

# Supplementary Material for

## An Intruder-Free Fock Space Coupled-Cluster Study of the Potential Energy Curves of $\text{LiMg}^+$ within the (2,0) Sector

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April 18, 2024

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Table S1: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $X^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.067712	8.0	-207.284103	19.2	-207.283351	30.4	-207.283336
1.5	-207.117425	8.2	-207.284026	19.4	-207.283350	30.6	-207.283336
1.6	-207.158798	8.4	-207.283959	19.6	-207.283350	30.8	-207.283336
1.7	-207.193188	8.6	-207.283899	19.8	-207.283349	31.0	-207.283336
1.8	-207.221467	8.8	-207.283847	20.0	-207.283348	31.2	-207.283336
1.9	-207.244392	9.0	-207.283798	20.2	-207.283348	31.4	-207.283336
2.0	-207.262690	9.2	-207.283759	20.4	-207.283347	31.6	-207.283336
2.1	-207.277058	9.4	-207.283723	20.6	-207.283347	31.8	-207.283336
2.2	-207.288143	9.6	-207.283692	20.8	-207.283346	32.0	-207.283336
2.3	-207.296525	9.8	-207.283664	21.0	-207.283346	33.0	-207.283336
2.4	-207.302710	10.0	-207.283638	21.2	-207.283345	34.0	-207.283336
2.5	-207.307127	10.2	-207.283615	21.4	-207.283345	35.0	-207.283335
2.6	-207.310133	10.4	-207.283594	21.6	-207.283344	36.0	-207.283335
2.7	-207.312020	10.6	-207.283575	21.8	-207.283344	37.0	-207.283335
2.8	-207.313027	10.8	-207.283557	22.0	-207.283343	38.0	-207.283335
2.9	-207.313340	11.0	-207.283541	22.2	-207.283343	39.0	-207.283335
3.0	-207.313122	11.2	-207.283527	22.4	-207.283343	40.0	-207.283335
3.1	-207.312506	11.4	-207.283513	22.6	-207.283342	42.0	-207.283335
3.2	-207.311589	11.6	-207.283489	22.8	-207.283342	44.0	-207.283335
3.3	-207.310452	11.8	-207.283478	23.0	-207.283342	46.0	-207.283335
3.4	-207.309160	12.0	-207.283468	23.2	-207.283341	48.0	-207.283335
3.5	-207.307768	12.2	-207.283459	23.4	-207.283341	50.0	-207.283335
3.6	-207.306317	12.4	-207.283451	23.6	-207.283341	52.0	-207.283335
3.7	-207.304843	12.6	-207.283443	23.8	-207.283340	54.0	-207.283335
3.8	-207.303372	12.8	-207.283436	24.0	-207.283340	56.0	-207.283335
3.9	-207.301927	13.0	-207.283429	24.2	-207.283340	58.0	-207.283335
4.0	-207.300523	13.2	-207.283423	24.4	-207.283340	60.0	-207.283334
4.1	-207.299174	13.4	-207.283418	24.6	-207.283340	62.0	-207.283334
4.2	-207.297890	13.6	-207.283413	24.8	-207.283339	64.0	-207.283334
4.3	-207.296678	13.8	-207.283408	25.0	-207.283339	66.0	-207.283334
4.4	-207.295540	14.0	-207.283403	25.2	-207.283339	68.0	-207.283334
4.5	-207.294480	14.2	-207.283399	25.4	-207.283339	70.0	-207.283334
4.6	-207.293498	14.4	-207.283395	25.6	-207.283339	72.0	-207.283334
4.7	-207.292593	14.6	-207.283392	25.8	-207.283338	74.0	-207.283334
4.8	-207.291763	14.8	-207.283388	26.0	-207.283338	76.0	-207.283334
4.9	-207.291005	15.0	-207.283385	26.2	-207.283338	78.0	-207.283334
5.0	-207.290314	15.2	-207.283382	26.4	-207.283338	80.0	-207.283334
5.1	-207.289687	15.4	-207.283379	26.6	-207.283338	82.0	-207.283334
5.2	-207.289119	15.6	-207.283377	26.8	-207.283338	84.0	-207.283334
5.3	-207.288605	15.8	-207.283374	27.0	-207.283338	86.0	-207.283334
5.4	-207.288142	16.0	-207.283372	27.2	-207.283338	88.0	-207.283334
5.5	-207.287723	16.2	-207.283370	27.4	-207.283337	90.0	-207.283334
5.6	-207.287347	16.4	-207.283368	27.6	-207.283337	92.0	-207.283334
5.7	-207.287008	16.6	-207.283366	27.8	-207.283337	94.0	-207.283334
5.8	-207.286703	16.8	-207.283365	28.0	-207.283337	96.0	-207.283334
5.9	-207.286428	17.0	-207.283363	28.2	-207.283337	98.0	-207.283334
6.0	-207.286182	17.2	-207.283362	28.4	-207.283337	100.0	-207.283334
6.2	-207.285760	17.4	-207.283360	28.6	-207.283337	150.0	-207.283334
6.4	-207.285417	17.6	-207.283359	28.8	-207.283337	200.0	-207.283334
6.6	-207.285136	17.8	-207.283358	29.0	-207.283337		
6.8	-207.284904	18.0	-207.283357	29.2	-207.283337		
7.0	-207.284711	18.2	-207.283356	29.4	-207.283337		
7.2	-207.284548	18.4	-207.283355	29.6	-207.283336		
7.4	-207.284410	18.6	-207.283354	29.8	-207.283336		
7.6	-207.284293	18.8	-207.283353	30.0	-207.283336		
7.8	-207.284191	19.0	-207.283352	30.2	-207.283336		

Table S2: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $2^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.890931	8.0	-207.203090	19.2	-207.201252	30.4	-207.201212
1.5	-206.938611	8.2	-207.202902	19.4	-207.201250	30.6	-207.201211
1.6	-206.978355	8.4	-207.202734	19.6	-207.201248	30.8	-207.201211
1.7	-207.012132	8.6	-207.202586	19.8	-207.201247	31.0	-207.201211
1.8	-207.040961	8.8	-207.202454	20.0	-207.201245	31.2	-207.201211
1.9	-207.065422	9.0	-207.202337	20.2	-207.201243	31.4	-207.201211
2.0	-207.085940	9.2	-207.202233	20.4	-207.201242	31.6	-207.201210
2.1	-207.102927	9.4	-207.202141	20.6	-207.201240	31.8	-207.201210
2.2	-207.116814	9.6	-207.202059	20.8	-207.201239	32.0	-207.201210
2.3	-207.128042	9.8	-207.201986	21.0	-207.201238	33.0	-207.201209
2.4	-207.137036	10.0	-207.201921	21.2	-207.201236	34.0	-207.201209
2.5	-207.144195	10.2	-207.201862	21.4	-207.201235	35.0	-207.201208
2.6	-207.149884	10.4	-207.201810	21.6	-207.201234	36.0	-207.201208
2.7	-207.154433	10.6	-207.201762	21.8	-207.201233	37.0	-207.201207
2.8	-207.158137	10.8	-207.201719	22.0	-207.201232	38.0	-207.201207
2.9	-207.161257	11.0	-207.201681	22.2	-207.201231	39.0	-207.201207
3.0	-207.164022	11.2	-207.201646	22.4	-207.201230	40.0	-207.201206
3.1	-207.166618	11.4	-207.201614	22.6	-207.201229	42.0	-207.201206
3.2	-207.169176	11.6	-207.201585	22.8	-207.201228	44.0	-207.201206
3.3	-207.171777	11.8	-207.201559	23.0	-207.201227	46.0	-207.201205
3.4	-207.174448	12.0	-207.201535	23.2	-207.201226	48.0	-207.201205
3.5	-207.177177	12.2	-207.201513	23.4	-207.201226	50.0	-207.201205
3.6	-207.179927	12.4	-207.201493	23.6	-207.201225	52.0	-207.201205
3.7	-207.182649	12.6	-207.201474	23.8	-207.201224	54.0	-207.201205
3.8	-207.185297	12.8	-207.201457	24.0	-207.201224	56.0	-207.201205
3.9	-207.187830	13.0	-207.201441	24.2	-207.201223	58.0	-207.201204
4.0	-207.190215	13.2	-207.201427	24.4	-207.201222	60.0	-207.201204
4.1	-207.192430	13.4	-207.201413	24.6	-207.201222	62.0	-207.201204
4.2	-207.194462	13.6	-207.201401	24.8	-207.201221	64.0	-207.201204
4.3	-207.196302	13.8	-207.201390	25.0	-207.201221	66.0	-207.201204
4.4	-207.197950	14.0	-207.201379	25.2	-207.201220	68.0	-207.201204
4.5	-207.199410	14.2	-207.201369	25.4	-207.201220	70.0	-207.201204
4.6	-207.200687	14.4	-207.201360	25.6	-207.201219	72.0	-207.201204
4.7	-207.201791	14.6	-207.201351	25.8	-207.201219	74.0	-207.201204
4.8	-207.202734	14.8	-207.201343	26.0	-207.201218	76.0	-207.201204
4.9	-207.203527	15.0	-207.201336	26.2	-207.201218	78.0	-207.201204
5.0	-207.204183	15.2	-207.201329	26.4	-207.201217	80.0	-207.201204
5.1	-207.204715	15.4	-207.201322	26.6	-207.201217	82.0	-207.201204
5.2	-207.205135	15.6	-207.201316	26.8	-207.201217	84.0	-207.201204
5.3	-207.205458	15.8	-207.201311	27.0	-207.201216	86.0	-207.201204
5.4	-207.205693	16.0	-207.201305	27.2	-207.201216	88.0	-207.201204
5.5	-207.205853	16.2	-207.201300	27.4	-207.201215	90.0	-207.201204
5.6	-207.205948	16.4	-207.201296	27.6	-207.201215	92.0	-207.201204
5.7	-207.205988	16.6	-207.201291	27.8	-207.201215	94.0	-207.201204
5.8	-207.205982	16.8	-207.201287	28.0	-207.201215	96.0	-207.201204
5.9	-207.205937	17.0	-207.201283	28.2	-207.201214	98.0	-207.201204
6.0	-207.205860	17.2	-207.201279	28.4	-207.201214	100.0	-207.201204
6.2	-207.205635	17.4	-207.201276	28.6	-207.201214	150.0	-207.201204
6.4	-207.205349	17.6	-207.201273	28.8	-207.201213	200.0	-207.201204
6.6	-207.205032	17.8	-207.201270	29.0	-207.201213		
6.8	-207.204705	18.0	-207.201267	29.2	-207.201213		
7.0	-207.204385	18.2	-207.201264	29.4	-207.201213		
7.2	-207.204080	18.4	-207.201261	29.6	-207.201212		
7.4	-207.203796	18.6	-207.201259	29.8	-207.201212		
7.6	-207.203536	18.8	-207.201257	30.0	-207.201212		
7.8	-207.203301	19.0	-207.201254	30.2	-207.201212		

Table S3: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $3^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.862316	8.0	-207.142261	19.2	-207.133519	30.4	-207.133312
1.5	-206.898835	8.2	-207.141702	19.4	-207.133510	30.6	-207.133311
1.6	-206.927399	8.4	-207.141126	19.6	-207.133502	30.8	-207.133309
1.7	-206.959124	8.6	-207.140545	19.8	-207.133494	31.0	-207.133308
1.8	-206.988447	8.8	-207.139968	20.0	-207.133486	31.2	-207.133307
1.9	-207.012857	9.0	-207.139406	20.2	-207.133478	31.4	-207.133306
2.0	-207.033020	9.2	-207.138865	20.4	-207.133471	31.6	-207.133305
2.1	-207.049632	9.4	-207.138351	20.6	-207.133464	31.8	-207.133304
2.2	-207.063331	9.6	-207.137869	20.8	-207.133458	32.0	-207.133303
2.3	-207.074663	9.8	-207.137423	21.0	-207.133451	33.0	-207.133298
2.4	-207.084086	10.0	-207.137013	21.2	-207.133445	34.0	-207.133293
2.5	-207.091974	10.2	-207.136642	21.4	-207.133440	35.0	-207.133289
2.6	-207.098623	10.4	-207.136308	21.6	-207.133434	36.0	-207.133286
2.7	-207.104257	10.6	-207.136010	21.8	-207.133429	37.0	-207.133283
2.8	-207.109042	10.8	-207.135746	22.0	-207.133424	38.0	-207.133280
2.9	-207.113091	11.0	-207.135514	22.2	-207.133419	39.0	-207.133278
3.0	-207.116463	11.2	-207.135309	22.4	-207.133414	40.0	-207.133276
3.1	-207.119221	11.4	-207.135130	22.6	-207.133409	42.0	-207.133272
3.2	-207.121409	11.6	-207.134974	22.8	-207.133405	44.0	-207.133269
3.3	-207.123085	11.8	-207.134837	23.0	-207.133401	46.0	-207.133266
3.4	-207.124330	12.0	-207.134716	23.2	-207.133396	48.0	-207.133264
3.5	-207.125248	12.2	-207.134609	23.4	-207.133392	50.0	-207.133262
3.6	-207.125952	12.4	-207.134515	23.6	-207.133389	52.0	-207.133261
3.7	-207.126557	12.6	-207.134431	23.8	-207.133385	54.0	-207.133259
3.8	-207.127157	12.8	-207.134356	24.0	-207.133381	56.0	-207.133258
3.9	-207.127820	13.0	-207.134288	24.2	-207.133378	58.0	-207.133257
4.0	-207.128578	13.2	-207.134227	24.4	-207.133375	60.0	-207.133256
4.1	-207.129434	13.4	-207.134172	24.6	-207.133371	62.0	-207.133256
4.2	-207.130370	13.6	-207.134122	24.8	-207.133368	64.0	-207.133255
4.3	-207.131359	13.8	-207.134075	25.0	-207.133365	66.0	-207.133254
4.4	-207.132375	14.0	-207.134033	25.2	-207.133362	68.0	-207.133254
4.5	-207.133394	14.2	-207.133994	25.4	-207.133360	70.0	-207.133253
4.6	-207.134400	14.4	-207.133957	25.6	-207.133357	72.0	-207.133253
4.7	-207.135377	14.6	-207.133923	25.8	-207.133354	74.0	-207.133253
4.8	-207.136317	14.8	-207.133892	26.0	-207.133352	76.0	-207.133252
4.9	-207.137213	15.0	-207.133863	26.2	-207.133349	78.0	-207.133252
5.0	-207.138060	15.2	-207.133835	26.4	-207.133347	80.0	-207.133252
5.1	-207.138854	15.4	-207.133810	26.6	-207.133345	82.0	-207.133252
5.2	-207.139595	15.6	-207.133785	26.8	-207.133342	84.0	-207.133251
5.3	-207.140280	15.8	-207.133763	27.0	-207.133340	86.0	-207.133251
5.4	-207.140910	16.0	-207.133741	27.2	-207.133338	88.0	-207.133251
5.5	-207.141484	16.2	-207.133721	27.4	-207.133336	90.0	-207.133251
5.6	-207.142002	16.4	-207.133702	27.6	-207.133334	92.0	-207.133251
5.7	-207.142468	16.6	-207.133684	27.8	-207.133332	94.0	-207.133251
5.8	-207.142881	16.8	-207.133667	28.0	-207.133330	96.0	-207.133250
5.9	-207.143243	17.0	-207.133651	28.2	-207.133329	98.0	-207.133250
6.0	-207.143554	17.2	-207.133636	28.4	-207.133327	100.0	-207.133250
6.2	-207.144033	17.4	-207.133622	28.6	-207.133325	150.0	-207.133249
6.4	-207.144332	17.6	-207.133608	28.8	-207.133324	200.0	-207.133249
6.6	-207.144466	17.8	-207.133595	29.0	-207.133322		
6.8	-207.144452	18.0	-207.133582	29.2	-207.133320		
7.0	-207.144308	18.2	-207.133570	29.4	-207.133319		
7.2	-207.144053	18.4	-207.133559	29.6	-207.133317		
7.4	-207.143703	18.6	-207.133548	29.8	-207.133316		
7.6	-207.143277	18.8	-207.133538	30.0	-207.133315		
7.8	-207.142791	19.0	-207.133528	30.2	-207.133313		

