Requirement for transient metal ions revealed through computational analysis for a DNA polymerase going in reverse

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Supplemental Appendix

Supplemental Materials and Methods

Unconstrained Optimization of the $Na_cMg_nMg_p$ Configuration at $P_\alpha - O_\beta = 1.7$ Å. Unconstrained optimization of the original $Na_cMg_nMg_p$ system was carried out to check whether the removal of constraints brings the system back to its starting configuration. The optimized system, after the removal of constraints, landed in a configuration near the reactant state of the system as indicated in Figure S1 (open triangle).

CM5 Charges for Quantum System. As described in the main text, the QM atom charges are calculated using the CM5 charge model (35) for each system at each selected geometry along the reaction path. The charges are given in Table S1*A*-*D* and the atom identities are given in Table S1*E*. The charge variations during the reaction profiles are illustrated in Figure S2.

Table S1. Initial CM5 charges (in electron units) on QM atoms and their variations along the reaction path.

(A) CM charges for the $Na_cMg_nMg_p$ system. Index is the atom identification; C_{is} is the initial charge; (C_{cs}-C_{is}) is the difference between the charges of the current systems (cs) and the initial system (is).

Index	C_{is}	(C_{cs}-C_{is})*10^{-2} along the reaction coordinate ------>												
1	0.333	0.0	0.1	0.1	0.3	0.2	0.2	0.3	0.3	0.4	0.4	0.5	0.5	0.5
2	-0.582	0.1	0.2	0.3	0.1	0.4	0.5	0.6	0.6	0.7	0.7	0.8	0.9	0.9
3	0.382	0.0	0.1	0.3	-0.2	0.5	0.5	0.6	0.6	0.7	0.7	0.8	0.8	0.8
4	0.416	0.0	0.0	-0.1	0.3	0.0	0.0	0.0	0.0	0.1	0.1	0.2	0.2	0.2
5	-0.589	0.0	0.0	-0.1	0.1	-0.1	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.2
6	0.378	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.2	0.2	0.2	0.3	0.3
7	0.327	0.0	0.0	-0.1	-0.2	-0.1	-0.1	-0.1	0.0	-0.1	-0.1	-0.1	-0.1	0.0
8	-0.581	0.0	0.0	-0.1	0.0	-0.1	-0.1	0.0	0.0	0.1	0.1	0.1	0.2	0.2
9	0.389	0.0	-0.1	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.1	-0.1	-0.1	-0.1	-0.1
10	0.321	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.3
11	0.092	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3
12	-0.242	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1
13	0.095	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.0
14	0.117	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.3
15	0.279	0.0	0.0	0.0	0.1	0.1	0.2	0.2	0.2	0.4	0.5	0.5	0.5	0.4
16	-0.427	0.0	-0.1	-0.2	-0.3	-0.4	-0.5	-0.6	-0.8	-0.8	-1.0	-1.3	-1.7	-2.1
17	-0.427	0.0	-0.1	0.2	0.2	0.2	0.3	0.4	0.6	0.6	0.8	1.1	1.4	2.0
18	0.103	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1
19	-0.243	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2
20	0.092	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.4	-0.5
21	0.101	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1
22	0.294	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2
23	-0.414	0.0	0.1	0.2	0.3	0.4	0.5	0.7	0.9	1.1	1.4	1.7	2.1	2.5
24	-0.423	-0.1	-0.2	-0.3	-0.4	-0.5	-0.6	-0.8	-1.0	-1.2	-1.5	-1.7	-2.1	-2.6
25	0.324	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2
26	-0.588	0.0	-0.1	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3
27	0.385	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1
28	0.416	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1
29	-0.590	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1
30	0.363	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3
31	0.362	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3
32	-0.578	0.0	0.0	0.1	0.1	0.2	0.2	0.3	0.3	0.4	0.4	0.5	0.6	0.6
33	0.325	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1
34	0.317	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
35	0.093	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5
36	-0.245	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.3
37	0.109	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2
38	0.092	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3
39	0.267	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2
40	-0.440	0.0	0.1	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.3	-0.4	-0.4	-0.6	-0.7
41	-0.430	0.1	0.0	0.1	0.1	0.2	0.3	0.4	0.5	0.6	0.8	1.0	1.2	1.6
42	0.361	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2
43	-0.484	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.3
44	0.498	0.0	-0.1	-0.2	-0.2	-0.3	-0.4	-0.4	-0.5	-0.6	-0.7	-0.8	-1.0	-1.3
45	-0.480	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.4	-0.5	-0.5	-0.7
46	-0.586	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.7	-0.7	-0.9	-1.1	-1.2	-1.4	-2.1
47	-0.306	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.4	-0.4	-0.4	-0.4
48	-0.054	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.4	-0.3
49	0.123	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5
50	0.125	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.2

