
1	-0.301665	-0.061079	-4.647739
1	-2.482097	-0.003897	-3.447318
1	-2.572330	0.005398	-1.012452
3	0.876306	1.782029	0.000000

**21a**

6	4.803499	0.715793	-0.133531
6	3.609133	1.412448	-0.108966
6	2.348290	0.729083	-0.076091
6	2.348293	-0.729080	-0.075969
6	3.609134	-1.412446	-0.108962
6	4.803499	-0.715791	-0.133532

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6	1.129802	1.414937	-0.039343	1	0.082034	-3.685646	2.504119
6	1.129803	-1.414935	-0.039320	1	0.082034	-3.685646	-2.504119
6	-0.096112	-0.728408	-0.025933	1	0.131910	-5.805471	-1.245986
6	-0.096116	0.728411	-0.026276	1	0.131910	-5.805471	1.245986
6	-1.323542	1.411998	-0.012146	3	-1.817105	-1.214027	0.000000
1	-1.326218	2.502050	-0.015875				
6	-2.538095	0.723835	-0.003134				
6	-2.538092	-0.723835	-0.002842				
6	-1.323540	-1.411998	-0.012084				
1	1.130948	2.505422	-0.048400				
1	5.747030	1.253977	-0.171806				
1	3.613704	2.501452	-0.125808				
1	3.613704	-2.501451	-0.125775				
1	5.747030	-1.253975	-0.171831				
1	1.130950	-2.505422	-0.048177				
1	-1.326212	-2.502051	-0.015488				
6	-3.786247	1.411949	0.005200				
6	-3.786244	-1.411950	0.005372				
6	-4.965667	0.711697	0.012899				
6	-4.965665	-0.711699	0.013034				
1	-3.788001	2.500021	0.003413				
1	-3.787996	-2.500023	0.003811				
1	-5.912393	-1.245249	0.018075				
1	-5.912396	1.245245	0.017932				
3	3.632352	-0.000009	1.749889				
<b>21b</b>							
6	0.049042	4.913420	0.711657				
6	0.035424	3.734507	1.412973				
6	0.023166	2.486460	0.724490				
6	0.023166	2.486460	-0.724490				
6	0.035424	3.734507	-1.412973				
6	0.049042	4.913420	-0.711657				
6	0.012080	1.272874	1.414276				
6	0.012080	1.272874	-1.414276				
6	0.025130	0.041716	-0.730861				
6	0.025130	0.041716	0.730861				
6	0.024696	-1.202034	1.410828				
1	0.036831	-1.204303	2.501493				
6	0.051227	-2.430273	0.727656				
6	0.051227	-2.430273	-0.727656				
6	0.024696	-1.202034	-1.410828				
1	0.022537	1.275116	2.504279				
1	0.062049	5.859762	1.245530				
1	0.039443	3.737422	2.500870				
1	0.039443	3.737422	-2.500870				
1	0.062049	5.859762	-1.245530				
1	0.022537	1.275116	-2.504279				
1	0.036831	-1.204303	-2.501493				
6	0.069737	-3.683290	1.416172				
6	0.069737	-3.683290	-1.416172				
6	0.101306	-4.859353	0.712665				
6	0.101306	-4.859353	-0.712665				

**Table S5:** The MP2(FULL)/6-31G\* optimized cartesian coordinates of the acyclic Mg<sup>2+</sup> complexes considered in the study.

<b>1</b>			
6	0.000000	0.687223	-0.979309
1	-0.933921	1.249955	-1.066914
1	0.933921	1.249955	-1.066914
6	0.000000	-0.687223	-0.979309
1	0.933921	-1.249955	-1.066914
1	-0.933921	-1.249955	-1.066914
12	0.000000	0.000000	1.334947

  

<b>2</b>			
6	0.000000	1.840897	-0.397870
1	-0.670710	2.697960	-0.393573
1	1.062920	2.049539	-0.237544
6	-0.448195	0.600766	-0.749038
1	-1.494428	0.457394	-1.039434
6	0.448195	-0.600766	-0.749038
1	1.494428	-0.457394	-1.039434
6	0.000000	-1.840897	-0.397870
1	0.670710	-2.697960	-0.393573
1	-1.062920	-2.049539	-0.237544
12	0.000000	0.000000	1.425333

  

<b>3a</b>			
6	1.085592	2.871235	-0.645385
1	0.128948	3.389414	-0.641273
1	1.968898	3.474751	-0.830639
6	1.182448	1.529506	-0.469619
1	2.155768	1.040102	-0.523119
6	0.000000	0.707858	-0.345054
1	-0.973866	1.209095	-0.441759
6	0.000000	-0.707858	-0.345054
1	0.973866	-1.209095	-0.441759
6	-1.182448	-1.529506	-0.469619
1	-2.155768	-1.040102	-0.523119
6	-1.085592	-2.871235	-0.645385