Table S4: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $4^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.775549	8.0	-207.123015	19.2	-207.124586	30.4	-207.124271
1.5	-206.822770	8.2	-207.123705	19.4	-207.124572	30.6	-207.124270
1.6	-206.859869	8.4	-207.124310	19.6	-207.124558	30.8	-207.124268
1.7	-206.890990	8.6	-207.124837	19.8	-207.124545	31.0	-207.124266
1.8	-206.918811	8.8	-207.125288	20.0	-207.124533	31.2	-207.124264
1.9	-206.943579	9.0	-207.125668	20.2	-207.124522	31.4	-207.124263
2.0	-206.965050	9.2	-207.125985	20.4	-207.124510	31.6	-207.124261
2.1	-206.983412	9.4	-207.126242	20.6	-207.124500	31.8	-207.124260
2.2	-206.999101	9.6	-207.126444	20.8	-207.124489	32.0	-207.124258
2.3	-207.012620	9.8	-207.126594	21.0	-207.124480	33.0	-207.124251
2.4	-207.024453	10.0	-207.126698	21.2	-207.124470	34.0	-207.124245
2.5	-207.035008	10.2	-207.126760	21.4	-207.124461	35.0	-207.124240
2.6	-207.044576	10.4	-207.126785	21.6	-207.124453	36.0	-207.124235
2.7	-207.053323	10.6	-207.126780	21.8	-207.124445	37.0	-207.124231
2.8	-207.061314	10.8	-207.126748	22.0	-207.124437	38.0	-207.124228
2.9	-207.068559	11.0	-207.126695	22.2	-207.124429	39.0	-207.124224
3.0	-207.075061	11.2	-207.126626	22.4	-207.124422	40.0	-207.124221
3.1	-207.080829	11.4	-207.126545	22.6	-207.124415	42.0	-207.124216
3.2	-207.085880	11.6	-207.126451	22.8	-207.124408	44.0	-207.124212
3.3	-207.090244	11.8	-207.126355	23.0	-207.124402	46.0	-207.124209
3.4	-207.093957	12.0	-207.126257	23.2	-207.124395	48.0	-207.124206
3.5	-207.097054	12.2	-207.126159	23.4	-207.124389	50.0	-207.124204
3.6	-207.099566	12.4	-207.126062	23.6	-207.124384	52.0	-207.124202
3.7	-207.101523	12.6	-207.125967	23.8	-207.124378	54.0	-207.124200
3.8	-207.102959	12.8	-207.125876	24.0	-207.124373	56.0	-207.124198
3.9	-207.103924	13.0	-207.125789	24.2	-207.124368	58.0	-207.124197
4.0	-207.104483	13.2	-207.125706	24.4	-207.124363	60.0	-207.124196
4.1	-207.104720	13.4	-207.125627	24.6	-207.124358	62.0	-207.124195
4.2	-207.104722	13.6	-207.125553	24.8	-207.124353	64.0	-207.124194
4.3	-207.104574	13.8	-207.125483	25.0	-207.124349	66.0	-207.124194
4.4	-207.104351	14.0	-207.125418	25.2	-207.124345	68.0	-207.124193
4.5	-207.104117	14.2	-207.125356	25.4	-207.124340	70.0	-207.124192
4.6	-207.103921	14.4	-207.125298	25.6	-207.124336	72.0	-207.124192
4.7	-207.103800	14.6	-207.125244	25.8	-207.124333	74.0	-207.124191
4.8	-207.103781	14.8	-207.125193	26.0	-207.124329	76.0	-207.124191
4.9	-207.103878	15.0	-207.125146	26.2	-207.124325	78.0	-207.124191
5.0	-207.104097	15.2	-207.125101	26.4	-207.124322	80.0	-207.124190
5.1	-207.104437	15.4	-207.125059	26.6	-207.124318	82.0	-207.124190
5.2	-207.104888	15.6	-207.125019	26.8	-207.124315	84.0	-207.124190
5.3	-207.105438	15.8	-207.124982	27.0	-207.124312	86.0	-207.124190
5.4	-207.106072	16.0	-207.124947	27.2	-207.124309	88.0	-207.124189
5.5	-207.106773	16.2	-207.124913	27.4	-207.124306	90.0	-207.124189
5.6	-207.107525	16.4	-207.124882	27.6	-207.124303	92.0	-207.124189
5.7	-207.108313	16.6	-207.124853	27.8	-207.124300	94.0	-207.124189
5.8	-207.109124	16.8	-207.124825	28.0	-207.124298	96.0	-207.124189
5.9	-207.109947	17.0	-207.124799	28.2	-207.124295	98.0	-207.124189
6.0	-207.110774	17.2	-207.124774	28.4	-207.124293	100.0	-207.124188
6.2	-207.112406	17.4	-207.124750	28.6	-207.124290	150.0	-207.124187
6.4	-207.113978	17.6	-207.124728	28.8	-207.124288	200.0	-207.124187
6.6	-207.115466	17.8	-207.124707	29.0	-207.124286		
6.8	-207.116857	18.0	-207.124687	29.2	-207.124283		
7.0	-207.118142	18.2	-207.124668	29.4	-207.124281		
7.2	-207.119321	18.4	-207.124650	29.6	-207.124279		
7.4	-207.120394	18.6	-207.124633	29.8	-207.124277		
7.6	-207.121365	18.8	-207.124616	30.0	-207.124275		
7.8	-207.122237	19.0	-207.124601	30.2	-207.124273		

Table S5: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $5^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.743975	8.0	-207.085882	19.2	-207.086519	30.4	-207.085974
1.5	-206.795021	8.2	-207.086880	19.4	-207.086485	30.6	-207.085972
1.6	-206.836864	8.4	-207.087811	19.6	-207.086454	30.8	-207.085970
1.7	-206.870133	8.6	-207.088669	19.8	-207.086425	31.0	-207.085968
1.8	-206.895716	8.8	-207.089451	20.0	-207.086398	31.2	-207.085966
1.9	-206.916212	9.0	-207.090150	20.2	-207.086374	31.4	-207.085964
2.0	-206.934577	9.2	-207.090778	20.4	-207.086351	31.6	-207.085963
2.1	-206.952220	9.4	-207.091327	20.6	-207.086329	31.8	-207.085961
2.2	-206.968397	9.6	-207.091801	20.8	-207.086309	32.0	-207.085959
2.3	-206.982585	9.8	-207.092200	21.0	-207.086290	33.0	-207.085952
2.4	-206.994795	10.0	-207.092528	21.2	-207.086273	34.0	-207.085946
2.5	-207.005170	10.2	-207.092786	21.4	-207.086256	35.0	-207.085940
2.6	-207.013881	10.4	-207.092979	21.6	-207.086241	36.0	-207.085936
2.7	-207.021133	10.6	-207.093109	21.8	-207.086226	37.0	-207.085932
2.8	-207.027151	10.8	-207.093180	22.0	-207.086212	38.0	-207.085928
2.9	-207.032161	11.0	-207.093197	22.2	-207.086199	39.0	-207.085925
3.0	-207.036383	11.2	-207.093163	22.4	-207.086187	40.0	-207.085922
3.1	-207.039996	11.4	-207.093084	22.6	-207.086176	42.0	-207.085918
3.2	-207.043141	11.6	-207.092962	22.8	-207.086165	44.0	-207.085915
3.3	-207.045928	11.8	-207.092806	23.0	-207.086154	46.0	-207.085912
3.4	-207.048443	12.0	-207.092618	23.2	-207.086144	48.0	-207.085910
3.5	-207.050749	12.2	-207.092404	23.4	-207.086135	50.0	-207.085908
3.6	-207.052891	12.4	-207.092168	23.6	-207.086126	52.0	-207.085906
3.7	-207.054904	12.6	-207.091915	23.8	-207.086118	54.0	-207.085905
3.8	-207.056810	12.8	-207.091649	24.0	-207.086109	56.0	-207.085904
3.9	-207.058625	13.0	-207.091374	24.2	-207.086102	58.0	-207.085904
4.0	-207.060359	13.2	-207.091094	24.4	-207.086094	60.0	-207.085903
4.1	-207.062016	13.4	-207.090810	24.6	-207.086087	62.0	-207.085902
4.2	-207.063597	13.6	-207.090528	24.8	-207.086081	64.0	-207.085902
4.3	-207.065099	13.8	-207.090248	25.0	-207.086074	66.0	-207.085901
4.4	-207.066518	14.0	-207.089973	25.2	-207.086068	68.0	-207.085901
4.5	-207.067846	14.2	-207.089706	25.4	-207.086063	70.0	-207.085901
4.6	-207.069074	14.4	-207.089446	25.6	-207.086057	72.0	-207.085900
4.7	-207.070195	14.6	-207.089197	25.8	-207.086052	74.0	-207.085900
4.8	-207.071204	14.8	-207.088960	26.0	-207.086047	76.0	-207.085900
4.9	-207.072097	15.0	-207.088734	26.2	-207.086042	78.0	-207.085900
5.0	-207.072879	15.2	-207.088521	26.4	-207.086037	80.0	-207.085900
5.1	-207.073553	15.4	-207.088321	26.6	-207.086033	82.0	-207.085900
5.2	-207.074131	15.6	-207.088134	26.8	-207.086028	84.0	-207.085899
5.3	-207.074626	15.8	-207.087961	27.0	-207.086024	86.0	-207.085899
5.4	-207.075050	16.0	-207.087801	27.2	-207.086020	88.0	-207.085899
5.5	-207.075418	16.2	-207.087654	27.4	-207.086016	90.0	-207.085899
5.6	-207.075744	16.4	-207.087520	27.6	-207.086013	92.0	-207.085899
5.7	-207.076039	16.6	-207.087396	27.8	-207.086009	94.0	-207.085899
5.8	-207.076315	16.8	-207.087284	28.0	-207.086006	96.0	-207.085899
5.9	-207.076582	17.0	-207.087182	28.2	-207.086003	98.0	-207.085899
6.0	-207.076846	17.2	-207.087090	28.4	-207.086000	100.0	-207.085899
6.2	-207.077394	17.4	-207.087005	28.6	-207.085997	150.0	-207.085898
6.4	-207.078005	17.6	-207.086929	28.8	-207.085994	200.0	-207.085898
6.6	-207.078715	17.8	-207.086860	29.0	-207.085991		
6.8	-207.079543	18.0	-207.086797	29.2	-207.085988		
7.0	-207.080489	18.2	-207.086739	29.4	-207.085986		
7.2	-207.081528	18.4	-207.086687	29.6	-207.085983		
7.4	-207.082622	18.6	-207.086639	29.8	-207.085981		
7.6	-207.083733	18.8	-207.086596	30.0	-207.085978		
7.8	-207.084828	19.0	-207.086556	30.2	-207.085976		