51	0.016	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.9
52	0.125	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4
53	-0.316	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.7	-1.0
54	-0.063	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.4	-0.5	-0.6	-0.7	-0.9
55	0.119	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.7	-0.9
56	0.049	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.7	-0.8	-1.1
57	0.031	0.0	-0.1	-0.1	-0.1	-0.3	-0.4	-0.5	-0.7	-0.9	-1.1	-1.4	-1.7	-2.2
58	0.121	0.0	-0.1	-0.1	-0.1	-0.3	-0.4	-0.5	-0.7	-0.8	-1.1	-1.3	-1.6	-2.5
59	-0.164	0.0	-0.1	-0.1	-0.1	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.7	-0.9	-1.1
60	0.102	0.0	-0.1	-0.2	-0.2	-0.3	-0.4	-0.4	-0.5	-0.6	-0.7	-0.8	-0.9	-1.2
61	0.113	0.0	0.0	0.0	0.0	-0.1	-0.2	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.8
62	-0.278	-0.2	-0.9	-1.1	-1.2	-2.1	-2.8	-3.6	-4.4	-5.3	-6.5	-7.8	-9.6	-14.0
63	0.587	-0.2	-0.2	-0.3	-0.3	-0.3	-0.4	-0.5	-0.6	-0.9	-1.1	-1.4	-1.5	-0.9
64	-0.454	0.1	0.2	0.1	-0.1	-0.1	-0.4	-0.8	-1.1	-1.9	-2.5	-3.3	-3.8	-3.0
65	-0.488	-0.1	-0.1	-0.4	0.5	-0.7	-0.9	-1.2	-1.5	-1.8	-2.4	-2.9	-3.4	-3.0
66	-0.277	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.4	-0.6	-0.8	-1.0	-1.2	-1.1
67	-0.031	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.0	-0.1	-0.2	-0.3	-0.2
68	0.131	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.1	0.1	0.1	0.3
69	0.130	0.0	0.0	0.1	0.0	0.1	0.0	0.0	0.0	-0.1	-0.2	-0.3	-0.4	-0.4
70	0.007	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
71	0.127	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1
72	-0.270	0.0	0.1	0.1	0.1	0.2	0.2	0.3	0.4	0.4	0.4	0.5	0.5	0.6
73	-0.061	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.2
74	0.122	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.2
75	0.041	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.0	0.0
76	-0.001	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.3	-0.4	-0.4
77	0.108	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.4	-0.5	-0.5
78	-0.174	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
79	0.098	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
80	0.112	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2
81	-0.471	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.2	0.2	0.2
82	0.306	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.3	0.3	0.4	0.4	0.4
83	-0.429	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.2	0.3	0.4	0.6	0.8
84	0.402	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.2	0.3	0.4
85	0.520	0.1	-0.1	-0.1	-0.1	0.0	0.1	0.2	0.3	0.6	0.8	1.0	1.2	1.3
86	-0.459	0.0	0.1	0.1	0.1	0.3	0.3	0.5	0.6	0.8	1.1	1.4	1.8	2.0
87	-0.632	0.1	0.0	0.0	0.0	0.1	0.2	0.3	0.4	0.5	0.7	0.8	1.0	1.2
88	-0.367	0.1	0.3	0.3	0.4	0.5	0.6	0.7	0.9	1.1	1.2	1.4	1.6	1.9
89	0.531	0.0	0.1	0.1	0.2	0.4	0.6	1.0	1.4	1.9	2.6	3.3	4.1	5.1
90	-0.518	-0.2	-0.2	-0.2	-0.1	-0.1	0.1	0.3	0.5	0.9	1.4	1.9	2.4	3.0
91	-0.511	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.4	0.4	0.6	0.8	1.1	1.6
92	-0.505	0.5	0.8	1.4	1.7	2.6	3.5	4.5	5.4	7.1	9.0	11.0	13.2	15.7
93	0.875	0.2	0.4	0.6	0.7	0.9	1.2	1.4	1.7	1.9	2.3	2.6	3.0	4.0
94	0.867	-0.1	-0.2	-0.3	-0.4	-0.4	-0.5	-0.5	-0.7	-0.6	-0.7	-0.9	-1.1	-2.0
95	0.855	0.1	0.1	0.2	0.5	0.5	0.7	0.8	1.0	1.1	1.3	1.4	1.4	1.4
96	-0.631	-0.1	-0.2	-0.3	-0.3	-0.3	-0.4	-0.3	-0.3	-0.3	-0.2	-0.2	0.0	0.8
97	0.337	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	0.0	0.0	0.1	0.5
98	0.390	0.0	0.0	0.1	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.5	0.5	1.4
99	-0.610	0.2	0.4	0.4	0.4	0.5	0.7	0.7	0.7	0.8	0.8	0.8	0.7	0.6
100	0.325	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.4
101	0.368	-0.1	-0.3	-0.3	-0.4	-0.7	-1.0	-1.5	-1.7	-2.3	-2.7	-2.9	-3.1	-3.3
102	-0.621	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	0.0
103	0.385	0.0	0.0	0.1	0.1	0.2	0.2	0.3	0.3	0.3	0.3	0.3	0.4	0.5
104	0.357	0.0	0.0	0.0	0.0	0.1	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
105	-0.602	0.0	0.1	0.1	0.1	0.1	0.0	0.0	-0.2	-0.2	-0.2	-0.3	-0.4	-0.6
106	0.384	0.1	0.1	0.2	0.2	0.3	0.3	0.4	0.4	0.5	0.5	0.5	0.5	0.5
107	0.385	0.1	0.1	0.1	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.7	0.5
108	-0.608	0.1	0.1	0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4
109	0.382	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.3	0.4	0.5	0.6	0.6