  

<b>3b</b>			
6	2.636429	-0.769801	0.228788
1	3.480601	-1.240750	-0.267341
1	2.824329	-0.384804	1.241250
6	1.361459	-0.894661	-0.259511
1	1.203301	-1.429485	-1.200175
12	1.618361	1.342880	-0.228220
6	0.186205	-0.254720	0.382577
1	0.238969	-0.117070	1.472382
6	-1.074764	-0.262995	-0.208362
1	-1.158003	-0.610394	-1.242678
6	-2.281372	0.103029	0.442521
1	-2.257787	0.429525	1.479712
6	-3.465736	-0.021239	-0.214682
1	-3.515699	-0.360704	-1.246698
1	-4.409365	0.201443	0.274204

  

<b>4a</b>			
6	-1.886460	-0.256604	-0.230202
1	-1.927900	-0.197984	-1.324988
6	-0.642795	-0.306662	0.381018
1	-0.591714	-0.521714	1.454873
6	0.642765	-0.306727	-0.380999
1	0.591672	-0.521859	-1.454837
6	1.886432	-0.256587	0.230211
1	1.927869	-0.197865	1.324993
12	0.000068	1.768708	-0.000042
6	3.137687	-0.393233	-0.453100
1	3.135722	-0.507028	-1.535332
6	-3.137714	-0.393174	0.453120

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1	-3.135756	-0.506862	1.535363
6	4.299917	-0.447670	0.239435
1	4.329790	-0.359019	1.322674
1	5.248443	-0.601610	-0.264631
6	-4.299942	-0.447664	-0.239416
1	-5.248475	-0.601526	0.264660
1	-4.329807	-0.359113	-1.322664

1	0.447464	-0.215077	-1.522402
6	0.803698	-0.252394	0.591515
1	0.359874	-0.523461	1.554736
12	-1.439250	1.363055	-0.162496
6	2.201228	0.075445	0.630632
6	3.028564	-0.032867	-0.438753
1	4.091634	0.160623	-0.333753
1	2.694795	-0.363771	-1.418762
1	2.620734	0.307286	1.605926

**4b**

6	-1.292348	-0.098709	0.355863
1	-1.339311	0.176540	1.419340
6	-2.424006	-0.925954	-0.127100
1	-2.235805	-1.608384	-0.960054
12	-2.825401	1.262385	-0.416325
6	-3.710012	-0.788281	0.330850
1	-3.922592	-0.244686	1.263805
6	0.005973	-0.260045	-0.190725
1	0.088068	-0.782699	-1.147986
6	1.186732	0.163301	0.406849
1	1.161856	0.669130	1.370704
6	2.410955	-0.110597	-0.192732
1	2.412514	-0.625537	-1.156117
6	3.667601	0.215480	0.371268
1	3.708595	0.726966	1.329584
6	4.815570	-0.118903	-0.280943
1	4.796064	-0.634572	-1.237916
1	-4.519184	-1.398675	-0.057166
1	5.791819	0.115538	0.131730

**7a**

6	0.500137	-0.172032	1.567110
1	1.500082	-0.220313	1.106995
6	-0.617156	-0.157212	0.746686
1	-1.603819	-0.175765	1.212691
6	-0.617156	-0.157212	-0.746686
1	-1.603819	-0.175765	-1.212691
6	0.500137	-0.172032	-1.567110
1	1.500082	-0.220313	-1.106995
12	0.223840	1.773703	0.000000
6	0.500137	-0.254755	3.013461
6	0.500137	-0.254755	-3.013461
6	-0.515744	-0.786877	3.729452
1	-0.444949	-0.866892	4.809207
6	-0.515744	-0.786877	-3.729452
1	-0.444949	-0.866892	-4.809207
1	1.414282	0.041435	3.521287
1	-1.412880	-1.195426	3.272124
1	-1.412880	-1.195426	-3.272124
1	1.414282	0.041435	-3.521287

**5**

6	-1.468433	-0.449239	0.554760
1	-2.528941	-0.690711	0.556057
1	-1.107467	0.058769	1.467956
6	-0.627388	-0.928022	-0.405738
1	-1.037812	-1.534011	-1.214751
6	0.843620	-0.633237	-0.478315
1	1.324491	-0.792646	-1.446291
6	1.609471	-0.237188	0.581316
1	2.672342	-0.046816	0.444887
1	1.243738	-0.224647	1.611180
12	-0.225831	1.393015	-0.244265