Table S6: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $6^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.728103	8.0	-207.073716	19.2	-207.078972	30.4	-207.077540
1.5	-206.777119	8.2	-207.073926	19.4	-207.078894	30.6	-207.077534
1.6	-206.817559	8.4	-207.074113	19.6	-207.078820	30.8	-207.077529
1.7	-206.851129	8.6	-207.074289	19.8	-207.078750	31.0	-207.077523
1.8	-206.878883	8.8	-207.074463	20.0	-207.078683	31.2	-207.077518
1.9	-206.901642	9.0	-207.074643	20.2	-207.078621	31.4	-207.077514
2.0	-206.922213	9.2	-207.074834	20.4	-207.078561	31.6	-207.077509
2.1	-206.938320	9.4	-207.075037	20.6	-207.078505	31.8	-207.077504
2.2	-206.951550	9.6	-207.075255	20.8	-207.078452	32.0	-207.077500
2.3	-206.963493	9.8	-207.075488	21.0	-207.078402	33.0	-207.077480
2.4	-206.974345	10.0	-207.075736	21.2	-207.078355	34.0	-207.077463
2.5	-206.983878	10.2	-207.075998	21.4	-207.078310	35.0	-207.077448
2.6	-206.992049	10.4	-207.076271	21.6	-207.078268	36.0	-207.077436
2.7	-206.998984	10.6	-207.076553	21.8	-207.078228	37.0	-207.077425
2.8	-207.004860	10.8	-207.076841	22.0	-207.078190	38.0	-207.077415
2.9	-207.009860	11.0	-207.077132	22.2	-207.078155	39.0	-207.077407
3.0	-207.014148	11.2	-207.077423	22.4	-207.078121	40.0	-207.077400
3.1	-207.017867	11.4	-207.077711	22.6	-207.078089	42.0	-207.077388
3.2	-207.021136	11.6	-207.077991	22.8	-207.078059	44.0	-207.077379
3.3	-207.024059	11.8	-207.078265	23.0	-207.078031	46.0	-207.077371
3.4	-207.026720	12.0	-207.078529	23.2	-207.078003	48.0	-207.077365
3.5	-207.029192	12.2	-207.078781	23.4	-207.077978	50.0	-207.077361
3.6	-207.031529	12.4	-207.079020	23.6	-207.077953	52.0	-207.077357
3.7	-207.033773	12.6	-207.079245	23.8	-207.077930	54.0	-207.077354
3.8	-207.035951	12.8	-207.079453	24.0	-207.077908	56.0	-207.077351
3.9	-207.038075	13.0	-207.079645	24.2	-207.077887	58.0	-207.077349
4.0	-207.040145	13.2	-207.079820	24.4	-207.077867	60.0	-207.077347
4.1	-207.042152	13.4	-207.079978	24.6	-207.077848	62.0	-207.077345
4.2	-207.044083	13.6	-207.080117	24.8	-207.077830	64.0	-207.077344
4.3	-207.045920	13.8	-207.080238	25.0	-207.077812	66.0	-207.077343
4.4	-207.047652	14.0	-207.080341	25.2	-207.077796	68.0	-207.077342
4.5	-207.049270	14.2	-207.080425	25.4	-207.077780	70.0	-207.077341
4.6	-207.050768	14.4	-207.080491	25.6	-207.077765	72.0	-207.077340
4.7	-207.052151	14.6	-207.080539	25.8	-207.077750	74.0	-207.077340
4.8	-207.053424	14.8	-207.080570	26.0	-207.077736	76.0	-207.077339
4.9	-207.054600	15.0	-207.080583	26.2	-207.077723	78.0	-207.077339
5.0	-207.055692	15.2	-207.080580	26.4	-207.077710	80.0	-207.077338
5.1	-207.056718	15.4	-207.080562	26.6	-207.077698	82.0	-207.077338
5.2	-207.057692	15.6	-207.080529	26.8	-207.077687	84.0	-207.077337
5.3	-207.058631	15.8	-207.080483	27.0	-207.077675	86.0	-207.077337
5.4	-207.059547	16.0	-207.080426	27.2	-207.077665	88.0	-207.077337
5.5	-207.060450	16.2	-207.080358	27.4	-207.077654	90.0	-207.077337
5.6	-207.061345	16.4	-207.080280	27.6	-207.077645	92.0	-207.077337
5.7	-207.062237	16.6	-207.080196	27.8	-207.077635	94.0	-207.077336
5.8	-207.063125	16.8	-207.080105	28.0	-207.077626	96.0	-207.077336
5.9	-207.064006	17.0	-207.080010	28.2	-207.077617	98.0	-207.077336
6.0	-207.064874	17.2	-207.079912	28.4	-207.077609	100.0	-207.077336
6.2	-207.066547	17.4	-207.079812	28.6	-207.077601	150.0	-207.077335
6.4	-207.068090	17.6	-207.079711	28.8	-207.077593	200.0	-207.077334
6.6	-207.069450	17.8	-207.079611	29.0	-207.077585		
6.8	-207.070591	18.0	-207.079511	29.2	-207.077578		
7.0	-207.071505	18.2	-207.079414	29.4	-207.077571		
7.2	-207.072211	18.4	-207.079319	29.6	-207.077564		
7.4	-207.072746	18.6	-207.079227	29.8	-207.077558		
7.6	-207.073152	18.8	-207.079138	30.0	-207.077552		
7.8	-207.073465	19.0	-207.079053	30.2	-207.077546		

Table S7: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $1^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.927881	8.0	-207.203512	19.2	-207.201252	30.4	-207.201212
1.5	-206.975890	8.2	-207.203200	19.4	-207.201250	30.6	-207.201211
1.6	-207.017805	8.4	-207.202943	19.6	-207.201248	30.8	-207.201211
1.7	-207.054947	8.6	-207.202731	19.8	-207.201247	31.0	-207.201211
1.8	-207.087508	8.8	-207.202555	20.0	-207.201245	31.2	-207.201211
1.9	-207.115514	9.0	-207.202406	20.2	-207.201243	31.4	-207.201211
2.0	-207.139185	9.2	-207.202281	20.4	-207.201242	31.6	-207.201210
2.1	-207.158931	9.4	-207.202174	20.6	-207.201240	31.8	-207.201210
2.2	-207.175246	9.6	-207.202082	20.8	-207.201239	32.0	-207.201210
2.3	-207.188626	9.8	-207.202001	21.0	-207.201238	33.0	-207.201209
2.4	-207.199532	10.0	-207.201931	21.2	-207.201236	34.0	-207.201209
2.5	-207.208369	10.2	-207.201869	21.4	-207.201235	35.0	-207.201208
2.6	-207.215484	10.4	-207.201814	21.6	-207.201234	36.0	-207.201208
2.7	-207.221167	10.6	-207.201765	21.8	-207.201233	37.0	-207.201207
2.8	-207.225659	10.8	-207.201722	22.0	-207.201232	38.0	-207.201207
2.9	-207.229158	11.0	-207.201682	22.2	-207.201231	39.0	-207.201207
3.0	-207.231832	11.2	-207.201647	22.4	-207.201230	40.0	-207.201206
3.1	-207.233821	11.4	-207.201615	22.6	-207.201229	42.0	-207.201206
3.2	-207.235237	11.6	-207.201586	22.8	-207.201228	44.0	-207.201206
3.3	-207.236176	11.8	-207.201559	23.0	-207.201227	46.0	-207.201205
3.4	-207.236716	12.0	-207.201535	23.2	-207.201226	48.0	-207.201205
3.5	-207.236923	12.2	-207.201513	23.4	-207.201226	50.0	-207.201205
3.6	-207.236854	12.4	-207.201493	23.6	-207.201225	52.0	-207.201205
3.7	-207.236553	12.6	-207.201474	23.8	-207.201224	54.0	-207.201205
3.8	-207.236061	12.8	-207.201457	24.0	-207.201224	56.0	-207.201205
3.9	-207.235411	13.0	-207.201441	24.2	-207.201223	58.0	-207.201204
4.0	-207.234631	13.2	-207.201427	24.4	-207.201222	60.0	-207.201204
4.1	-207.233745	13.4	-207.201413	24.6	-207.201222	62.0	-207.201204
4.2	-207.232773	13.6	-207.201401	24.8	-207.201221	64.0	-207.201204
4.3	-207.231734	13.8	-207.201390	25.0	-207.201221	66.0	-207.201204
4.4	-207.230643	14.0	-207.201379	25.2	-207.201220	68.0	-207.201204
4.5	-207.229512	14.2	-207.201369	25.4	-207.201220	70.0	-207.201204
4.6	-207.228354	14.4	-207.201360	25.6	-207.201219	72.0	-207.201204
4.7	-207.227177	14.6	-207.201351	25.8	-207.201219	74.0	-207.201204
4.8	-207.225991	14.8	-207.201343	26.0	-207.201218	76.0	-207.201204
4.9	-207.224804	15.0	-207.201336	26.2	-207.201218	78.0	-207.201204
5.0	-207.223621	15.2	-207.201329	26.4	-207.201217	80.0	-207.201204
5.1	-207.222449	15.4	-207.201322	26.6	-207.201217	82.0	-207.201204
5.2	-207.221293	15.6	-207.201316	26.8	-207.201217	84.0	-207.201204
5.3	-207.220158	15.8	-207.201311	27.0	-207.201216	86.0	-207.201204
5.4	-207.219047	16.0	-207.201305	27.2	-207.201216	88.0	-207.201204
5.5	-207.217965	16.2	-207.201300	27.4	-207.201215	90.0	-207.201204
5.6	-207.216914	16.4	-207.201296	27.6	-207.201215	92.0	-207.201204
5.7	-207.215898	16.6	-207.201291	27.8	-207.201215	94.0	-207.201204
5.8	-207.214919	16.8	-207.201287	28.0	-207.201215	96.0	-207.201204
5.9	-207.213979	17.0	-207.201283	28.2	-207.201214	98.0	-207.201204
6.0	-207.213079	17.2	-207.201279	28.4	-207.201214	100.0	-207.201204
6.2	-207.211406	17.4	-207.201276	28.6	-207.201214	150.0	-207.201204
6.4	-207.209908	17.6	-207.201273	28.8	-207.201213	200.0	-207.201204
6.6	-207.208586	17.8	-207.201270	29.0	-207.201213		
6.8	-207.207437	18.0	-207.201267	29.2	-207.201213		
7.0	-207.206453	18.2	-207.201264	29.4	-207.201213		
7.2	-207.205624	18.4	-207.201261	29.6	-207.201212		
7.4	-207.204932	18.6	-207.201259	29.8	-207.201212		
7.6	-207.204362	18.8	-207.201257	30.0	-207.201212		
7.8	-207.203895	19.0	-207.201254	30.2	-207.201212		



Table S8: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $2^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.838899	8.0	-207.188091	19.2	-207.184827	30.4	-207.184665
1.5	-206.896836	8.2	-207.187931	19.4	-207.184821	30.6	-207.184664
1.6	-206.943510	8.4	-207.187753	19.6	-207.184814	30.8	-207.184663
1.7	-206.980731	8.6	-207.187569	19.8	-207.184808	31.0	-207.184662
1.8	-207.010363	8.8	-207.187385	20.0	-207.184802	31.2	-207.184661
1.9	-207.034084	9.0	-207.187201	20.2	-207.184796	31.4	-207.184660
2.0	-207.053198	9.2	-207.187031	20.4	-207.184790	31.6	-207.184659
2.1	-207.068683	9.4	-207.186872	20.6	-207.184785	31.8	-207.184658
2.2	-207.081289	9.6	-207.186722	20.8	-207.184780	32.0	-207.184657
2.3	-207.091612	9.8	-207.186583	21.0	-207.184775	33.0	-207.184653
2.4	-207.100131	10.0	-207.186455	21.2	-207.184770	34.0	-207.184650
2.5	-207.107235	10.2	-207.186337	21.4	-207.184766	35.0	-207.184647
2.6	-207.113234	10.4	-207.186227	21.6	-207.184761	36.0	-207.184644
2.7	-207.118378	10.6	-207.186127	21.8	-207.184757	37.0	-207.184642
2.8	-207.122862	10.8	-207.186034	22.0	-207.184753	38.0	-207.184640
2.9	-207.126841	11.0	-207.185948	22.2	-207.184749	39.0	-207.184638
3.0	-207.130428	11.2	-207.185869	22.4	-207.184745	40.0	-207.184636
3.1	-207.133719	11.4	-207.185796	22.6	-207.184742	42.0	-207.184633
3.2	-207.136781	11.6	-207.185724	22.8	-207.184738	44.0	-207.184631
3.3	-207.139666	11.8	-207.185661	23.0	-207.184735	46.0	-207.184629
3.4	-207.142410	12.0	-207.185603	23.2	-207.184731	48.0	-207.184627
3.5	-207.145041	12.2	-207.185550	23.4	-207.184728	50.0	-207.184626
3.6	-207.147577	12.4	-207.185500	23.6	-207.184725	52.0	-207.184624
3.7	-207.150031	12.6	-207.185453	23.8	-207.184722	54.0	-207.184623
3.8	-207.152408	12.8	-207.185410	24.0	-207.184720	56.0	-207.184622
3.9	-207.154714	13.0	-207.185370	24.2	-207.184717	58.0	-207.184622
4.0	-207.156950	13.2	-207.185333	24.4	-207.184714	60.0	-207.184621
4.1	-207.159114	13.4	-207.185298	24.6	-207.184712	62.0	-207.184620
4.2	-207.161204	13.6	-207.185265	24.8	-207.184709	64.0	-207.184620
4.3	-207.163219	13.8	-207.185235	25.0	-207.184707	66.0	-207.184619
4.4	-207.165154	14.0	-207.185206	25.2	-207.184705	68.0	-207.184619
4.5	-207.167008	14.2	-207.185179	25.4	-207.184702	70.0	-207.184619
4.6	-207.168778	14.4	-207.185154	25.6	-207.184700	72.0	-207.184618
4.7	-207.170462	14.6	-207.185130	25.8	-207.184698	74.0	-207.184618
4.8	-207.172059	14.8	-207.185107	26.0	-207.184696	76.0	-207.184618
4.9	-207.173569	15.0	-207.185086	26.2	-207.184694	78.0	-207.184618
5.0	-207.174990	15.2	-207.185066	26.4	-207.184692	80.0	-207.184617
5.1	-207.176325	15.4	-207.185048	26.6	-207.184691	82.0	-207.184617
5.2	-207.177573	15.6	-207.185030	26.8	-207.184689	84.0	-207.184617
5.3	-207.178737	15.8	-207.185013	27.0	-207.184687	86.0	-207.184617
5.4	-207.179818	16.0	-207.184997	27.2	-207.184685	88.0	-207.184617
5.5	-207.180819	16.2	-207.184982	27.4	-207.184684	90.0	-207.184617
5.6	-207.181742	16.4	-207.184968	27.6	-207.184682	92.0	-207.184617
5.7	-207.182590	16.6	-207.184954	27.8	-207.184681	94.0	-207.184616
5.8	-207.183366	16.8	-207.184941	28.0	-207.184679	96.0	-207.184616
5.9	-207.184072	17.0	-207.184929	28.2	-207.184678	98.0	-207.184616
6.0	-207.184712	17.2	-207.184917	28.4	-207.184676	100.0	-207.184616
6.2	-207.185803	17.4	-207.184906	28.6	-207.184675	150.0	-207.184615
6.4	-207.186663	17.6	-207.184896	28.8	-207.184674	200.0	-207.184615
6.6	-207.187317	17.8	-207.184886	29.0	-207.184672		
6.8	-207.187786	18.0	-207.184876	29.2	-207.184671		
7.0	-207.188095	18.2	-207.184867	29.4	-207.184670		
7.2	-207.188269	18.4	-207.184858	29.6	-207.184669		
7.4	-207.188333	18.6	-207.184850	29.8	-207.184668		
7.6	-207.188310	18.8	-207.184842	30.0	-207.184667		
7.8	-207.188223	19.0	-207.184835	30.2	-207.184666		