110	0.387	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.1	0.1
111	-0.611	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.0	0.0	0.1
112	0.386	0.0	0.2	0.3	0.3	0.4	0.5	0.5	0.6	0.7	0.8	0.9	1.0	1.3
113	0.404	0.0	0.1	0.2	0.2	0.3	0.3	0.4	0.4	0.5	0.6	0.7	0.9	0.9

(B) CM charges for the $Mg_cMg_nMg_p$ system.

Index	**C_{is}**	**$\mid (C_{cs}-C_{is})*10^{-2}$ along the reaction coordinate ----------$>\mid$**												
1	0.332	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.3	0.3	0.3	0.3	0.3	0.3	0.3
2	-0.586	0.1	0.1	0.2	0.3	0.3	0.4	0.4	0.5	0.7	0.8	0.8	0.8	0.9	0.9
3	0.378	0.1	0.1	0.3	0.3	0.4	0.5	0.5	0.6	0.8	0.9	0.9	0.9	1.0	1.0
4	0.413	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.2	0.1	0.2	0.2	0.3
5	-0.590	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.0	0.0	-0.1	0.0	0.0	0.1
6	0.375	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.1	0.1	0.1	0.1	0.2	0.2
7	0.326	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2
8	-0.580	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.2	0.4	0.3	0.5	0.5
9	0.379	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.8	0.9	0.9	1.0	1.0
10	0.326	0.1	0.0	0.0	0.0	0.1	0.1	0.1	0.2	-0.2	-0.2	-0.2	-0.2	-0.3	-0.3
11	0.080	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.3	-0.3	-0.4	-0.5	-0.3	-0.4
12	-0.255	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	0.0	-0.1	0.0	-0.1	0.1	0.2
13	0.082	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.1	0.0
14	0.098	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.2	0.3	0.2	0.7	0.8
15	0.228	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.6	0.4	0.6	1.2	1.5
16	-0.443	-0.3	-0.3	-0.4	-0.5	-0.7	-0.8	-0.9	-1.1	-1.1	-1.2	-1.5	-1.6	-1.8	-1.7
17	-0.458	0.1	0.2	0.3	0.4	0.6	0.8	1.1	1.3	1.0	1.4	1.9	2.4	1.9	1.7
18	0.096	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	0.0	-0.1
19	-0.259	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.2	0.2
20	0.065	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1
21	0.090	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.0
22	0.260	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	0.0	0.0	-0.1	-0.1	0.0	0.0
23	-0.431	0.2	0.1	0.2	0.2	0.3	0.4	0.5	0.7	0.9	1.2	0.2	0.8	-2.3	-2.1
24	-0.479	-0.2	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.7	-0.9	-1.0	-0.5	-0.8	0.3	0.3
25	0.319	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	0.0	-0.1
26	-0.593	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	0.0	0.0
27	0.377	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.2	-0.2	0.0	0.0
28	0.416	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1
29	-0.590	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.2	0.0	0.0
30	0.356	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.3	-0.3
31	0.352	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.2	0.1	0.1	0.1
32	-0.571	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.2	0.3	0.4	0.6	0.6	0.7	0.8
33	0.326	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1
34	0.317	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.2	0.2	0.1	0.2
35	0.086	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.2	-0.3
36	-0.252	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.1	-0.1
37	0.111	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2
38	0.081	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	0.0	0.0
39	0.233	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.1	-0.1
40	-0.487	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.4	-0.4	-0.5	-0.7	0.0	-0.1
41	-0.459	0.0	0.1	0.1	0.2	0.3	0.4	0.5	0.6	0.6	0.7	0.4	0.6	-0.1	0.3
42	0.351	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	0.1	0.0	0.1	0.1	0.0	-0.1
43	-0.472	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	0.2	0.2	0.2	0.2	0.1	0.0
44	0.495	0.0	0.0	-0.1	-0.1	-0.2	-0.3	-0.4	-0.4	-0.2	-0.2	-0.3	-0.4	-0.4	-0.6
45	-0.480	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.4	-0.4	0.2	0.2
46	-0.612	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.7	-0.8	-0.8	-0.9	-0.7	-0.9
47	-0.308	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.3	-0.3	-0.4	-0.4	-0.4
48	-0.051	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.1	-0.1