**7b**

6	3.287160	-0.905586	-0.057156
1	4.245276	-1.333323	0.221650
1	3.003855	-1.039184	-1.116720
6	2.399182	-0.447173	0.870427
1	2.700848	-0.436502	1.919784
6	1.051555	0.137997	0.547570
1	0.635175	0.762823	1.338811
6	0.143764	-0.632844	-0.235218
1	0.587328	-1.449113	-0.810835
12	2.487384	1.225376	-0.681964
6	-1.247192	-0.525839	-0.345204
6	-2.025496	0.341847	0.408830
6	-3.446109	0.458419	0.390584
1	-3.887611	1.173567	1.078300
6	-4.269266	-0.265455	-0.418111
1	-5.345066	-0.127239	-0.374334
1	-3.907412	-1.001666	-1.129817
1	-1.725462	-1.221672	-1.028222

**6**

6	-2.295742	-0.709757	0.500538
1	-3.280286	-1.168943	0.477968
1	-2.020328	-0.241475	1.462983
6	-1.385675	-0.906844	-0.498809
1	-1.687130	-1.482978	-1.375921
6	-0.011366	-0.311729	-0.535261

1	-1.517127	0.999606	1.114632
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<b>8a</b>			
6	1.030701	0.010446	0.767548
1	0.820928	0.096111	1.838257
6	-0.033627	-0.311748	-0.065253
1	0.160999	-0.510545	-1.128290
6	-1.334595	-0.788345	0.475996
1	-1.394500	-1.009606	1.545432
6	-2.465936	-0.887577	-0.290061
1	-3.406287	-1.229640	0.134163
1	-2.423048	-0.825783	-1.386011
12	-1.527048	1.341872	-0.236047
6	2.392171	0.230172	0.378966
6	2.938477	-0.300031	-0.744160
1	3.993691	-0.165918	-0.961210
1	3.030011	0.748678	1.089638
1	2.379635	-0.923259	-1.437619

<b>8b</b>			
6	2.114229	-0.943970	-0.606373
1	3.047776	-1.487614	-0.722523
1	1.588420	-0.705786	-1.548803
6	1.520636	-0.775769	0.612386
1	2.038826	-1.131786	1.505186
6	0.227565	-0.053890	0.829994
1	0.055155	0.346264	1.832858
6	-0.889710	-0.273117	0.022034
1	-0.781375	-0.915475	-0.857679
12	1.546197	1.314895	-0.321270
6	-2.197293	0.209183	0.304036
1	-2.364519	0.827084	1.183411
6	-3.239193	-0.169725	-0.482765
1	-4.256781	0.134180	-0.256390
1	-3.099272	-0.801879	-1.356696

<b>9a</b>			
6	-1.786207	-0.342687	-0.125189
1	-1.699023	-0.807678	-1.113556
6	-0.623140	0.014696	0.541529
1	-0.696790	0.318137	1.593347
6	0.739966	-0.282478	0.011912
1	0.820677	-0.982285	-0.826596
6	1.892820	0.231530	0.581234
1	1.781223	0.878305	1.465379
12	0.156609	1.770372	-0.559145
6	3.254503	-0.098938	0.209674

6	3.600018	-1.267107	-0.372772
1	4.638896	-1.487384	-0.594355
6	-3.101955	-0.232818	0.418871
1	-3.229985	0.184431	1.415546
6	-4.170330	-0.703047	-0.270560
1	-5.170352	-0.672362	0.150048
1	-4.068007	-1.142444	-1.259867
1	4.029113	0.602121	0.509165
1	2.880897	-2.050218	-0.597568

<b>9b</b>			
6	1.298975	0.035779	0.082021
1	1.401575	0.787780	0.861055
6	0.035953	-0.435784	-0.259202
1	-0.015125	-1.206550	-1.033331
6	-1.185090	-0.026744	0.332407
1	-1.107537	0.539969	1.271077
6	-2.400903	-0.868004	0.206671
1	-2.331655	-1.774111	-0.400918
12	-2.718136	1.166554	-0.685311
6	2.413642	-0.504350	-0.548343
1	2.221259	-1.244089	-1.327598
6	3.786847	-0.214693	-0.294792
1	4.516462	-0.712264	-0.926686
6	4.225799	0.611633	0.692293
1	3.556671	1.123917	1.377530
6	-3.624815	-0.506841	0.709482
1	-3.715886	0.298960	1.453282
1	-4.498197	-1.139332	0.585987
1	5.287621	0.781095	0.840112