Table S9: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $3^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.762869	8.0	-207.137094	19.2	-207.133519	30.4	-207.133312
1.5	-206.812403	8.2	-207.137120	19.4	-207.133510	30.6	-207.133311
1.6	-206.853590	8.4	-207.137088	19.6	-207.133502	30.8	-207.133309
1.7	-206.888154	8.6	-207.137010	19.8	-207.133494	31.0	-207.133308
1.8	-206.917500	8.8	-207.136896	20.0	-207.133486	31.2	-207.133307
1.9	-206.943885	9.0	-207.136756	20.2	-207.133478	31.4	-207.133306
2.0	-206.965881	9.2	-207.136598	20.4	-207.133471	31.6	-207.133305
2.1	-206.984095	9.4	-207.136429	20.6	-207.133464	31.8	-207.133304
2.2	-206.999090	9.6	-207.136254	20.8	-207.133458	32.0	-207.133303
2.3	-207.011377	9.8	-207.136079	21.0	-207.133451	33.0	-207.133298
2.4	-207.021408	10.0	-207.135906	21.2	-207.133445	34.0	-207.133293
2.5	-207.029578	10.2	-207.135738	21.4	-207.133440	35.0	-207.133289
2.6	-207.036226	10.4	-207.135578	21.6	-207.133434	36.0	-207.133286
2.7	-207.041640	10.6	-207.135426	21.8	-207.133429	37.0	-207.133283
2.8	-207.046060	10.8	-207.135283	22.0	-207.133424	38.0	-207.133280
2.9	-207.049690	11.0	-207.135150	22.2	-207.133419	39.0	-207.133278
3.0	-207.052708	11.2	-207.135025	22.4	-207.133414	40.0	-207.133276
3.1	-207.055272	11.4	-207.134910	22.6	-207.133409	42.0	-207.133272
3.2	-207.057578	11.6	-207.134804	22.8	-207.133405	44.0	-207.133269
3.3	-207.060359	11.8	-207.134707	23.0	-207.133401	46.0	-207.133266
3.4	-207.064706	12.0	-207.134617	23.2	-207.133396	48.0	-207.133264
3.5	-207.069376	12.2	-207.134534	23.4	-207.133392	50.0	-207.133262
3.6	-207.073951	12.4	-207.134458	23.6	-207.133389	52.0	-207.133261
3.7	-207.078365	12.6	-207.134388	23.8	-207.133385	54.0	-207.133259
3.8	-207.082592	12.8	-207.134324	24.0	-207.133381	56.0	-207.133258
3.9	-207.086618	13.0	-207.134264	24.2	-207.133378	58.0	-207.133257
4.0	-207.090431	13.2	-207.134209	24.4	-207.133375	60.0	-207.133256
4.1	-207.094028	13.4	-207.134159	24.6	-207.133371	62.0	-207.133256
4.2	-207.097407	13.6	-207.134112	24.8	-207.133368	64.0	-207.133255
4.3	-207.100570	13.8	-207.134068	25.0	-207.133365	66.0	-207.133254
4.4	-207.103522	14.0	-207.134027	25.2	-207.133362	68.0	-207.133254
4.5	-207.106273	14.2	-207.133989	25.4	-207.133360	70.0	-207.133253
4.6	-207.108832	14.4	-207.133954	25.6	-207.133357	72.0	-207.133253
4.7	-207.111209	14.6	-207.133921	25.8	-207.133354	74.0	-207.133253
4.8	-207.113415	14.8	-207.133890	26.0	-207.133352	76.0	-207.133252
4.9	-207.115461	15.0	-207.133861	26.2	-207.133349	78.0	-207.133252
5.0	-207.117359	15.2	-207.133834	26.4	-207.133347	80.0	-207.133252
5.1	-207.119118	15.4	-207.133809	26.6	-207.133345	82.0	-207.133252
5.2	-207.120748	15.6	-207.133785	26.8	-207.133342	84.0	-207.133251
5.3	-207.122259	15.8	-207.133762	27.0	-207.133340	86.0	-207.133251
5.4	-207.123658	16.0	-207.133741	27.2	-207.133338	88.0	-207.133251
5.5	-207.124954	16.2	-207.133721	27.4	-207.133336	90.0	-207.133251
5.6	-207.126153	16.4	-207.133702	27.6	-207.133334	92.0	-207.133251
5.7	-207.127262	16.6	-207.133684	27.8	-207.133332	94.0	-207.133251
5.8	-207.128287	16.8	-207.133667	28.0	-207.133330	96.0	-207.133250
5.9	-207.129233	17.0	-207.133651	28.2	-207.133329	98.0	-207.133250
6.0	-207.130104	17.2	-207.133636	28.4	-207.133327	100.0	-207.133250
6.2	-207.131641	17.4	-207.133621	28.6	-207.133325	150.0	-207.133249
6.4	-207.132931	17.6	-207.133608	28.8	-207.133324	200.0	-207.133249
6.6	-207.134000	17.8	-207.133595	29.0	-207.133322		
6.8	-207.134873	18.0	-207.133582	29.2	-207.133320		
7.0	-207.135571	18.2	-207.133570	29.4	-207.133319		
7.2	-207.136115	18.4	-207.133559	29.6	-207.133317		
7.4	-207.136522	18.6	-207.133548	29.8	-207.133316		
7.6	-207.136809	18.8	-207.133538	30.0	-207.133315		
7.8	-207.136995	19.0	-207.133528	30.2	-207.133313		

Table S10: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $4^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.710397	8.0	-207.097411	19.2	-207.096838	30.4	-207.096416
1.5	-206.761501	8.2	-207.098352	19.4	-207.096816	30.6	-207.096414
1.6	-206.807281	8.4	-207.099191	19.6	-207.096794	30.8	-207.096412
1.7	-206.847067	8.6	-207.099927	19.8	-207.096774	31.0	-207.096410
1.8	-206.881121	8.8	-207.100561	20.0	-207.096756	31.2	-207.096409
1.9	-206.909891	9.0	-207.101092	20.2	-207.096738	31.4	-207.096407
2.0	-206.934010	9.2	-207.101530	20.4	-207.096721	31.6	-207.096405
2.1	-206.954161	9.4	-207.101877	20.6	-207.096705	31.8	-207.096404
2.2	-206.971000	9.6	-207.102137	20.8	-207.096690	32.0	-207.096402
2.3	-206.985122	9.8	-207.102318	21.0	-207.096676	33.0	-207.096396
2.4	-206.997050	10.0	-207.102426	21.2	-207.096663	34.0	-207.096390
2.5	-207.007236	10.2	-207.102468	21.4	-207.096650	35.0	-207.096385
2.6	-207.016059	10.4	-207.102451	21.6	-207.096638	36.0	-207.096381
2.7	-207.023834	10.6	-207.102381	21.8	-207.096627	37.0	-207.096377
2.8	-207.030813	10.8	-207.102266	22.0	-207.096616	38.0	-207.096374
2.9	-207.037192	11.0	-207.102113	22.2	-207.096605	39.0	-207.096371
3.0	-207.043117	11.2	-207.101928	22.4	-207.096596	40.0	-207.096369
3.1	-207.048684	11.4	-207.101717	22.6	-207.096586	42.0	-207.096365
3.2	-207.053881	11.6	-207.101485	22.8	-207.096577	44.0	-207.096362
3.3	-207.058113	11.8	-207.101241	23.0	-207.096569	46.0	-207.096359
3.4	-207.060384	12.0	-207.100988	23.2	-207.096561	48.0	-207.096357
3.5	-207.061999	12.2	-207.100730	23.4	-207.096553	50.0	-207.096355
3.6	-207.063415	12.4	-207.100473	23.6	-207.096546	52.0	-207.096354
3.7	-207.064720	12.6	-207.100219	23.8	-207.096539	54.0	-207.096353
3.8	-207.065949	12.8	-207.099972	24.0	-207.096532	56.0	-207.096352
3.9	-207.067119	13.0	-207.099733	24.2	-207.096526	58.0	-207.096351
4.0	-207.068242	13.2	-207.099504	24.4	-207.096520	60.0	-207.096351
4.1	-207.069323	13.4	-207.099288	24.6	-207.096514	62.0	-207.096350
4.2	-207.070364	13.6	-207.099083	24.8	-207.096508	64.0	-207.096350
4.3	-207.071369	13.8	-207.098892	25.0	-207.096503	66.0	-207.096349
4.4	-207.072336	14.0	-207.098713	25.2	-207.096497	68.0	-207.096349
4.5	-207.073268	14.2	-207.098548	25.4	-207.096493	70.0	-207.096349
4.6	-207.074166	14.4	-207.098394	25.6	-207.096488	72.0	-207.096348
4.7	-207.075030	14.6	-207.098252	25.8	-207.096483	74.0	-207.096348
4.8	-207.075864	14.8	-207.098122	26.0	-207.096479	76.0	-207.096348
4.9	-207.076668	15.0	-207.098001	26.2	-207.096475	78.0	-207.096348
5.0	-207.077447	15.2	-207.097891	26.4	-207.096471	80.0	-207.096348
5.1	-207.078202	15.4	-207.097789	26.6	-207.096467	82.0	-207.096348
5.2	-207.078938	15.6	-207.097696	26.8	-207.096463	84.0	-207.096347
5.3	-207.079658	15.8	-207.097610	27.0	-207.096460	86.0	-207.096347
5.4	-207.080365	16.0	-207.097531	27.2	-207.096456	88.0	-207.096347
5.5	-207.081062	16.2	-207.097458	27.4	-207.096453	90.0	-207.096347
5.6	-207.081752	16.4	-207.097391	27.6	-207.096450	92.0	-207.096347
5.7	-207.082439	16.6	-207.097330	27.8	-207.096447	94.0	-207.096347
5.8	-207.083124	16.8	-207.097273	28.0	-207.096444	96.0	-207.096347
5.9	-207.083810	17.0	-207.097220	28.2	-207.096441	98.0	-207.096347
6.0	-207.084497	17.2	-207.097171	28.4	-207.096438	100.0	-207.096347
6.2	-207.085878	17.4	-207.097126	28.6	-207.096435	150.0	-207.096346
6.4	-207.087270	17.6	-207.097085	28.8	-207.096433	200.0	-207.096346
6.6	-207.088664	17.8	-207.097046	29.0	-207.096430		
6.8	-207.090053	18.0	-207.097010	29.2	-207.096428		
7.0	-207.091421	18.2	-207.096976	29.4	-207.096426		
7.2	-207.092752	18.4	-207.096945	29.6	-207.096424		
7.4	-207.094031	18.6	-207.096915	29.8	-207.096422		
7.6	-207.095242	18.8	-207.096888	30.0	-207.096419		
7.8	-207.096372	19.0	-207.096862	30.2	-207.096418		

Table S11: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $5^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.708963	8.0	-207.069937	19.2	-207.079057	30.4	-207.077540
1.5	-206.751350	8.2	-207.071260	19.4	-207.078964	30.6	-207.077534
1.6	-206.790944	8.4	-207.072481	19.6	-207.078878	30.8	-207.077529
1.7	-206.827380	8.6	-207.073607	19.8	-207.078797	31.0	-207.077523
1.8	-206.857790	8.8	-207.074646	20.0	-207.078722	31.2	-207.077518
1.9	-206.883059	9.0	-207.075607	20.2	-207.078652	31.4	-207.077514
2.0	-206.904017	9.2	-207.076494	20.4	-207.078587	31.6	-207.077509
2.1	-206.921380	9.4	-207.077314	20.6	-207.078526	31.8	-207.077504
2.2	-206.935775	9.6	-207.078070	20.8	-207.078469	32.0	-207.077500
2.3	-206.947781	9.8	-207.078768	21.0	-207.078416	33.0	-207.077480
2.4	-206.957986	10.0	-207.079410	21.2	-207.078366	34.0	-207.077463
2.5	-206.967092	10.2	-207.079999	21.4	-207.078319	35.0	-207.077448
2.6	-206.975411	10.4	-207.080536	21.6	-207.078275	36.0	-207.077436
2.7	-206.982771	10.6	-207.081025	21.8	-207.078234	37.0	-207.077425
2.8	-206.989180	10.8	-207.081466	22.0	-207.078195	38.0	-207.077415
2.9	-206.994748	11.0	-207.081860	22.2	-207.078159	39.0	-207.077407
3.0	-206.999598	11.2	-207.082210	22.4	-207.078124	40.0	-207.077400
3.1	-207.003844	11.4	-207.082517	22.6	-207.078092	42.0	-207.077388
3.2	-207.007593	11.6	-207.082781	22.8	-207.078061	44.0	-207.077379
3.3	-207.010942	11.8	-207.083005	23.0	-207.078032	46.0	-207.077371
3.4	-207.013982	12.0	-207.083189	23.2	-207.078005	48.0	-207.077365
3.5	-207.016798	12.2	-207.083336	23.4	-207.077979	50.0	-207.077361
3.6	-207.019474	12.4	-207.083446	23.6	-207.077954	52.0	-207.077357
3.7	-207.022087	12.6	-207.083522	23.8	-207.077931	54.0	-207.077354
3.8	-207.024669	12.8	-207.083566	24.0	-207.077908	56.0	-207.077351
3.9	-207.027182	13.0	-207.083578	24.2	-207.077887	58.0	-207.077349
4.0	-207.029550	13.2	-207.083562	24.4	-207.077867	60.0	-207.077347
4.1	-207.031721	13.4	-207.083519	24.6	-207.077848	62.0	-207.077345
4.2	-207.033677	13.6	-207.083452	24.8	-207.077830	64.0	-207.077344
4.3	-207.035420	13.8	-207.083362	25.0	-207.077812	66.0	-207.077343
4.4	-207.036967	14.0	-207.083253	25.2	-207.077796	68.0	-207.077342
4.5	-207.038347	14.2	-207.083125	25.4	-207.077780	70.0	-207.077341
4.6	-207.039597	14.4	-207.082982	25.6	-207.077765	72.0	-207.077340
4.7	-207.040767	14.6	-207.082824	25.8	-207.077750	74.0	-207.077340
4.8	-207.041916	14.8	-207.082656	26.0	-207.077736	76.0	-207.077339
4.9	-207.043090	15.0	-207.082477	26.2	-207.077723	78.0	-207.077339
5.0	-207.044298	15.2	-207.082291	26.4	-207.077710	80.0	-207.077338
5.1	-207.045522	15.4	-207.082100	26.6	-207.077698	82.0	-207.077338
5.2	-207.046738	15.6	-207.081904	26.8	-207.077687	84.0	-207.077337
5.3	-207.047929	15.8	-207.081707	27.0	-207.077675	86.0	-207.077337
5.4	-207.049086	16.0	-207.081509	27.2	-207.077665	88.0	-207.077337
5.5	-207.050203	16.2	-207.081312	27.4	-207.077654	90.0	-207.077337
5.6	-207.051275	16.4	-207.081117	27.6	-207.077645	92.0	-207.077337
5.7	-207.052303	16.6	-207.080926	27.8	-207.077635	94.0	-207.077336
5.8	-207.053284	16.8	-207.080740	28.0	-207.077626	96.0	-207.077336
5.9	-207.054220	17.0	-207.080559	28.2	-207.077617	98.0	-207.077336
6.0	-207.055111	17.2	-207.080385	28.4	-207.077609	100.0	-207.077336
6.2	-207.056762	17.4	-207.080217	28.6	-207.077601	150.0	-207.077335
6.4	-207.058253	17.6	-207.080057	28.8	-207.077593	200.0	-207.077334
6.6	-207.059611	17.8	-207.079905	29.0	-207.077585		
6.8	-207.060891	18.0	-207.079760	29.2	-207.077578		
7.0	-207.062207	18.2	-207.079624	29.4	-207.077571		
7.2	-207.063700	18.4	-207.079495	29.6	-207.077564		
7.4	-207.065335	18.6	-207.079375	29.8	-207.077558		
7.6	-207.066963	18.8	-207.079261	30.0	-207.077552		
7.8	-207.068504	19.0	-207.079156	30.2	-207.077546		