49	0.121	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	-0.1
50	0.130	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.2	-0.2	-0.3	-0.1	0.0
51	0.014	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.4	-0.4	-0.7	-0.8
52	0.126	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.5	-0.6
53	-0.323	0.0	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.3	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4
54	-0.067	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.3	-0.4	-0.5	-0.6	-0.6	-0.7
55	0.113	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.3	-0.4	-0.5	-0.5	-0.6
56	0.041	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.4	-0.5	-0.6	-0.7	-0.7	-0.9
57	0.024	0.0	-0.1	-0.1	-0.2	-0.3	-0.3	-0.5	-0.6	-0.8	-1.0	-1.3	-1.6	-1.9	-2.2
58	0.116	0.0	-0.1	-0.1	-0.1	-0.2	-0.3	-0.4	-0.5	-0.6	-0.7	-1.0	-1.2	-1.3	-1.7
59	-0.165	0.0	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.5	-0.7	-0.9	-1.0	-1.1	-1.3
60	0.099	0.0	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.5	-0.6	-0.8	-0.9	-1.0	-1.1
61	0.113	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.4	-0.5	-0.6	-0.7
62	-0.313	-0.3	-0.5	-0.7	-1.1	-1.4	-1.8	-2.3	-2.8	-3.2	-3.7	-4.3	-5.2	-7.9	-9.3
63	0.559	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.5	-0.7	-0.9	-1.4	-1.5	-1.5
64	-0.494	0.1	0.0	0.0	-0.2	-0.3	-0.6	-1.0	-1.6	-2.3	-3.1	-3.1	-4.4	-3.3	-3.5
65	-0.518	-0.1	-0.3	-0.4	-0.6	-0.7	-0.9	-1.2	-1.5	-2.1	-2.5	-2.6	-3.4	-3.5	-4.3
66	-0.285	0.0	0.0	0.1	0.1	0.1	0.0	0.0	-0.1	-0.1	-0.1	0.1	0.2	0.2	0.1
67	-0.028	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	-0.1	-0.3	-0.4	-0.6	-0.7
68	0.131	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.1	0.0	-0.1	-0.1	-0.1
69	0.130	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.3	-0.4	-0.5	-0.6	-0.7	-0.8
70	0.007	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
71	0.118	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	-0.1	-0.1	-0.1
72	-0.268	0.0	0.1	0.1	0.1	0.2	0.3	0.3	0.4	0.3	0.4	0.4	0.4	0.4	0.5
73	-0.063	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.1	0.2	0.2
74	0.116	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.3	0.2	0.3	0.3
75	0.038	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.1	0.0
76	-0.002	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.3	-0.4	-0.3	-0.4	-0.3	-0.3
77	0.113	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.3	-0.4	-0.5	-0.5	-0.6	-0.6
78	-0.178	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.1
79	0.093	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1
80	0.107	0.1	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.3	0.3	0.3	0.2
81	-0.476	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	0.0	0.1	0.5	0.5	0.8	0.9
82	0.307	-0.1	-0.1	0.0	-0.1	-0.1	-0.1	-0.1	0.0	0.2	0.2	0.6	0.6	0.8	0.9
83	-0.435	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.3	-4.2	-3.7	-4.0	-3.9
84	0.389	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	1.1	0.9	0.1	0.0	0.2	0.2
85	0.528	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	0.0	-0.5	-0.5	-1.7	-1.3	-1.6	-1.6
86	-0.431	0.2	0.2	0.2	0.2	0.4	0.4	0.5	0.6	1.5	1.6	0.9	1.5	0.5	0.3
87	-0.627	0.1	0.1	0.2	0.2	0.2	0.3	0.3	0.4	1.4	1.5	0.7	0.9	0.8	0.8
88	-0.350	-0.1	0.0	-0.1	0.0	0.0	0.0	0.1	0.2	-2.4	-2.3	-1.3	-1.3	-0.9	-0.8
89	0.527	0.0	-0.1	-0.1	-0.1	0.0	0.1	0.3	0.6	0.7	1.2	1.7	2.4	3.0	3.6
90	-0.518	0.1	-0.1	-0.2	-0.3	-0.2	-0.2	-0.1	0.1	0.7	1.0	1.4	1.9	2.1	2.6
91	-0.516	-0.1	-0.1	-0.1	-0.1	-0.2	-0.1	-0.1	-0.1	0.0	0.1	0.4	0.5	0.9	1.1
92	-0.497	0.5	0.8	1.2	1.7	2.2	2.8	3.6	4.4	5.2	6.4	7.2	9.3	11.4	13.6
93	0.884	0.1	0.4	0.6	0.8	1.1	1.3	1.5	1.8	2.0	2.4	2.3	2.6	2.8	2.9
94	0.763	0.0	-0.1	-0.2	-0.4	-0.5	-0.7	-0.9	-1.0	-0.9	-1.1	-2.1	-1.9	-1.2	-1.5
95	0.825	0.1	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.7	0.8	0.7	0.6	0.7	0.6
96	-0.618	0.0	0.1	0.1	0.2	0.2	0.3	0.4	0.5	2.9	2.9	1.3	1.5	1.1	1.3
97	0.343	0.1	0.1	0.1	0.2	0.2	0.3	0.3	0.4	0.1	0.2	0.3	0.3	1.0	1.5
98	0.388	0.1	0.0	0.1	0.1	0.1	0.1	0.2	0.2	-0.2	-0.1	-0.2	0.0	-0.7	-0.6
99	-0.652	-0.1	0.0	0.0	0.2	0.2	0.2	0.3	0.4	-0.1	-0.2	0.9	0.7	-1.8	-2.2
100	0.298	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.4	-0.4	-0.6	-0.6	-0.9	-0.9
101	0.350	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.4	-3.8	-3.8	-3.3	-3.4	-3.0	-3.1
102	-0.606	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.4	-0.4	-0.3	-0.4	-0.4	-0.4
103	0.368	0.1	0.1	0.2	0.2	0.2	0.3	0.3	0.4	0.5	0.5	0.6	0.6	0.5	0.4
104	0.363	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.2	0.1	0.0	-0.1
105	-0.620	-0.5	-0.3	-0.4	-0.5	-0.7	-0.8	-0.9	-0.9	-1.1	-0.9	0.9	0.8	0.7	0.7
106	0.374	-0.5	-0.2	-0.3	-0.2	-0.2	-0.2	-0.2	-0.1	0.6	0.8	0.7	0.7	0.8	1.0
107	0.334	-0.6	-0.3	-0.5	-0.5	-0.5	-0.5	-0.6	-0.5	0.0	0.4	4.7	4.5	4.8	4.9