<b>9c</b>			
6	-3.089464	1.230677	-0.322853
1	-3.937643	1.903986	-0.245978
1	-2.586242	1.216230	-1.306036
6	-2.545667	0.616611	0.765701
1	-3.030768	0.743860	1.735736
6	-1.358747	-0.302996	0.712323
1	-1.266890	-0.986454	1.560071
6	-0.130472	0.165144	0.162805
1	-0.156842	1.083375	-0.430941
12	-2.759936	-1.085234	-0.750905
6	1.110597	-0.424490	0.375614
1	1.189632	-1.328017	0.978034
6	2.263936	0.175910	-0.117680
1	2.161627	1.085562	-0.713889
6	3.574897	-0.301047	0.120487
1	3.718362	-1.202306	0.711106
6	4.647935	0.372920	-0.379996
1	5.663677	0.031172	-0.207225

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1	4.526230	1.279027	-0.968431
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**10a**

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6	1.752558	-0.073163	0.709821
1	1.487573	0.079506	1.764459
6	0.718560	-0.198430	-0.202776
1	0.951076	-0.423109	-1.250020
6	-0.718624	-0.198279	0.202747
1	-0.951143	-0.422547	1.250082
6	-1.752623	-0.073439	-0.709907
1	-1.487640	0.078812	-1.764598
12	0.000146	1.884909	-0.000152
6	3.162561	-0.214849	0.426457
6	3.641151	-0.950165	-0.601991
1	4.710085	-1.068084	-0.746027
1	3.854228	0.215365	1.145892
1	2.998182	-1.493930	-1.289047
6	-3.162615	-0.214988	-0.426475
6	-3.641210	-0.949828	0.602317
1	-4.710144	-1.067683	0.746404
1	-3.854283	0.214885	-1.146112
1	-2.998242	-1.493275	1.289627

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**10b**

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6	3.175977	-1.066745	-0.115239
1	4.084836	-1.629553	0.074444
1	2.749595	-1.187493	-1.127158
6	2.486963	-0.439380	0.879822
1	2.908507	-0.435692	1.887158
6	1.213456	0.330146	0.672262
1	0.980760	1.055826	1.455255
6	0.095417	-0.312575	0.069185
1	0.274832	-1.255558	-0.454863
12	2.633935	1.152937	-0.755423
6	-1.220774	0.132825	0.145258
1	-1.446322	1.055402	0.675306
6	-2.230094	-0.646717	-0.407569
1	-1.915634	-1.550223	-0.933333
6	-3.635962	-0.414003	-0.362281
6	-4.221448	0.610678	0.314679
1	-5.300740	0.725660	0.317866
1	-3.657728	1.343824	0.884333
1	-4.266541	-1.122816	-0.890645

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**11**

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6	0.840399	1.269513	0.683682
6	0.150789	0.408803	1.639291
6	0.150789	-0.966906	1.714033
6	0.150789	-0.966906	-1.714033
6	0.150789	0.408803	-1.639291

6	0.840399	1.269513	-0.683682
1	1.298878	2.140927	1.153128
1	-0.353882	0.943590	2.450644
1	-0.314009	-1.456376	2.571324
1	-0.314009	-1.456376	-2.571324
1	-0.353882	0.943590	-2.450644
1	1.298878	2.140927	-1.153128
1	0.836839	-1.567867	-1.116071
1	0.836839	-1.567867	1.116071
12	-1.386615	-0.721455	0.000000

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**12a**

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6	0.885684	-1.481116	-0.474141
6	-0.393127	-1.161674	0.192239
6	-1.320817	-0.220747	-0.264040
6	1.435030	1.766832	-0.230159
6	2.274278	0.698113	-0.455448
6	1.968428	-0.692867	-0.796668
1	1.022691	-2.548446	-0.655357
1	-0.798832	-1.966317	0.814771
1	1.860797	2.724824	0.062299
1	3.342294	0.892240	-0.327125
1	2.812423	-1.225500	-1.231410
1	0.395225	1.780695	-0.543805
1	-1.046281	0.417336	-1.107039
12	0.943387	0.136471	1.406124
6	-2.664074	-0.128340	0.197040
6	-3.535241	0.712132	-0.421333
1	-4.580345	0.755848	-0.130047
1	-3.001705	-0.779603	1.000524
1	-3.227877	1.357272	-1.241244

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**12b**

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6	1.580081	-1.361072	-0.464944
6	0.250274	-1.000533	-0.776855
6	-0.590278	-0.034724	-0.195597
6	2.237379	1.708366	-0.169458
6	2.560980	0.703726	0.678199
6	2.521926	-0.684368	0.286090
1	1.888544	-2.329597	-0.852619
1	-0.214396	-1.630042	-1.541814
1	2.421558	2.744102	0.097718
1	3.073928	0.937685	1.609533
1	3.398222	-1.268508	0.574624
1	1.871551	1.513359	-1.174317
1	-0.144098	0.717396	0.462363
6	-1.870730	0.338202	-0.837076
12	-2.268664	-0.723455	1.090111
6	-2.802269	1.156027	-0.245027
1	-3.735914	1.401476	-0.742306