Table S12: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $1^1\Pi$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.921608	8.0	-207.133260	19.2	-207.133172	30.4	-207.133226
1.5	-206.962856	8.2	-207.133178	19.4	-207.133174	30.6	-207.133226
1.6	-206.996139	8.4	-207.133115	19.6	-207.133175	30.8	-207.133227
1.7	-207.023670	8.6	-207.133067	19.8	-207.133177	31.0	-207.133227
1.8	-207.046679	8.8	-207.133031	20.0	-207.133179	31.2	-207.133227
1.9	-207.065897	9.0	-207.133006	20.2	-207.133181	31.4	-207.133228
2.0	-207.081845	9.2	-207.132988	20.4	-207.133183	31.6	-207.133228
2.1	-207.094938	9.4	-207.132976	20.6	-207.133184	31.8	-207.133228
2.2	-207.105556	9.6	-207.132970	20.8	-207.133186	32.0	-207.133229
2.3	-207.114065	9.8	-207.132967	21.0	-207.133187	33.0	-207.133230
2.4	-207.120793	10.0	-207.132966	21.2	-207.133189	34.0	-207.133232
2.5	-207.126045	10.2	-207.132968	21.4	-207.133190	35.0	-207.133233
2.6	-207.130081	10.4	-207.132972	21.6	-207.133192	36.0	-207.133234
2.7	-207.133130	10.6	-207.132977	21.8	-207.133193	37.0	-207.133235
2.8	-207.135388	10.8	-207.132982	22.0	-207.133194	38.0	-207.133236
2.9	-207.137018	11.0	-207.132988	22.2	-207.133196	39.0	-207.133237
3.0	-207.138159	11.2	-207.132995	22.4	-207.133197	40.0	-207.133238
3.1	-207.138929	11.4	-207.133002	22.6	-207.133198	42.0	-207.133239
3.2	-207.139422	11.6	-207.133009	22.8	-207.133199	44.0	-207.133240
3.3	-207.139715	11.8	-207.133016	23.0	-207.133200	46.0	-207.133241
3.4	-207.139873	12.0	-207.133023	23.2	-207.133201	48.0	-207.133242
3.5	-207.139939	12.2	-207.133030	23.4	-207.133202	50.0	-207.133243
3.6	-207.139946	12.4	-207.133037	23.6	-207.133203	52.0	-207.133243
3.7	-207.139915	12.6	-207.133043	23.8	-207.133204	54.0	-207.133244
3.8	-207.139860	12.8	-207.133050	24.0	-207.133205	56.0	-207.133244
3.9	-207.139787	13.0	-207.133056	24.2	-207.133206	58.0	-207.133245
4.0	-207.139698	13.2	-207.133062	24.4	-207.133207	60.0	-207.133245
4.1	-207.139599	13.4	-207.133068	24.6	-207.133208	62.0	-207.133245
4.2	-207.139483	13.6	-207.133073	24.8	-207.133209	64.0	-207.133246
4.3	-207.139351	13.8	-207.133079	25.0	-207.133210	66.0	-207.133246
4.4	-207.139206	14.0	-207.133084	25.2	-207.133211	68.0	-207.133246
4.5	-207.139048	14.2	-207.133089	25.4	-207.133211	70.0	-207.133246
4.6	-207.138872	14.4	-207.133094	25.6	-207.133212	72.0	-207.133247
4.7	-207.138684	14.6	-207.133099	25.8	-207.133213	74.0	-207.133247
4.8	-207.138488	14.8	-207.133104	26.0	-207.133214	76.0	-207.133247
4.9	-207.138279	15.0	-207.133108	26.2	-207.133214	78.0	-207.133247
5.0	-207.138061	15.2	-207.133112	26.4	-207.133215	80.0	-207.133247
5.1	-207.137833	15.4	-207.133116	26.6	-207.133216	82.0	-207.133247
5.2	-207.137604	15.6	-207.133120	26.8	-207.133216	84.0	-207.133247
5.3	-207.137371	15.8	-207.133124	27.0	-207.133217	86.0	-207.133247
5.4	-207.137136	16.0	-207.133128	27.2	-207.133218	88.0	-207.133247
5.5	-207.136902	16.2	-207.133131	27.4	-207.133218	90.0	-207.133247
5.6	-207.136669	16.4	-207.133135	27.6	-207.133219	92.0	-207.133248
5.7	-207.136439	16.6	-207.133138	27.8	-207.133219	94.0	-207.133248
5.8	-207.136212	16.8	-207.133141	28.0	-207.133220	96.0	-207.133248
5.9	-207.135991	17.0	-207.133144	28.2	-207.133221	98.0	-207.133248
6.0	-207.135775	17.2	-207.133147	28.4	-207.133221	100.0	-207.133248
6.2	-207.135365	17.4	-207.133150	28.6	-207.133222	150.0	-207.133248
6.4	-207.134987	17.6	-207.133153	28.8	-207.133222	200.0	-207.133248
6.6	-207.134644	17.8	-207.133155	29.0	-207.133223		
6.8	-207.134340	18.0	-207.133158	29.2	-207.133223		
7.0	-207.134074	18.2	-207.133160	29.4	-207.133224		
7.2	-207.133846	18.4	-207.133163	29.6	-207.133224		
7.4	-207.133654	18.6	-207.133165	29.8	-207.133224		
7.6	-207.133494	18.8	-207.133167	30.0	-207.133225		
7.8	-207.133364	19.0	-207.133169	30.2	-207.133225		

Table S13: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $2^1\Pi$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.819661	8.0	-207.123425	19.2	-207.124111	30.4	-207.124163
1.5	-206.868022	8.2	-207.123538	19.4	-207.124113	30.6	-207.124164
1.6	-206.909460	8.4	-207.123626	19.6	-207.124115	30.8	-207.124164
1.7	-206.944904	8.6	-207.123695	19.8	-207.124117	31.0	-207.124164
1.8	-206.974897	8.8	-207.123749	20.0	-207.124118	31.2	-207.124165
1.9	-207.000031	9.0	-207.123791	20.2	-207.124120	31.4	-207.124165
2.0	-207.020964	9.2	-207.123824	20.4	-207.124122	31.6	-207.124165
2.1	-207.038336	9.4	-207.123850	20.6	-207.124123	31.8	-207.124166
2.2	-207.052721	9.6	-207.123872	20.8	-207.124125	32.0	-207.124166
2.3	-207.064635	9.8	-207.123889	21.0	-207.124126	33.0	-207.124168
2.4	-207.074496	10.0	-207.123903	21.2	-207.124127	34.0	-207.124169
2.5	-207.082666	10.2	-207.123914	21.4	-207.124129	35.0	-207.124171
2.6	-207.089432	10.4	-207.123924	21.6	-207.124130	36.0	-207.124172
2.7	-207.095028	10.6	-207.123933	21.8	-207.124131	37.0	-207.124173
2.8	-207.099647	10.8	-207.123942	22.0	-207.124133	38.0	-207.124174
2.9	-207.103438	11.0	-207.123949	22.2	-207.124134	39.0	-207.124175
3.0	-207.106525	11.2	-207.123957	22.4	-207.124135	40.0	-207.124175
3.1	-207.109012	11.4	-207.123963	22.6	-207.124136	42.0	-207.124177
3.2	-207.110980	11.6	-207.123968	22.8	-207.124137	44.0	-207.124178
3.3	-207.112500	11.8	-207.123975	23.0	-207.124138	46.0	-207.124179
3.4	-207.113634	12.0	-207.123981	23.2	-207.124139	48.0	-207.124180
3.5	-207.114441	12.2	-207.123987	23.4	-207.124140	50.0	-207.124181
3.6	-207.114976	12.4	-207.123993	23.6	-207.124141	52.0	-207.124181
3.7	-207.115291	12.6	-207.123999	23.8	-207.124142	54.0	-207.124182
3.8	-207.115437	12.8	-207.124004	24.0	-207.124143	56.0	-207.124182
3.9	-207.115461	13.0	-207.124009	24.2	-207.124144	58.0	-207.124183
4.0	-207.115405	13.2	-207.124015	24.4	-207.124145	60.0	-207.124183
4.1	-207.115306	13.4	-207.124020	24.6	-207.124146	62.0	-207.124183
4.2	-207.115198	13.6	-207.124025	24.8	-207.124147	64.0	-207.124184
4.3	-207.115107	13.8	-207.124029	25.0	-207.124148	66.0	-207.124184
4.4	-207.115051	14.0	-207.124033	25.2	-207.124148	68.0	-207.124184
4.5	-207.115045	14.2	-207.124038	25.4	-207.124149	70.0	-207.124184
4.6	-207.115096	14.4	-207.124042	25.6	-207.124150	72.0	-207.124184
4.7	-207.115208	14.6	-207.124046	25.8	-207.124151	74.0	-207.124185
4.8	-207.115379	14.8	-207.124050	26.0	-207.124151	76.0	-207.124185
4.9	-207.115604	15.0	-207.124054	26.2	-207.124152	78.0	-207.124185
5.0	-207.115877	15.2	-207.124058	26.4	-207.124153	80.0	-207.124185
5.1	-207.116190	15.4	-207.124061	26.6	-207.124153	82.0	-207.124185
5.2	-207.116534	15.6	-207.124065	26.8	-207.124154	84.0	-207.124185
5.3	-207.116902	15.8	-207.124068	27.0	-207.124155	86.0	-207.124185
5.4	-207.117285	16.0	-207.124071	27.2	-207.124155	88.0	-207.124185
5.5	-207.117677	16.2	-207.124074	27.4	-207.124156	90.0	-207.124185
5.6	-207.118071	16.4	-207.124077	27.6	-207.124156	92.0	-207.124185
5.7	-207.118462	16.6	-207.124080	27.8	-207.124157	94.0	-207.124186
5.8	-207.118847	16.8	-207.124083	28.0	-207.124157	96.0	-207.124186
5.9	-207.119222	17.0	-207.124086	28.2	-207.124158	98.0	-207.124186
6.0	-207.119585	17.2	-207.124089	28.4	-207.124159	100.0	-207.124186
6.2	-207.120264	17.4	-207.124091	28.6	-207.124159	150.0	-207.124186
6.4	-207.120875	17.6	-207.124094	28.8	-207.124160	200.0	-207.124186
6.6	-207.121413	17.8	-207.124096	29.0	-207.124160		
6.8	-207.121878	18.0	-207.124099	29.2	-207.124161		
7.0	-207.122274	18.2	-207.124101	29.4	-207.124161		
7.2	-207.122605	18.4	-207.124103	29.6	-207.124161		
7.4	-207.122879	18.6	-207.124105	29.8	-207.124162		
7.6	-207.123103	18.8	-207.124107	30.0	-207.124162		
7.8	-207.123282	19.0	-207.124109	30.2	-207.124163		