108	-0.609	0.2	0.2	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.5	0.7	0.8	0.5	0.2
109	0.382	0.1	0.1	0.2	0.1	0.2	0.2	0.2	0.3	0.4	0.4	0.4	0.4	0.6	0.8
110	0.383	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.4	0.3	0.6	0.6	0.7	1.0
111	-0.617	0.0	0.0	0.0	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.7	0.5	0.6	0.6
112	0.381	0.4	0.2	0.3	0.4	0.6	0.7	0.9	0.9	0.8	0.7	1.3	1.4	1.5	1.6
113	0.395	0.1	0.1	0.2	0.2	0.2	0.3	0.3	0.4	0.7	0.8	1.1	1.1	1.4	1.5

(C) CM charges for the Mg_cMg_n system.

Index C_{is}	**$(C_{cs}-C_{is})*10^{-2}$ along the reaction coordinate ----------\>|**																		
1	0.330	0.0	0.0	-0.1	-0.1	-0.1	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.3
2	-0.591	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	-0.2	0.0	0.2
3	0.371	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	0.0	0.0	0.0	-0.1	-0.2	-0.2	-0.1	-0.4	-0.3	0.0
4	0.415	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	0.0	0.0	0.0	0.1	0.0	0.1	0.1	0.2	0.4	0.2
5	-0.583	0.1	0.1	-0.1	0.0	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.4	0.8	0.8	0.9	0.9	1.2	0.9
6	0.376	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	-0.1	0.0	0.0	-0.1	0.4	0.1
7	0.326	0.0	0.0	0.1	0.0	0.1	0.0	0.1	0.0	0.1	0.1	0.1	0.0	-0.2	-0.2	-0.2	-0.1	-0.2	-0.1
8	-0.568	0.0	0.0	-0.2	-0.2	-0.1	-0.2	-0.1	0.0	0.1	0.2	0.3	0.4	0.2	0.3	0.3	0.4	0.3	0.3
9	0.391	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	0.0	0.1	0.1	0.1	0.0	0.0	0.1	0.1	0.1	0.1
10	0.343	0.2	0.2	-0.6	-0.4	-0.3	-0.4	-0.3	-0.2	-0.1	0.1	0.2	0.3	1.9	2.0	2.3	3.2	3.0	2.5
11	0.090	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.2	-0.2	-0.3	-0.2	-0.3	-0.4
12	-0.244	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5
13	0.099	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.4	-0.5	-0.1
14	0.108	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.1	-0.4	-0.4	-0.4	-0.5	-0.8	-0.5
15	0.278	0.0	0.0	-0.1	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.3	-0.3	-0.3	-0.2	-0.2	-0.2	-0.1	0.1	-0.1
16	-0.427	0.0	0.1	0.6	0.5	0.4	0.4	0.3	0.3	0.1	-0.1	-0.2	-0.4	-0.4	-0.7	-1.0	-1.0	-1.3	-2.0
17	-0.416	0.1	0.2	0.5	0.4	0.4	0.5	0.3	0.5	0.6	0.7	0.7	0.8	0.5	0.7	0.9	0.9	1.5	1.7
18	0.102	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.1
19	-0.244	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.4	-0.2
20	0.092	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.3	-0.5	-0.4
21	0.101	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.3	-0.5	-0.1
22	0.293	0.0	0.0	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.3
23	-0.410	-0.2	-0.3	-0.3	-0.3	-0.2	-0.2	-0.1	-0.1	-0.1	0.0	0.1	0.2	0.3	0.6	0.8	0.7	1.3	2.0
24	-0.427	0.1	0.1	0.1	0.0	0.0	-0.1	0.0	-0.1	-0.1	-0.2	-0.3	-0.4	-0.4	-0.7	-0.9	-0.6	-1.1	-1.9