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1	-2.542718	1.772336	0.627675
1	-2.116894	-0.130496	-1.794188

**13**

6	-0.607948	1.540393	-0.228443
6	0.639184	0.840927	0.146990
6	1.232114	-0.198571	-0.567037
6	-1.947686	-1.488261	-0.463691
6	-2.490138	-0.235553	-0.284405
6	-1.888972	1.090319	-0.451501
1	-0.501009	2.626346	-0.222855
1	1.284554	1.399322	0.833380
1	-1.046281	0.417336	-1.107039
12	0.943387	0.136471	1.406124
6	-2.664074	-0.128340	0.197040
6	-3.535241	0.712132	-0.421333
1	-4.580345	0.755848	-0.130047
1	-3.001705	-0.779603	1.000524
1	-3.227877	1.357272	-1.241244

**14**

6	2.623604	-1.035084	-0.339631
6	-2.072796	-0.965390	0.980118
6	-2.185728	-0.548424	-0.318906
6	2.092906	0.220050	-0.315832
6	-1.620657	0.681973	-0.927727

1	-2.557448	-2.366707	-0.259854
1	-3.529130	-0.205656	0.054922
1	-2.624965	1.873632	-0.625488
1	-1.027313	-1.660104	-1.015229
1	0.666123	-0.635851	-1.391329
12	-0.762666	-0.454955	1.300011
6	2.576225	-0.688955	-0.409999
6	3.585339	0.037790	0.129830
1	4.595033	-0.359897	0.157637
1	2.800008	-1.651190	-0.863239
1	3.457437	1.051035	0.501458

6	1.392877	0.767841	0.885888
6	0.145061	1.308251	0.814741
1	3.143039	-1.409070	-1.219528
1	-2.554154	-1.890468	1.291199
1	-2.765063	-1.175050	-1.000608
1	2.179629	0.857979	-1.199850
1	1.904821	0.704422	1.847718
1	-2.052654	0.950363	-1.890818
1	-0.321562	1.691134	1.725188
6	-0.602766	1.467039	-0.464871
1	-0.312519	2.319500	-1.083779
1	2.665445	-1.658681	0.558971
1	-1.656011	-0.345854	1.773530
12	0.094502	-0.951817	-0.223726

**Table S6:** The MP2(FULL)/6-31G\* optimized cartesian coordinates of the cyclic Mg<sup>2+</sup> complexes considered in the study.

<b>15</b>			
6	0.682695	0.806082	-0.607587
6	-0.682695	0.806082	-0.607587
6	-0.682695	-0.806082	-0.607587
6	0.682695	-0.806082	-0.607587
1	1.440815	1.549222	-0.853267
1	1.440815	-1.549222	-0.853267
1	-1.440815	1.549222	-0.853267
1	-1.440815	-1.549222	-0.853267
12	0.000000	0.000000	1.499596

  

<b>16</b>			
6	0.000000	1.417241	-0.426610
6	1.227367	0.708620	-0.426610
6	1.227367	-0.708620	-0.426610
6	0.000000	-1.417241	-0.426610
6	-1.227367	-0.708620	-0.426610
6	-1.227367	0.708620	-0.426610
1	0.000000	2.505976	-0.466254
1	2.170239	1.252988	-0.466254
1	2.170239	-1.252988	-0.466254
1	0.000000	-2.505976	-0.466254
1	-2.170239	-1.252988	-0.466254
1	-2.170239	1.252988	-0.466254
12	0.000000	0.000000	1.512958

  

<b>17</b>			
6	-0.444058	0.531748	1.569718
6	0.491864	-0.485701	1.570444
6	0.491864	-1.652131	0.677832
6	-1.607458	0.625867	0.677613
6	0.491864	-1.652131	-0.677832
6	-1.607458	0.625867	-0.677613
6	-0.444058	0.531748	-1.569718

  

<b>18</b>			
6	0.012306	2.651570	0.707549
6	0.088695	1.470400	1.422991
6	0.207152	0.238754	0.732012
6	0.207152	0.238754	-0.732012
6	0.088695	1.470400	-1.422991
6	0.012306	2.651570	-0.707549
1	0.438510	-1.015905	2.510338
1	-0.040858	3.597329	1.240974
1	0.102735	1.480694	2.511118
6	0.393556	-1.013718	1.420777
6	0.393556	-1.013718	-1.420777
1	0.102735	1.480694	-2.511118
1	-0.040858	3.597329	-1.240974
6	0.564548	-2.212713	-0.718217
6	0.564548	-2.212713	0.718217
1	0.438510	-1.015905	-2.510338
1	0.741857	-3.140854	-1.259033
1	0.741857	-3.140854	1.259033
12	-1.473297	-1.287837	0.000000

  