Table S14: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $1^3\Pi$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.999024	8.0	-207.184202	19.2	-207.184548	30.4	-207.184596
1.5	-207.040844	8.2	-207.184211	19.4	-207.184550	30.6	-207.184596
1.6	-207.074324	8.4	-207.184222	19.6	-207.184552	30.8	-207.184596
1.7	-207.101481	8.6	-207.184233	19.8	-207.184554	31.0	-207.184597
1.8	-207.123536	8.8	-207.184245	20.0	-207.184555	31.2	-207.184597
1.9	-207.141335	9.0	-207.184257	20.2	-207.184557	31.4	-207.184597
2.0	-207.155556	9.2	-207.184269	20.4	-207.184558	31.6	-207.184598
2.1	-207.166770	9.4	-207.184281	20.6	-207.184560	31.8	-207.184598
2.2	-207.175480	9.6	-207.184295	20.8	-207.184561	32.0	-207.184598
2.3	-207.182123	9.8	-207.184307	21.0	-207.184562	33.0	-207.184600
2.4	-207.187083	10.0	-207.184319	21.2	-207.184564	34.0	-207.184601
2.5	-207.190684	10.2	-207.184329	21.4	-207.184565	35.0	-207.184602
2.6	-207.193200	10.4	-207.184340	21.6	-207.184566	36.0	-207.184603
2.7	-207.194858	10.6	-207.184351	21.8	-207.184567	37.0	-207.184604
2.8	-207.195845	10.8	-207.184361	22.0	-207.184568	38.0	-207.184605
2.9	-207.196310	11.0	-207.184371	22.2	-207.184569	39.0	-207.184606
3.0	-207.196380	11.2	-207.184380	22.4	-207.184571	40.0	-207.184606
3.1	-207.196160	11.4	-207.184389	22.6	-207.184572	42.0	-207.184607
3.2	-207.195730	11.6	-207.184391	22.8	-207.184573	44.0	-207.184608
3.3	-207.195152	11.8	-207.184399	23.0	-207.184574	46.0	-207.184609
3.4	-207.194479	12.0	-207.184407	23.2	-207.184574	48.0	-207.184610
3.5	-207.193751	12.2	-207.184415	23.4	-207.184575	50.0	-207.184610
3.6	-207.192998	12.4	-207.184422	23.6	-207.184576	52.0	-207.184611
3.7	-207.192244	12.6	-207.184429	23.8	-207.184577	54.0	-207.184611
3.8	-207.191505	12.8	-207.184436	24.0	-207.184578	56.0	-207.184612
3.9	-207.190795	13.0	-207.184442	24.2	-207.184579	58.0	-207.184612
4.0	-207.190120	13.2	-207.184448	24.4	-207.184580	60.0	-207.184612
4.1	-207.189490	13.4	-207.184454	24.6	-207.184580	62.0	-207.184612
4.2	-207.188905	13.6	-207.184459	24.8	-207.184581	64.0	-207.184613
4.3	-207.188364	13.8	-207.184464	25.0	-207.184582	66.0	-207.184613
4.4	-207.187871	14.0	-207.184469	25.2	-207.184583	68.0	-207.184613
4.5	-207.187426	14.2	-207.184474	25.4	-207.184583	70.0	-207.184613
4.6	-207.187020	14.4	-207.184479	25.6	-207.184584	72.0	-207.184613
4.7	-207.186658	14.6	-207.184483	25.8	-207.184585	74.0	-207.184613
4.8	-207.186336	14.8	-207.184487	26.0	-207.184585	76.0	-207.184613
4.9	-207.186048	15.0	-207.184491	26.2	-207.184586	78.0	-207.184614
5.0	-207.185793	15.2	-207.184495	26.4	-207.184586	80.0	-207.184614
5.1	-207.185565	15.4	-207.184499	26.6	-207.184587	82.0	-207.184614
5.2	-207.185367	15.6	-207.184502	26.8	-207.184588	84.0	-207.184614
5.3	-207.185193	15.8	-207.184506	27.0	-207.184588	86.0	-207.184614
5.4	-207.185041	16.0	-207.184509	27.2	-207.184589	88.0	-207.184614
5.5	-207.184908	16.2	-207.184512	27.4	-207.184589	90.0	-207.184614
5.6	-207.184793	16.4	-207.184516	27.6	-207.184590	92.0	-207.184614
5.7	-207.184694	16.6	-207.184519	27.8	-207.184590	94.0	-207.184614
5.8	-207.184608	16.8	-207.184521	28.0	-207.184591	96.0	-207.184614
5.9	-207.184535	17.0	-207.184524	28.2	-207.184591	98.0	-207.184614
6.0	-207.184472	17.2	-207.184527	28.4	-207.184592	100.0	-207.184614
6.2	-207.184373	17.4	-207.184529	28.6	-207.184592	150.0	-207.184615
6.4	-207.184303	17.6	-207.184532	28.8	-207.184593	200.0	-207.184615
6.6	-207.184254	17.8	-207.184534	29.0	-207.184593		
6.8	-207.184222	18.0	-207.184536	29.2	-207.184593		
7.0	-207.184202	18.2	-207.184539	29.4	-207.184594		
7.2	-207.184192	18.4	-207.184541	29.6	-207.184594		
7.4	-207.184188	18.6	-207.184543	29.8	-207.184595		
7.6	-207.184190	18.8	-207.184545	30.0	-207.184595		
7.8	-207.184195	19.0	-207.184547	30.2	-207.184595		

Table S15: Total IH-FS-CCSD (2,0)/unANO-RCC+ energies for the  $2^3\Pi$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.803500	8.0	-207.132864	19.2	-207.133172	30.4	-207.133226
1.5	-206.849861	8.2	-207.132875	19.4	-207.133174	30.6	-207.133226
1.6	-206.892290	8.4	-207.132885	19.6	-207.133175	30.8	-207.133227
1.7	-206.928168	8.6	-207.132893	19.8	-207.133177	31.0	-207.133227
1.8	-206.958480	8.8	-207.132900	20.0	-207.133179	31.2	-207.133227
1.9	-206.983978	9.0	-207.132908	20.2	-207.133181	31.4	-207.133228
2.0	-207.005322	9.2	-207.132915	20.4	-207.133183	31.6	-207.133228
2.1	-207.023112	9.4	-207.132922	20.6	-207.133184	31.8	-207.133228
2.2	-207.037896	9.6	-207.132929	20.8	-207.133186	32.0	-207.133229
2.3	-207.050177	9.8	-207.132937	21.0	-207.133187	33.0	-207.133230
2.4	-207.060390	10.0	-207.132945	21.2	-207.133189	34.0	-207.133232
2.5	-207.068918	10.2	-207.132952	21.4	-207.133190	35.0	-207.133233
2.6	-207.076078	10.4	-207.132960	21.6	-207.133192	36.0	-207.133234
2.7	-207.082135	10.6	-207.132968	21.8	-207.133193	37.0	-207.133235
2.8	-207.087308	10.8	-207.132976	22.0	-207.133194	38.0	-207.133236
2.9	-207.091773	11.0	-207.132984	22.2	-207.133196	39.0	-207.133237
3.0	-207.095670	11.2	-207.132992	22.4	-207.133197	40.0	-207.133238
3.1	-207.099112	11.4	-207.133000	22.6	-207.133198	42.0	-207.133239
3.2	-207.102186	11.6	-207.133007	22.8	-207.133199	44.0	-207.133240
3.3	-207.104958	11.8	-207.133015	23.0	-207.133200	46.0	-207.133241
3.4	-207.107479	12.0	-207.133022	23.2	-207.133201	48.0	-207.133242
3.5	-207.109788	12.2	-207.133029	23.4	-207.133202	50.0	-207.133243
3.6	-207.111913	12.4	-207.133036	23.6	-207.133203	52.0	-207.133243
3.7	-207.113875	12.6	-207.133043	23.8	-207.133204	54.0	-207.133244
3.8	-207.115689	12.8	-207.133050	24.0	-207.133205	56.0	-207.133244
3.9	-207.117367	13.0	-207.133056	24.2	-207.133206	58.0	-207.133245
4.0	-207.118916	13.2	-207.133062	24.4	-207.133207	60.0	-207.133245
4.1	-207.120344	13.4	-207.133068	24.6	-207.133208	62.0	-207.133245
4.2	-207.121657	13.6	-207.133073	24.8	-207.133209	64.0	-207.133246
4.3	-207.122860	13.8	-207.133079	25.0	-207.133210	66.0	-207.133246
4.4	-207.123959	14.0	-207.133084	25.2	-207.133211	68.0	-207.133246
4.5	-207.124959	14.2	-207.133089	25.4	-207.133211	70.0	-207.133246
4.6	-207.125866	14.4	-207.133094	25.6	-207.133212	72.0	-207.133247
4.7	-207.126686	14.6	-207.133099	25.8	-207.133213	74.0	-207.133247
4.8	-207.127425	14.8	-207.133104	26.0	-207.133214	76.0	-207.133247
4.9	-207.128089	15.0	-207.133108	26.2	-207.133214	78.0	-207.133247
5.0	-207.128682	15.2	-207.133112	26.4	-207.133215	80.0	-207.133247
5.1	-207.129211	15.4	-207.133116	26.6	-207.133216	82.0	-207.133247
5.2	-207.129682	15.6	-207.133120	26.8	-207.133216	84.0	-207.133247
5.3	-207.130099	15.8	-207.133124	27.0	-207.133217	86.0	-207.133247
5.4	-207.130468	16.0	-207.133128	27.2	-207.133218	88.0	-207.133247
5.5	-207.130793	16.2	-207.133131	27.4	-207.133218	90.0	-207.133247
5.6	-207.131079	16.4	-207.133135	27.6	-207.133219	92.0	-207.133248
5.7	-207.131330	16.6	-207.133138	27.8	-207.133219	94.0	-207.133248
5.8	-207.131549	16.8	-207.133141	28.0	-207.133220	96.0	-207.133248
5.9	-207.131741	17.0	-207.133144	28.2	-207.133221	98.0	-207.133248
6.0	-207.131907	17.2	-207.133147	28.4	-207.133221	100.0	-207.133248
6.2	-207.132176	17.4	-207.133150	28.6	-207.133222	150.0	-207.133248
6.4	-207.132375	17.6	-207.133153	28.8	-207.133222	200.0	-207.133248
6.6	-207.132522	17.8	-207.133155	29.0	-207.133223		
6.8	-207.132629	18.0	-207.133158	29.2	-207.133223		
7.0	-207.132706	18.2	-207.133160	29.4	-207.133224		
7.2	-207.132761	18.4	-207.133163	29.6	-207.133224		
7.4	-207.132800	18.6	-207.133165	29.8	-207.133224		
7.6	-207.132828	18.8	-207.133167	30.0	-207.133225		
7.8	-207.132849	19.0	-207.133169	30.2	-207.133225		



Table S16: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $X^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.352573	8.0	-207.565415	14.6	-207.564735
1.6	-207.442780	8.2	-207.565341	14.8	-207.564731
1.8	-207.504499	8.4	-207.565276	15.0	-207.564729
2.0	-207.545018	8.6	-207.565219	15.2	-207.564726
2.2	-207.570040	8.8	-207.565168	15.4	-207.564723
2.4	-207.584342	9.0	-207.565123	15.6	-207.564721
2.6	-207.591631	9.2	-207.565084	15.8	-207.564718
2.8	-207.594396	9.4	-207.565048	16.0	-207.564716
3.0	-207.594425	9.6	-207.565016	17.0	-207.564706
3.2	-207.592843	9.8	-207.564988	18.0	-207.564700
3.4	-207.590389	10.0	-207.564962	19.0	-207.564695
3.6	-207.587499	10.2	-207.564939	20.0	-207.564690
3.8	-207.584556	10.4	-207.564918	21.0	-207.564687
4.0	-207.581718	10.6	-207.564899	22.0	-207.564685
4.2	-207.579100	10.8	-207.564882	23.0	-207.564683
4.4	-207.576765	11.0	-207.564866	24.0	-207.564681
4.6	-207.574737	11.2	-207.564852	25.0	-207.564680
4.8	-207.573013	11.4	-207.564840	26.0	-207.564679
5.0	-207.571573	11.6	-207.564828	27.0	-207.564678
5.2	-207.570385	11.8	-207.564818	28.0	-207.564677
5.4	-207.569414	12.0	-207.564808	29.0	-207.564677
5.6	-207.568625	12.2	-207.564799	30.0	-207.564676
5.8	-207.567986	12.4	-207.564791	50.0	-207.564673
6.0	-207.567468	12.6	-207.564784	100.0	-207.564673
6.2	-207.567049	12.8	-207.564777	200.0	-207.564673
6.4	-207.566701	13.0	-207.564771	300.0	-207.564673
6.6	-207.566425	13.2	-207.564765		
6.8	-207.566197	13.4	-207.564760		
7.0	-207.566008	13.6	-207.564755		
7.2	-207.565848	13.8	-207.564750		
7.4	-207.565714	14.0	-207.564746		
7.6	-207.565599	14.2	-207.564742		
7.8	-207.565500	14.4	-207.564738		

Table S17: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $2^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.175475	8.0	-207.484060	14.6	-207.482333
1.6	-207.261966	8.2	-207.483873	14.8	-207.482325
1.8	-207.323567	8.4	-207.483707	15.0	-207.482317
2.0	-207.367810	8.6	-207.483559	15.2	-207.482310
2.2	-207.398230	8.8	-207.483429	15.4	-207.482304
2.4	-207.418180	9.0	-207.483313	15.6	-207.482298
2.6	-207.430964	9.2	-207.483210	15.8	-207.482292
2.8	-207.439126	9.4	-207.483119	16.0	-207.482287
3.0	-207.444993	9.6	-207.483038	17.0	-207.482265
3.2	-207.450169	9.8	-207.482965	18.0	-207.482248
3.4	-207.455476	10.0	-207.482900	19.0	-207.482236
3.6	-207.460999	10.2	-207.482842	20.0	-207.482227
3.8	-207.466381	10.4	-207.482790	21.0	-207.482219
4.0	-207.471299	10.6	-207.482743	22.0	-207.482213
4.2	-207.475538	10.8	-207.482700	23.0	-207.482209
4.4	-207.479013	11.0	-207.482662	24.0	-207.482205
4.6	-207.481735	11.2	-207.482627	25.0	-207.482202
4.8	-207.483767	11.4	-207.482596	26.0	-207.482200
5.0	-207.485202	11.6	-207.482567	27.0	-207.482198
5.2	-207.486142	11.8	-207.482541	28.0	-207.482196
5.4	-207.486688	12.0	-207.482516	29.0	-207.482195
5.6	-207.486934	12.2	-207.482494	30.0	-207.482194
5.8	-207.486960	12.4	-207.482474	50.0	-207.482187
6.0	-207.486831	12.6	-207.482456	100.0	-207.482186
6.2	-207.486603	12.8	-207.482439	200.0	-207.482186
6.4	-207.486315	13.0	-207.482423	300.0	-207.482186
6.6	-207.485996	13.2	-207.482408		
6.8	-207.485669	13.4	-207.482395		
7.0	-207.485349	13.6	-207.482383		
7.2	-207.485044	13.8	-207.482371		
7.4	-207.484762	14.0	-207.482360		
7.6	-207.484503	14.2	-207.482351		
7.8	-207.484270	14.4	-207.482341		

Table S18: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $3^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.146100	8.0	-207.422942	14.6	-207.414876
1.6	-207.210328	8.2	-207.422355	14.8	-207.414846
1.8	-207.270946	8.4	-207.421752	15.0	-207.414819
2.0	-207.314901	8.6	-207.421146	15.2	-207.414793
2.2	-207.344830	8.8	-207.420548	15.4	-207.414768
2.4	-207.365347	9.0	-207.419970	15.6	-207.414745
2.6	-207.379714	9.2	-207.419419	15.8	-207.414723
2.8	-207.389989	9.4	-207.418902	16.0	-207.414702
3.0	-207.397301	9.6	-207.418425	17.0	-207.414615
3.2	-207.402168	9.8	-207.417991	18.0	-207.414548
3.4	-207.405047	10.0	-207.417602	19.0	-207.414495
3.6	-207.406682	10.2	-207.417256	20.0	-207.414453
3.8	-207.407927	10.4	-207.416951	21.0	-207.414419
4.0	-207.409402	10.6	-207.416685	22.0	-207.414391
4.2	-207.411235	10.8	-207.416454	23.0	-207.414368
4.4	-207.413266	11.0	-207.416253	24.0	-207.414349
4.6	-207.415304	11.2	-207.416079	25.0	-207.414333
4.8	-207.417228	11.4	-207.415928	26.0	-207.414320
5.0	-207.418971	11.6	-207.415796	27.0	-207.414308
5.2	-207.420502	11.8	-207.415680	28.0	-207.414298
5.4	-207.421811	12.0	-207.415578	29.0	-207.414290
5.6	-207.422896	12.2	-207.415488	30.0	-207.414283
5.8	-207.423765	12.4	-207.415407	50.0	-207.414230
6.0	-207.424426	12.6	-207.415334	100.0	-207.414218
6.2	-207.424892	12.8	-207.415269	200.0	-207.414217
6.4	-207.425181	13.0	-207.415209	300.0	-207.414217
6.6	-207.425299	13.2	-207.415155		
6.8	-207.425269	13.4	-207.415105		
7.0	-207.425107	13.6	-207.415060		
7.2	-207.424832	13.8	-207.415017		
7.4	-207.424460	14.0	-207.414978		
7.6	-207.424010	14.2	-207.414942		
7.8	-207.423499	14.4	-207.414908		