25	0.325	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.7	-0.1
26	-0.584	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2
27	0.381	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	0.0	0.0	-0.1	0.2
28	0.418	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.5	-0.1
29	-0.587	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	1.2	-0.1
30	0.363	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	0.0	-1.1	-0.2
31	0.360	0.0	-0.1	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1	0.1	0.1	0.1	0.1	0.0	-0.1	-1.3	-0.1
32	-0.576	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.2	0.2	0.3	0.3	0.5	0.6	0.4
33	0.327	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	-0.1	-0.1	0.0
34	0.316	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.1	0.0
35	0.096	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.2	-0.1	-0.2	-0.4
36	-0.243	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.1	-0.2	-0.1
37	0.108	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	0.0	-0.3	-0.2
38	0.093	0.0	0.0	0.1	0.0	0.1	0.0	0.1	0.1	0.2	0.2	0.2	0.2	0.1	0.1	0.1	0.2	-0.3	0.0
39	0.266	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.3	-0.3
40	-0.440	0.0	0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	0.0	0.1	0.0	-0.1	0.0	0.0	0.0	-0.2	-0.2
41	-0.433	0.0	0.0	0.1	0.2	0.2	0.2	0.3	0.3	0.3	0.3	0.3	0.4	0.4	0.5	0.6	0.3	1.1	1.0
42	0.360	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	0.0	0.0	-0.1	-0.2	-0.2	-0.3	-0.3	-0.3	0.0
43	-0.466	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.1	-0.1	-0.2	0.0	0.0	-0.1	0.0	0.5	0.6
44	0.530	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.6	-0.3	-0.3	-0.4	-0.5	-0.7	-1.0	-1.2	-1.4	-1.5	-1.0	-2.3
45	-0.432	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	-0.1	0.0	0.0	-0.1	-0.1	-0.2	0.0	-0.1
46	-0.566	0.0	0.0	-0.1	-0.2	-0.2	-0.3	-0.4	-0.4	-0.5	-0.8	-0.9	-0.8	-0.2	-0.5	-1.0	-1.2	-1.3	-4.8
47	-0.302	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.4	-0.4	-0.5	-0.5	-0.3	0.0
48	-0.052	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	0.0	-0.1	-0.6
49	0.111	0.0	0.0	0.0	0.0	-0.1	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	0.0	0.0	-0.1	0.1	0.1
50	0.126	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.1	0.3	0.3
51	0.016	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.6	-0.7	-0.8	-0.9	-1.3
52	0.127	0.0	-0.1	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.4	-0.5	-0.5	-0.7	-1.1	-0.7
53	-0.311	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.8	-0.9	-1.0	-1.2	-1.3	-1.3	-1.4	-2.1
54	-0.061	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.7	-0.7	-1.0	-1.1
55	0.119	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.3	-0.4	-0.4	-0.7	-0.7
56	0.053	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.6	-0.7	-0.8	-0.9	-1.2	-1.3