<b>19a</b>			
1	-0.432892	1.212243	2.428042
1	1.169859	-0.530495	2.429662
1	0.615634	-2.607618	1.188805
1	-2.549506	0.824667	1.189914
1	-2.549506	0.824667	-1.189914
1	0.615634	-2.607618	-1.188805
1	-0.432892	1.212243	-2.428042
6	0.491864	-0.485701	-1.570444
1	1.169859	-0.530495	-2.429662
12	1.267272	1.163752	0.000000



6	-0.031743	3.950089	0.709917
6	0.005783	2.768996	1.418591
6	0.053234	1.531578	0.728345
6	0.053234	1.531578	-0.728345
6	0.005783	2.768996	-1.418591
6	-0.031743	3.950089	-0.709917
6	0.111802	0.315508	1.422258
6	0.111802	0.315508	-1.422258
6	0.208801	-0.906107	-0.739384
6	0.208801	-0.906107	0.739384
6	0.388133	-2.166101	1.423744
1	0.439278	-2.170348	2.512975
6	0.528620	-3.365396	0.721808
6	0.528620	-3.365396	-0.721808
6	0.388133	-2.166101	-1.423744
1	0.125380	0.319870	2.512594
1	-0.060052	4.897091	1.242291
1	0.010543	2.776983	2.506146
1	0.010543	2.776983	-2.506146
1	-0.060052	4.897091	-1.242291
1	0.125380	0.319870	-2.512594
1	0.691199	-4.296615	1.260773
1	0.691199	-4.296615	-1.260773
1	0.439278	-2.170348	-2.512975
12	-1.465688	-2.383066	0.000000

**19b**

6	-3.667942	0.711606	-0.310566
6	-2.495672	1.425204	-0.214086
6	-1.250206	0.734968	-0.149295
6	-1.250206	-0.734968	-0.149295
6	-2.495672	-1.425204	-0.214086
6	-3.667942	-0.711606	-0.310566
6	0.000000	1.419651	-0.127923
6	0.000000	-1.419651	-0.127923
6	1.250206	-0.734968	-0.149295
6	1.250206	0.734968	-0.149295
6	2.495672	1.425204	-0.214086
1	2.501858	2.513141	-0.231490
6	3.667942	0.711606	-0.310566
6	3.667942	-0.711606	-0.310566
6	2.495672	-1.425204	-0.214086
1	0.000000	2.510775	-0.163215
1	-4.612263	1.242750	-0.397377
1	-2.501858	2.513141	-0.231490
1	-2.501858	-2.513141	-0.231490
1	-4.612263	-1.242750	-0.397377
1	0.000000	-2.510775	-0.163215
1	4.612263	1.242750	-0.397377
1	4.612263	-1.242750	-0.397377
1	2.501858	-2.513141	-0.231490

12	0.000000	0.000000	1.712641
<b>20a</b>			
6	3.809120	-0.345267	0.054036
6	3.120475	0.853812	0.041875
6	1.711052	0.865557	-0.010966
6	0.996404	-0.375800	-0.113934
6	1.725411	-1.585794	-0.079407
6	3.107783	-1.564762	-0.020815
6	1.010731	2.105366	-0.054360
6	-0.440590	-0.323498	-0.189643
6	-1.115061	0.977468	-0.223982
6	-0.357747	2.174115	-0.114728
6	-2.543768	1.018691	-0.386508
1	-3.033905	1.991396	-0.434169
6	-3.305791	-0.148260	-0.545508
6	-2.651753	-1.417709	-0.540115
6	-1.259252	-1.494398	-0.370023
1	1.587942	3.027470	-0.009701
1	4.894764	-0.349134	0.097560
1	3.657317	1.798078	0.094700
1	1.230743	-2.550053	-0.150843
1	3.657449	-2.502034	-0.017425
1	-0.866917	3.134471	-0.156805
1	-4.379056	-0.084229	-0.714752
1	-3.225882	-2.327275	-0.706709
1	-0.793305	-2.475750	-0.410040
12	-2.130936	-0.341672	1.477721

**20b**

6	-0.422432	-0.227895	3.572983
6	0.761696	-0.308288	2.863336
6	0.746950	-0.257661	1.447936
6	-0.511233	-0.095605	0.740076
6	-1.693509	0.017958	1.509607
6	-1.645031	-0.064571	2.892782
6	1.976658	-0.427876	0.692224
6	-0.511233	-0.095605	-0.740076
6	0.746950	-0.257661	-1.447936
6	1.976658	-0.427876	-0.692224
6	0.761696	-0.308288	-2.863336
1	1.709541	-0.446135	-3.380146
6	-0.422432	-0.227895	-3.572983
6	-1.645031	-0.064571	-2.892782
6	-1.693509	0.017958	-1.509607
1	2.906998	-0.592374	1.235665
1	-0.410750	-0.298806	4.657291
1	1.709541	-0.446135	3.380146
1	-2.659133	0.129123	1.026980
1	-2.570692	-0.006959	3.459701
1	2.906998	-0.592374	-1.235665
1	-0.410750	-0.298806	-4.657291