Table S19: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $4^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.121479	8.0	-207.403623	14.6	-207.404785
1.6	-207.207748	8.2	-207.404275	14.8	-207.404751
1.8	-207.251771	8.4	-207.404835	15.0	-207.404719
2.0	-207.280816	8.6	-207.405309	15.2	-207.404688
2.2	-207.301303	8.8	-207.405699	15.4	-207.404660
2.4	-207.315288	9.0	-207.406012	15.6	-207.404633
2.6	-207.325400	9.2	-207.406252	15.8	-207.404608
2.8	-207.342097	9.4	-207.406424	16.0	-207.404585
3.0	-207.355826	9.6	-207.406535	17.0	-207.404485
3.2	-207.366607	9.8	-207.406591	18.0	-207.404409
3.4	-207.374636	10.0	-207.406599	19.0	-207.404349
3.6	-207.380172	10.2	-207.406567	20.0	-207.404302
3.8	-207.383487	10.4	-207.406503	21.0	-207.404264
4.0	-207.384940	10.6	-207.406415	22.0	-207.404233
4.2	-207.385131	10.8	-207.406311	23.0	-207.404208
4.4	-207.384745	11.0	-207.406196	24.0	-207.404187
4.6	-207.384319	11.2	-207.406076	25.0	-207.404170
4.8	-207.384203	11.4	-207.405955	26.0	-207.404155
5.0	-207.384558	11.6	-207.405837	27.0	-207.404143
5.2	-207.385395	11.8	-207.405724	28.0	-207.404132
5.4	-207.386623	12.0	-207.405616	29.0	-207.404123
5.6	-207.388114	12.2	-207.405516	30.0	-207.404115
5.8	-207.389745	12.4	-207.405423	50.0	-207.404060
6.0	-207.391422	12.6	-207.405337	100.0	-207.404048
6.2	-207.393076	12.8	-207.405258	200.0	-207.404047
6.4	-207.394645	13.0	-207.405186	300.0	-207.404047
6.6	-207.396149	13.2	-207.405120		
6.8	-207.397547	13.4	-207.405059		
7.0	-207.398834	13.6	-207.405004		
7.2	-207.400009	13.8	-207.404953		
7.4	-207.401071	14.0	-207.404906		
7.6	-207.402025	14.2	-207.404862		
7.8	-207.402874	14.4	-207.404822		

Table S20: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $5^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.028206	8.0	-207.365308	14.6	-207.365144
1.6	-207.120052	8.2	-207.366230	14.8	-207.365095
1.8	-207.177816	8.4	-207.367051	15.0	-207.365056
2.0	-207.216127	8.6	-207.367768	15.2	-207.365025
2.2	-207.249517	8.8	-207.368380	15.4	-207.365001
2.4	-207.275805	9.0	-207.368887	15.6	-207.364981
2.6	-207.294920	9.2	-207.369291	15.8	-207.364965
2.8	-207.308036	9.4	-207.369594	16.0	-207.364952
3.0	-207.317151	9.6	-207.369802	17.0	-207.364920
3.2	-207.323822	9.8	-207.369918	18.0	-207.364910
3.4	-207.329069	10.0	-207.369948	19.0	-207.364907
3.6	-207.333441	10.2	-207.369901	20.0	-207.364906
3.8	-207.337341	10.4	-207.369783	21.0	-207.364905
4.0	-207.340869	10.6	-207.369605	22.0	-207.364905
4.2	-207.344073	10.8	-207.369375	23.0	-207.364905
4.4	-207.346932	11.0	-207.369104	24.0	-207.364904
4.6	-207.349381	11.2	-207.368802	25.0	-207.364904
4.8	-207.351347	11.4	-207.368480	26.0	-207.364904
5.0	-207.352796	11.6	-207.368147	27.0	-207.364904
5.2	-207.353770	11.8	-207.367812	28.0	-207.364904
5.4	-207.354378	12.0	-207.367481	29.0	-207.364904
5.6	-207.354760	12.2	-207.367165	30.0	-207.364904
5.8	-207.355057	12.4	-207.366867	50.0	-207.364904
6.0	-207.355391	12.6	-207.366591	100.0	-207.364904
6.2	-207.355857	12.8	-207.366339	200.0	-207.364904
6.4	-207.356514	13.0	-207.366114	300.0	-207.364904
6.6	-207.357387	13.2	-207.365916		
6.8	-207.358437	13.4	-207.365743		
7.0	-207.359600	13.6	-207.365595		
7.2	-207.360812	13.8	-207.365469		
7.4	-207.362022	14.0	-207.365363		
7.6	-207.363190	14.2	-207.365275		
7.8	-207.364291	14.4	-207.365203		

Table S21: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $6^1\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.012239	8.0	-207.349135	14.6	-207.355653
1.6	-207.100448	8.2	-207.349243	14.8	-207.355612
1.8	-207.160320	8.4	-207.349368	15.0	-207.355569
2.0	-207.201624	8.6	-207.349515	15.2	-207.355524
2.2	-207.230169	8.8	-207.349690	15.4	-207.355479
2.4	-207.252355	9.0	-207.349901	15.6	-207.355433
2.6	-207.269946	9.2	-207.350150	15.8	-207.355388
2.8	-207.282772	9.4	-207.350438	16.0	-207.355345
3.0	-207.292197	9.6	-207.350765	17.0	-207.355151
3.2	-207.299383	9.8	-207.351122	18.0	-207.355002
3.4	-207.305200	10.0	-207.351503	19.0	-207.354890
3.6	-207.310297	10.2	-207.351897	20.0	-207.354805
3.8	-207.315008	10.4	-207.352296	21.0	-207.354742
4.0	-207.319481	10.6	-207.352693	22.0	-207.354692
4.2	-207.323662	10.8	-207.353079	23.0	-207.354654
4.4	-207.327430	11.0	-207.353449	24.0	-207.354624
4.6	-207.330705	11.2	-207.353798	25.0	-207.354600
4.8	-207.333490	11.4	-207.354124	26.0	-207.354580
5.0	-207.335859	11.6	-207.354421	27.0	-207.354564
5.2	-207.337917	11.8	-207.354687	28.0	-207.354551
5.4	-207.339762	12.0	-207.354922	29.0	-207.354540
5.6	-207.341465	12.2	-207.355126	30.0	-207.354531
5.8	-207.343049	12.4	-207.355298	50.0	-207.354479
6.0	-207.344493	12.6	-207.355439	100.0	-207.354472
6.2	-207.345751	12.8	-207.355551	200.0	-207.354472
6.4	-207.346731	13.0	-207.355636	300.0	-207.354472
6.6	-207.347496	13.2	-207.355696		
6.8	-207.348034	13.4	-207.355733		
7.0	-207.348396	13.6	-207.355751		
7.2	-207.348637	13.8	-207.355753		
7.4	-207.348804	14.0	-207.355742		
7.6	-207.348928	14.2	-207.355720		
7.8	-207.349033	14.4	-207.355689		

Table S22: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $1^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.212409	8.0	-207.484468	14.6	-207.482333
1.6	-207.301367	8.2	-207.484161	14.8	-207.482325
1.8	-207.370080	8.4	-207.483908	15.0	-207.482317
2.0	-207.421066	8.6	-207.483700	15.2	-207.482310
2.2	-207.456723	8.8	-207.483526	15.4	-207.482304
2.4	-207.480772	9.0	-207.483380	15.6	-207.482298
2.6	-207.496676	9.2	-207.483256	15.8	-207.482292
2.8	-207.506730	9.4	-207.483150	16.0	-207.482287
3.0	-207.512832	9.6	-207.483059	17.0	-207.482265
3.2	-207.516191	9.8	-207.482980	18.0	-207.482248
3.4	-207.517643	10.0	-207.482910	19.0	-207.482236
3.6	-207.517749	10.2	-207.482849	20.0	-207.482227
3.8	-207.516953	10.4	-207.482794	21.0	-207.482219
4.0	-207.515523	10.6	-207.482746	22.0	-207.482213
4.2	-207.513667	10.8	-207.482703	23.0	-207.482209
4.4	-207.511538	11.0	-207.482663	24.0	-207.482205
4.6	-207.509249	11.2	-207.482628	25.0	-207.482202
4.8	-207.506885	11.4	-207.482596	26.0	-207.482200
5.0	-207.504512	11.6	-207.482567	27.0	-207.482198
5.2	-207.502181	11.8	-207.482541	28.0	-207.482196
5.4	-207.499932	12.0	-207.482517	29.0	-207.482195
5.6	-207.497797	12.2	-207.482495	30.0	-207.482194
5.8	-207.495801	12.4	-207.482474	50.0	-207.482187
6.0	-207.493961	12.6	-207.482456	100.0	-207.482186
6.2	-207.492291	12.8	-207.482439	200.0	-207.482186
6.4	-207.490796	13.0	-207.482423	300.0	-207.482186
6.6	-207.489480	13.2	-207.482408		
6.8	-207.488340	13.4	-207.482395		
7.0	-207.487367	13.6	-207.482383		
7.2	-207.486548	13.8	-207.482371		
7.4	-207.485866	14.0	-207.482360		
7.6	-207.485304	14.2	-207.482351		
7.8	-207.484844	14.4	-207.482341		

Table S23: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $2^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.123408	8.0	-207.468856	14.6	-207.465973
1.6	-207.227173	8.2	-207.468696	14.8	-207.465951
1.8	-207.293123	8.4	-207.468521	15.0	-207.465931
2.0	-207.335288	8.6	-207.468341	15.2	-207.465912
2.2	-207.362959	8.8	-207.468160	15.4	-207.465893
2.4	-207.381534	9.0	-207.467986	15.6	-207.465876
2.6	-207.394460	9.2	-207.467819	15.8	-207.465860
2.8	-207.403959	9.4	-207.467662	16.0	-207.465844
3.0	-207.411446	9.6	-207.467515	17.0	-207.465778
3.2	-207.417753	9.8	-207.467379	18.0	-207.465726
3.4	-207.423355	10.0	-207.467253	19.0	-207.465685
3.6	-207.428498	10.2	-207.467137	20.0	-207.465652
3.8	-207.433317	10.4	-207.467030	21.0	-207.465626
4.0	-207.437851	10.6	-207.466932	22.0	-207.465604
4.2	-207.442100	10.8	-207.466842	23.0	-207.465587
4.4	-207.446044	11.0	-207.466759	24.0	-207.465572
4.6	-207.449663	11.2	-207.466682	25.0	-207.465559
4.8	-207.452939	11.4	-207.466612	26.0	-207.465549
5.0	-207.455864	11.6	-207.466547	27.0	-207.465540
5.2	-207.458441	11.8	-207.466487	28.0	-207.465532
5.4	-207.460680	12.0	-207.466431	29.0	-207.465525
5.6	-207.462597	12.2	-207.466379	30.0	-207.465519
5.8	-207.464214	12.4	-207.466331	50.0	-207.465478
6.0	-207.465552	12.6	-207.466286	100.0	-207.465469
6.2	-207.466636	12.8	-207.466245	200.0	-207.465468
6.4	-207.467469	13.0	-207.466206	300.0	-207.465468
6.6	-207.468114	13.2	-207.466170		
6.8	-207.468575	13.4	-207.466136		
7.0	-207.468877	13.6	-207.466104		
7.2	-207.469044	13.8	-207.466075		
7.4	-207.469103	14.0	-207.466047		
7.6	-207.469077	14.2	-207.466021		
7.8	-207.468988	14.4	-207.465996		



Table S24: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $3^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.037340	8.0	-207.417924	14.6	-207.414875
1.6	-207.132332	8.2	-207.417944	14.8	-207.414846
1.8	-207.199409	8.4	-207.417906	15.0	-207.414818
2.0	-207.242571	8.6	-207.417822	15.2	-207.414792
2.2	-207.280226	8.8	-207.417704	15.4	-207.414768
2.4	-207.302217	9.0	-207.417561	15.6	-207.414745
2.6	-207.316805	9.2	-207.417402	15.8	-207.414723
2.8	-207.326468	9.4	-207.417234	16.0	-207.414702
3.0	-207.333039	9.6	-207.417062	17.0	-207.414615
3.2	-207.338051	9.8	-207.416891	18.0	-207.414548
3.4	-207.345562	10.0	-207.416724	19.0	-207.414495
3.6	-207.354783	10.2	-207.416564	20.0	-207.414453
3.8	-207.363456	10.4	-207.416411	21.0	-207.414419
4.0	-207.371323	10.6	-207.416268	22.0	-207.414391
4.2	-207.378317	10.8	-207.416135	23.0	-207.414368
4.4	-207.384442	11.0	-207.416011	24.0	-207.414349
4.6	-207.389756	11.2	-207.415897	25.0	-207.414333
4.8	-207.394340	11.4	-207.415791	26.0	-207.414320
5.0	-207.398282	11.6	-207.415694	27.0	-207.414308
5.2	-207.401668	11.8	-207.415605	28.0	-207.414298
5.4	-207.404574	12.0	-207.415522	29.0	-207.414290
5.6	-207.407064	12.2	-207.415446	30.0	-207.414283
5.8	-207.409193	12.4	-207.415377	50.0	-207.414230
6.0	-207.411005	12.6	-207.415312	100.0	-207.414218
6.2	-207.412537	12.8	-207.415253	200.0	-207.414217
6.4	-207.413813	13.0	-207.415198	300.0	-207.414217
6.6	-207.414878	13.2	-207.415147		
6.8	-207.415746	13.4	-207.415099		
7.0	-207.416438	13.6	-207.415055		
7.2	-207.416975	13.8	-207.415014		
7.4	-207.417375	14.0	-207.414976		
7.6	-207.417655	14.2	-207.414940		
7.8	-207.417833	14.4	-207.414907		