57	0.028	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.6	-1.0	-1.4	-1.8
58	0.117	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.8	-1.0	-1.2	-1.3	-1.9	-2.5
59	-0.163	0.0	-0.1	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.4	-0.4	-0.5	-0.6	-0.7	-1.5	-1.1
60	0.104	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.4	-0.6	-0.5	-0.6	-0.7	-0.8	-1.0	-1.2
61	0.112	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.4	-0.4	-0.5
62	-0.276	-0.2	-0.6	-0.7	-0.9	-1.2	-1.1	-1.5	-1.8	-2.2	-2.7	-3.2	-3.6	-4.5	-5.3	-6.4	-6.5	-8.5	-12.9
63	0.561	-0.2	-0.5	-0.9	-1.0	-1.0	-1.0	-1.1	-0.8	-0.7	-0.6	-0.5	-0.3	0.2	0.3	0.3	0.3	-0.1	1.1
64	-0.478	0.5	0.8	1.1	1.1	1.2	1.1	1.1	1.0	1.0	0.8	0.6	0.3	0.1	-0.3	-0.8	0.2	-1.9	-1.1
65	-0.464	0.1	0.3	0.5	0.4	0.4	0.5	-0.1	0.5	0.5	0.4	0.3	0.3	-0.2	-0.3	-0.4	-0.7	-1.9	-1.6
66	-0.288	0.0	0.0	-0.4	-0.4	-0.4	-0.4	-0.4	-0.3	-0.3	-0.3	-0.3	-0.4	-0.2	-0.4	-0.5	-1.0	-1.0	-0.5
67	-0.036	0.0	0.0	0.2	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.5	0.5	0.4	0.3	0.8	0.4
68	0.128	0.0	0.1	0.0	0.0	0.1	0.1	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.0	0.1	0.4
69	0.127	0.0	0.0	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.2	0.2	0.3	0.3	0.2	0.1	0.1	-0.1
70	0.006	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1
71	0.122	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.4	0.0
72	-0.272	0.0	0.1	0.1	0.1	0.2	0.1	0.2	0.3	0.3	0.4	0.4	0.5	0.4	0.5	0.5	0.6	1.6	0.6
73	-0.061	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.2	0.1
74	0.118	0.0	0.0	0.1	0.0	0.0	0.1	0.0	0.1	0.1	0.1	0.1	0.0	0.0	0.0	0.0	-0.2	0.1	0.1
75	0.042	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.3	-0.3	-0.2	-0.2	-0.3	-0.5
76	-0.001	0.0	-0.1	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.3	-0.2	-0.5
77	0.111	-0.1	-0.2	-0.1	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	-0.3	-0.2	-0.4	-0.4	-0.5	-0.5	-0.3	-0.5
78	-0.174	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.2	-0.2
79	0.100	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	-0.1	-0.1	-0.1	-0.3	-0.3	-0.3	-0.2	-0.2	-0.3
80	0.111	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	-0.1	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.2	0.1
81	-0.477	0.0	-0.1	0.3	0.3	0.2	0.2	0.2	0.2	0.1	0.1	0.0	0.1	-0.3	-0.3	-0.3	-0.2	0.1	-0.2
82	0.304	0.0	0.0	0.1	0.1	0.1	0.1	0.0	0.0	-0.1	0.0	-0.1	-0.1	-0.2	-0.2	-0.1	0.1	-0.1	0.1
83	-0.501	0.1	0.4	-0.1	-0.2	-0.2	-0.2	-0.4	-0.3	-0.4	-0.4	-0.4	-0.4	-0.8	-0.7	-0.6	-0.5	-0.3	0.1