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1	-2.570692	-0.006959	-3.459701
1	-2.659133	0.129123	-1.026980
12	0.957572	1.566462	0.000000

**21a**

6	-4.544941	-0.722677	-0.504511
6	-3.343366	-1.423581	-0.381601
6	-2.081693	-0.742273	-0.205967
6	-2.081589	0.742757	-0.206101
6	-3.343397	1.424205	-0.379228
6	-4.545072	0.723389	-0.502753
6	-0.859779	-1.424610	-0.120305
6	-0.859679	1.424964	-0.120331
6	0.359347	0.735302	-0.069028
6	0.359276	-0.735046	-0.068567
6	1.584036	-1.418081	-0.031245
1	1.588746	-2.507930	-0.034743
6	2.799233	-0.727871	-0.006859
6	2.799303	0.727876	-0.007128
6	1.584170	1.418199	-0.031599
1	-0.858335	-2.515436	-0.135230
1	-5.477513	-1.261537	-0.657155
1	-3.348098	-2.512731	-0.434661
1	-3.348317	2.513443	-0.430493
1	-5.477727	1.262498	-0.654007
1	-0.858170	2.515793	-0.134991
1	1.588999	2.508046	-0.035490
6	4.041233	-1.417191	0.016342
6	4.041365	1.417075	0.015948
6	5.220943	-0.711537	0.036467
6	5.221013	0.711319	0.036269
1	4.046702	-2.504761	0.013981
1	4.046941	2.504645	0.013276
1	6.168488	1.243166	0.050942
1	6.168367	-1.243469	0.051278
12	-3.528541	-0.001254	1.464040

**21b**

6	0.206062	5.003540	0.711222
6	0.146598	3.825155	1.418304
6	0.089860	2.584979	0.728443
6	0.089860	2.584979	-0.728443
6	0.146598	3.825155	-1.418304
6	0.206062	5.003540	-0.711222
6	0.043793	1.371997	1.423454
6	0.043793	1.371997	-1.423454
6	0.040445	0.141411	-0.742145
6	0.040445	0.141411	0.742145
6	0.083633	-1.118773	1.422632
1	0.123835	-1.120829	2.513596
6	0.164535	-2.360264	0.736568
6	0.164535	-2.360264	-0.736568

6	0.083633	-1.118773	-1.422632
1	0.058856	1.376339	2.513588
1	0.255997	5.949625	1.243509
1	0.152532	3.831877	2.505869
1	0.152532	3.831877	-2.505869
1	0.255997	5.949625	-1.243509
1	0.058856	1.376339	-2.513588
1	0.123835	-1.120829	-2.513596
6	0.287034	-3.606327	1.425214
6	0.287034	-3.606327	-1.425214
6	0.432674	-4.771040	0.713324
6	0.432674	-4.771040	-0.713324
1	0.306177	-3.611328	2.513089
1	0.306177	-3.611328	-2.513089
1	0.560387	-5.710646	-1.244269
1	0.560387	-5.710646	1.244269
12	-1.737600	-1.189851	0.000000

**Table S7:** The total energy of the Li<sup>+</sup> and Mg<sup>2+</sup> complexes of the acyclic systems at the MP2(FULL)/6-311++G\*\* level.

System	BSSE Corrected		BSSE Uncorrected	
	Li <sup>+</sup>	Mg <sup>2+</sup>	Li <sup>+</sup>	Mg <sup>2+</sup>
<b>1</b>	-85.663628	-277.442298	-85.665914	-277.445283
<b>2</b>	-162.892459	-354.695861	-162.896130	-354.700730
<b>3a</b>	-240.113087	-431.928143	-240.116923	-431.932611
<b>3b</b>	-240.117190	-431.940980	-240.121064	-431.946230
<b>4a</b>	-317.341209	-509.174861	-317.345158	-509.180196
<b>4b</b>	-317.341726	-509.185597	-317.345523	-509.190768
<b>5</b>	-162.888946	-354.692682	-162.893720	-354.698460
<b>6</b>	-240.109359	-431.930320	-240.113691	-431.935649
<b>7a</b>	-317.328160	-509.157804	-317.332760	-509.164081
<b>7b</b>	-317.328814	-509.167967	-317.333400	-509.173002
<b>8a</b>	-240.112657	-431.933047	-240.116421	-431.938228
<b>8b</b>	-240.114648	-431.938390	-240.119239	-431.943719
<b>9a</b>	-317.336775	-509.168862	-317.340767	-509.174261
<b>9b</b>	-317.337081	-509.178409	-317.340982	-509.183573
<b>9c</b>	-317.339578	-509.183377	-317.344238	-509.188450
<b>10a</b>	-317.332341	-509.162420	-317.336193	-509.167735
<b>10b</b>	-317.334867	-509.176317	-317.339435	-509.181410
<b>11</b>	-240.111905	-431.951234	-240.117574	-431.957640
<b>12a</b>	-317.336808	-509.190804	-317.342737	-509.198185
<b>12b</b>	-317.326939	-509.158163	-317.330830	-509.163488
<b>13</b>	-317.334576	-509.182917	-317.340463	-509.190246
<b>14</b>	-317.341851	-509.202400	-317.348873	-509.211833