Table S25: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $4^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.994033	8.0	-207.377068	14.6	-207.376862
1.6	-207.089249	8.2	-207.377910	14.8	-207.376833
1.8	-207.162104	8.4	-207.378625	15.0	-207.376808
2.0	-207.214517	8.6	-207.379213	15.2	-207.376786
2.2	-207.251275	8.8	-207.379677	15.4	-207.376768
2.4	-207.277235	9.0	-207.380024	15.6	-207.376751
2.6	-207.296289	9.2	-207.380262	15.8	-207.376737
2.8	-207.311096	9.4	-207.380399	16.0	-207.376724
3.0	-207.323474	9.6	-207.380447	17.0	-207.376678
3.2	-207.334136	9.8	-207.380416	18.0	-207.376648
3.4	-207.340303	10.0	-207.380319	19.0	-207.376628
3.6	-207.343386	10.2	-207.380169	20.0	-207.376612
3.8	-207.345918	10.4	-207.379976	21.0	-207.376600
4.0	-207.348187	10.6	-207.379754	22.0	-207.376591
4.2	-207.350269	10.8	-207.379513	23.0	-207.376583
4.4	-207.352186	11.0	-207.379262	24.0	-207.376578
4.6	-207.353950	11.2	-207.379010	25.0	-207.376573
4.8	-207.355577	11.4	-207.378763	26.0	-207.376569
5.0	-207.357088	11.6	-207.378528	27.0	-207.376566
5.2	-207.358514	11.8	-207.378306	28.0	-207.376563
5.4	-207.359889	12.0	-207.378102	29.0	-207.376561
5.6	-207.361245	12.2	-207.377916	30.0	-207.376559
5.8	-207.362608	12.4	-207.377750	50.0	-207.376548
6.0	-207.363996	12.6	-207.377601	100.0	-207.376546
6.2	-207.365414	12.8	-207.377471	200.0	-207.376546
6.4	-207.366856	13.0	-207.377357	300.0	-207.376546
6.6	-207.368309	13.2	-207.377258		
6.8	-207.369755	13.4	-207.377172		
7.0	-207.371171	13.6	-207.377099		
7.2	-207.372534	13.8	-207.377036		
7.4	-207.373821	14.0	-207.376982		
7.6	-207.375015	14.2	-207.376935		
7.8	-207.376101	14.4	-207.376896		

Table S26: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $5^3\Sigma^+$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-206.992518	8.0	-207.347823	14.6	-207.355798
1.6	-207.073635	8.2	-207.348972	14.8	-207.355727
1.8	-207.139808	8.4	-207.350007	15.0	-207.355659
2.0	-207.185227	8.6	-207.350935	15.2	-207.355595
2.2	-207.216366	8.8	-207.351765	15.4	-207.355534
2.4	-207.238085	9.0	-207.352505	15.6	-207.355477
2.6	-207.255150	9.2	-207.353164	15.8	-207.355422
2.8	-207.268767	9.4	-207.353749	16.0	-207.355371
3.0	-207.279055	9.6	-207.354266	17.0	-207.355159
3.2	-207.286970	9.8	-207.354720	18.0	-207.355004
3.4	-207.293398	10.0	-207.355117	19.0	-207.354890
3.6	-207.299143	10.2	-207.355460	20.0	-207.354806
3.8	-207.304655	10.4	-207.355753	21.0	-207.354742
4.0	-207.309651	10.6	-207.355999	22.0	-207.354692
4.2	-207.313794	10.8	-207.356201	23.0	-207.354654
4.4	-207.317074	11.0	-207.356362	24.0	-207.354624
4.6	-207.319647	11.2	-207.356485	25.0	-207.354600
4.8	-207.321760	11.4	-207.356574	26.0	-207.354580
5.0	-207.323725	11.6	-207.356630	27.0	-207.354564
5.2	-207.325746	11.8	-207.356657	28.0	-207.354551
5.4	-207.327770	12.0	-207.356660	29.0	-207.354540
5.6	-207.329691	12.2	-207.356642	30.0	-207.354531
5.8	-207.331466	12.4	-207.356606	50.0	-207.354479
6.0	-207.333095	12.6	-207.356556	100.0	-207.354472
6.2	-207.334606	12.8	-207.356496	200.0	-207.354472
6.4	-207.336047	13.0	-207.356426	300.0	-207.354472
6.6	-207.337476	13.2	-207.356351		
6.8	-207.338952	13.4	-207.356272		
7.0	-207.340502	13.6	-207.356191		
7.2	-207.342094	13.8	-207.356110		
7.4	-207.343667	14.0	-207.356028		
7.6	-207.345163	14.2	-207.355949		
7.8	-207.346553	14.4	-207.355872		

Table S27: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $1^1\Pi$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.206075	8.0	-207.414083	14.6	-207.414066
1.6	-207.279738	8.2	-207.414018	14.8	-207.414070
1.8	-207.329354	8.4	-207.413970	15.0	-207.414075
2.0	-207.363834	8.6	-207.413937	15.2	-207.414079
2.2	-207.387108	8.8	-207.413915	15.4	-207.414083
2.4	-207.402068	9.0	-207.413902	15.6	-207.414088
2.6	-207.411175	9.2	-207.413894	15.8	-207.414091
2.8	-207.416305	9.4	-207.413892	16.0	-207.414095
3.0	-207.419055	9.6	-207.413893	17.0	-207.414112
3.2	-207.420280	9.8	-207.413897	18.0	-207.414126
3.4	-207.420707	10.0	-207.413903	19.0	-207.414137
3.6	-207.420774	10.2	-207.413910	20.0	-207.414147
3.8	-207.420704	10.4	-207.413917	21.0	-207.414155
4.0	-207.420555	10.6	-207.413926	22.0	-207.414162
4.2	-207.420344	10.8	-207.413934	23.0	-207.414168
4.4	-207.420068	11.0	-207.413943	24.0	-207.414173
4.6	-207.419732	11.2	-207.413952	25.0	-207.414178
4.8	-207.419341	11.4	-207.413960	26.0	-207.414182
5.0	-207.418905	11.6	-207.413969	27.0	-207.414185
5.2	-207.418437	11.8	-207.413977	28.0	-207.414188
5.4	-207.417955	12.0	-207.413985	29.0	-207.414191
5.6	-207.417471	12.2	-207.413993	30.0	-207.414193
5.8	-207.416999	12.4	-207.414000	50.0	-207.414211
6.0	-207.416548	12.6	-207.414007	100.0	-207.414216
6.2	-207.416126	12.8	-207.414014	200.0	-207.414217
6.4	-207.415739	13.0	-207.414021	300.0	-207.414217
6.6	-207.415393	13.2	-207.414027		
6.8	-207.415089	13.4	-207.414033		
7.0	-207.414828	13.6	-207.414039		
7.2	-207.414609	13.8	-207.414045		
7.4	-207.414429	14.0	-207.414050		
7.6	-207.414284	14.2	-207.414056		
7.8	-207.414170	14.4	-207.414061		

Table S28: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $2^1\Pi$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.103776	8.0	-207.403546	14.6	-207.403893
1.6	-207.192743	8.2	-207.403608	14.8	-207.403898
1.8	-207.257276	8.4	-207.403650	15.0	-207.403902
2.0	-207.302707	8.6	-207.403678	15.2	-207.403907
2.2	-207.334080	8.8	-207.403697	15.4	-207.403911
2.4	-207.355615	9.0	-207.403709	15.6	-207.403916
2.6	-207.370403	9.2	-207.403717	15.8	-207.403920
2.8	-207.380427	9.4	-207.403723	16.0	-207.403923
3.0	-207.387279	9.6	-207.403727	17.0	-207.403941
3.2	-207.391665	9.8	-207.403732	18.0	-207.403955
3.4	-207.394259	10.0	-207.403736	19.0	-207.403966
3.6	-207.395530	10.2	-207.403741	20.0	-207.403976
3.8	-207.395960	10.4	-207.403747	21.0	-207.403984
4.0	-207.395926	10.6	-207.403753	22.0	-207.403991
4.2	-207.395734	10.8	-207.403760	23.0	-207.403997
4.4	-207.395615	11.0	-207.403767	24.0	-207.404002
4.6	-207.395694	11.2	-207.403775	25.0	-207.404006
4.8	-207.396010	11.4	-207.403783	26.0	-207.404010
5.0	-207.396535	11.6	-207.403791	27.0	-207.404013
5.2	-207.397209	11.8	-207.403799	28.0	-207.404016
5.4	-207.397966	12.0	-207.403806	29.0	-207.404019
5.6	-207.398748	12.2	-207.403814	30.0	-207.404021
5.8	-207.399512	12.4	-207.403822	50.0	-207.404038
6.0	-207.400227	12.6	-207.403830	100.0	-207.404046
6.2	-207.400876	12.8	-207.403837	200.0	-207.404047
6.4	-207.401444	13.0	-207.403844	300.0	-207.404047
6.6	-207.401937	13.2	-207.403851		
6.8	-207.402350	13.4	-207.403858		
7.0	-207.402690	13.6	-207.403864		
7.2	-207.402962	13.8	-207.403870		
7.4	-207.403174	14.0	-207.403876		
7.6	-207.403337	14.2	-207.403882		
7.8	-207.403458	14.4	-207.403887		

Table S29: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $1^3\Pi$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.283387	8.0	-207.465021	14.6	-207.465335
1.6	-207.357797	8.2	-207.465033	14.8	-207.465339
1.8	-207.406068	8.4	-207.465046	15.0	-207.465343
2.0	-207.437409	8.6	-207.465059	15.2	-207.465347
2.2	-207.456920	8.8	-207.465073	15.4	-207.465351
2.4	-207.468266	9.0	-207.465087	15.6	-207.465355
2.6	-207.474221	9.2	-207.465100	15.8	-207.465359
2.8	-207.476681	9.4	-207.465114	16.0	-207.465362
3.0	-207.477202	9.6	-207.465127	17.0	-207.465377
3.2	-207.476500	9.8	-207.465140	18.0	-207.465390
3.4	-207.475204	10.0	-207.465152	19.0	-207.465400
3.6	-207.473660	10.2	-207.465164	20.0	-207.465408
3.8	-207.472157	10.4	-207.465176	21.0	-207.465416
4.0	-207.470774	10.6	-207.465187	22.0	-207.465422
4.2	-207.469562	10.8	-207.465198	23.0	-207.465427
4.4	-207.468540	11.0	-207.465208	24.0	-207.465431
4.6	-207.467705	11.2	-207.465218	25.0	-207.465435
4.8	-207.467036	11.4	-207.465228	26.0	-207.465438
5.0	-207.466509	11.6	-207.465237	27.0	-207.465441
5.2	-207.466098	11.8	-207.465246	28.0	-207.465444
5.4	-207.465783	12.0	-207.465254	29.0	-207.465446
5.6	-207.465545	12.2	-207.465262	30.0	-207.465448
5.8	-207.465368	12.4	-207.465270	50.0	-207.465462
6.0	-207.465239	12.6	-207.465277	100.0	-207.465467
6.2	-207.465147	12.8	-207.465284	200.0	-207.465467
6.4	-207.465081	13.0	-207.465291	300.0	-207.465468
6.6	-207.465040	13.2	-207.465297		
6.8	-207.465015	13.4	-207.465303		
7.0	-207.465002	13.6	-207.465309		
7.2	-207.464996	13.8	-207.465315		
7.4	-207.464997	14.0	-207.465320		
7.6	-207.465002	14.2	-207.465325		
7.8	-207.465011	14.4	-207.465330		

Table S30: Total IH-FS-CCSD (2,0) DK3/ANO-RCC energies for the  $2^3\Pi$  state of  $\text{LiMg}^+$ .

R (Å)	E (a.u.)	R (Å)	E (a.u.)	R (Å)	E (a.u.)
1.4	-207.087240	8.0	-207.413751	14.6	-207.414066
1.6	-207.175876	8.2	-207.413770	14.8	-207.414070
1.8	-207.241108	8.4	-207.413786	15.0	-207.414075
2.0	-207.287256	8.6	-207.413801	15.2	-207.414079
2.2	-207.319409	8.8	-207.413815	15.4	-207.414083
2.4	-207.341647	9.0	-207.413829	15.6	-207.414088
2.6	-207.357172	9.2	-207.413841	15.8	-207.414091
2.8	-207.368244	9.4	-207.413854	16.0	-207.414095
3.0	-207.376598	9.6	-207.413865	17.0	-207.414112
3.2	-207.383084	9.8	-207.413877	18.0	-207.414126
3.4	-207.388361	10.0	-207.413889	19.0	-207.414137
3.6	-207.392773	10.2	-207.413900	20.0	-207.414147
3.8	-207.396542	10.4	-207.413910	21.0	-207.414155
4.0	-207.399772	10.6	-207.413920	22.0	-207.414162
4.2	-207.402517	10.8	-207.413931	23.0	-207.414168
4.4	-207.404821	11.0	-207.413940	24.0	-207.414173
4.6	-207.406731	11.2	-207.413950	25.0	-207.414178
4.8	-207.408291	11.4	-207.413959	26.0	-207.414182
5.0	-207.409546	11.6	-207.413968	27.0	-207.414185
5.2	-207.410543	11.8	-207.413976	28.0	-207.414188
5.4	-207.411326	12.0	-207.413984	29.0	-207.414191
5.6	-207.411933	12.2	-207.413992	30.0	-207.414193
5.8	-207.412400	12.4	-207.414000	50.0	-207.414211
6.0	-207.412755	12.6	-207.414007	100.0	-207.414216
6.2	-207.413022	12.8	-207.414014	200.0	-207.414217
6.4	-207.413223	13.0	-207.414021	300.0	-207.414217
6.6	-207.413371	13.2	-207.414027		
6.8	-207.413481	13.4	-207.414033		
7.0	-207.413561	13.6	-207.414039		
7.2	-207.413622	13.8	-207.414045		
7.4	-207.413667	14.0	-207.414050		
7.6	-207.413702	14.2	-207.414056		
7.8	-207.413729	14.4	-207.414061		