**Table S8:** The total energy of the Li<sup>+</sup> and Mg<sup>2+</sup> complexes of the cyclic systems at the MP2(FULL)/6-311++G\*\* level.

System	BSSE Corrected		BSSE Uncorrected	
	Li <sup>+</sup>	Mg <sup>2+</sup>	Li <sup>+</sup>	Mg <sup>2+</sup>
<b>15</b>	-161.602512	-353.402099	-161.606400	-353.407283
<b>16</b>	-239.002443	-430.819605	-239.009222	-430.828269
<b>17</b>	-316.155645	-508.003180	-316.161035	-508.010041
<b>18</b>	-392.305620	-584.143739	-392.313075	-584.153489
<b>19a</b>	-545.601830	-737.455092	-545.609424	-737.464886
<b>19b</b>	-545.600820	-737.453110	-545.609168	-737.464097
<b>20a</b>	-545.613806	-737.462800	-545.620874	-737.472364
<b>20b</b>	-545.610852	-737.464838	-545.618817	-737.475427
<b>21a</b>	-698.895035	-890.758861	-698.902511	-890.768745
<b>21b</b>	-698.894278	-890.758516	-698.902805	-890.769748

**Table S9:** The MP2(FULL)/cc-pVDZ //MP2(FULL)/6-31G\* charges (in amu) on the Li<sup>+</sup> and Mg<sup>2+</sup> ions in the various acyclic complexes considered in the study.

	Li <sup>+</sup>		Mg <sup>2+</sup>	
	Mulliken	NPA	Mulliken	NPA
<b>1</b>	0.681	0.971	1.381	1.822
<b>2</b>	0.590	0.967	1.187	1.840
<b>3a</b>	0.639	0.974	1.238	1.725
<b>3b</b>	0.578	0.966	1.135	1.831
<b>4a</b>	0.583	0.967	1.151	1.802
<b>4b</b>	0.559	0.964	1.058	1.795
<b>5</b>	0.536	0.966	1.158	1.858
<b>6</b>	0.534	0.967	1.133	1.836
<b>7a</b>	0.536	0.968	1.121	1.846
<b>7b</b>	0.513	0.965	1.061	1.763
<b>8a</b>	0.579	0.967	1.151	1.834
<b>8b</b>	0.534	0.966	1.128	1.828
<b>9a</b>	0.581	0.967	1.147	1.813
<b>9b</b>	0.564	0.964	1.062	1.795
<b>9c</b>	0.516	0.965	1.061	1.756
<b>10a</b>	0.580	0.968	1.158	1.817
<b>10b</b>	0.520	0.965	1.063	1.761
<b>11</b>	0.430	0.943	0.996	1.713
<b>12a</b>	0.426	0.946	0.944	1.742
<b>12b</b>	0.565	0.966	1.097	1.814
<b>13</b>	0.426	0.929	0.950	1.744
<b>14</b>	0.299	0.924	0.751	1.773

**Table S10:** The MP2(FULL)/cc-pVDZ //MP2(FULL)/6-31G\* charges (in amu) on the Li<sup>+</sup> and Mg<sup>2+</sup> ions in the various cyclic complexes considered in the study.

	Li <sup>+</sup>		Mg <sup>2+</sup>	
	Mulliken	NPA	Mulliken	NPA
<b>15</b>	0.603	0.969	1.256	1.891
<b>16</b>	0.482	0.966	1.064	1.880
<b>17</b>	0.476	0.941	1.019	1.678
<b>18</b>	0.499	0.967	1.040	1.877
<b>19a</b>	0.489	0.966	1.007	1.871
<b>19b</b>	0.521	0.969	1.039	1.876
<b>20a</b>	0.495	0.967	1.017	1.866
<b>20b</b>	0.524	0.970	1.036	1.880
<b>21a</b>	0.480	0.966	0.982	1.867
<b>21b</b>	0.515	0.969	1.015	1.870

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