84	0.344	0.2	0.7	-0.5	-0.6	-0.7	-0.6	-1.0	-0.8	-0.8	-0.9	-0.9	-1.0	-1.4	-1.4	-1.4	-1.3	-0.9	-1.0
85	0.494	-0.2	0.1	0.7	0.8	0.8	0.8	0.7	0.7	0.7	0.6	0.6	0.6	0.5	0.6	0.8	1.0	1.2	1.7
86	-0.451	-0.2	-0.4	-1.5	-1.2	-1.3	-1.2	-1.1	-1.2	-1.2	-1.1	-1.0	-0.9	-0.9	-0.6	-0.4	-0.2	-0.3	0.5
87	-0.622	-0.2	-0.3	-0.9	-0.9	-0.9	-0.9	-1.1	-0.9	-0.9	-0.9	-0.8	-0.8	-1.3	-1.2	-1.0	-0.7	-0.8	-0.3
88	-0.378	-0.1	-0.1	0.3	0.3	0.4	0.4	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.5	0.7	1.0	1.4	1.5
89	0.494	-0.2	-0.2	-0.3	-0.3	-0.3	-0.3	-0.5	-0.2	0.0	0.1	0.4	0.7	-0.2	0.5	1.5	2.5	4.2	5.9
90	-0.509	-0.4	-0.9	-1.9	-2.2	-2.3	-2.3	-2.5	-2.4	-2.5	-2.4	-2.4	-2.4	-2.9	-2.6	-2.2	-2.1	-2.0	-0.7
91	-0.505	-0.1	-0.3	-0.2	-0.4	-0.5	-0.5	-0.7	-0.7	-0.7	-0.8	-0.8	-0.9	-1.3	-1.2	-1.0	-0.8	-0.7	0.4
92	-0.500	0.4	0.7	0.7	1.2	1.8	1.9	2.3	3.0	3.6	4.1	4.7	5.5	4.9	6.0	7.4	9.0	12.2	14.7
93	0.870	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.8	-0.8	-1.0	-1.1	-3.5	-1.7	-2.8
94	0.856	-0.3	-0.5	-1.1	-1.1	-1.0	-0.9	-0.9	-0.8	-0.6	-0.4	-0.3	0.0	0.1	0.2	0.4	0.3	0.7	0.7
95	-0.630	-0.2	-0.2	-0.5	-0.5	-0.5	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.5	-0.2	-0.2	-0.1	0.9	-1.0	0.4
96	0.320	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.3	-0.3	-0.4	-1.2	-0.4	-0.5
97	0.317	0.0	0.0	-0.1	-0.2	-0.2	-0.2	-0.1	-0.2	-0.2	-0.3	-0.3	-0.2	-0.4	-0.4	-0.4	-1.0	-0.6	-0.6
98	-0.618	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.2	-0.1
99	0.378	0.0	0.1	0.3	0.3	0.3	0.3	0.2	0.4	0.4	0.4	0.4	0.5	0.2	0.3	0.3	0.2	0.4	0.4
100	0.349	0.1	0.2	0.6	0.7	0.7	0.7	0.6	0.7	0.7	0.7	0.7	0.7	0.8	0.8	0.8	0.9	0.9	0.9
101	-0.726	-0.1	-0.2	-0.5	-0.5	-0.5	-0.4	-0.8	-0.4	-0.4	-0.4	-0.4	-0.5	-1.6	-1.5	-1.4	-1.4	-2.1	-2.6
102	0.292	-0.1	-0.1	-0.4	-0.4	-0.4	-0.4	-0.3	-0.3	-0.3	-0.3	-0.3	-0.1	0.1	0.1	0.1	0.2	0.3	-0.5
103	0.276	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.3	0.0	0.0	0.0	0.0	0.0	0.2	0.4	0.6	0.8	1.0	1.1
104	-0.664	0.0	0.1	0.6	0.6	0.6	0.6	0.9	0.7	0.7	0.8	0.8	1.0	0.5	0.4	0.4	0.3	0.8	0.2
105	0.299	0.0	0.1	0.8	0.9	0.9	0.9	1.2	1.0	1.1	1.1	1.2	1.5	0.8	0.8	0.7	0.7	0.8	0.6
106	0.314	0.1	0.3	0.5	0.5	0.5	0.5	0.6	0.6	0.7	0.7	0.8	0.7	0.8	0.8	0.8	0.8	0.8	0.8
107	-0.678	0.7	0.7	2.9	3.2	3.2	3.2	4.9	3.3	3.3	3.4	3.5	3.9	7.9	7.8	7.7	7.4	8.3	7.4
108	0.309	0.2	0.4	1.2	1.4	1.4	1.4	3.0	1.3	1.3	1.4	1.5	2.0	5.6	5.6	5.6	5.7	5.6	5.9
109	0.298	0.4	0.6	1.0	1.1	1.1	1.1	1.3	1.2	1.2	1.3	1.4	1.4	1.8	1.7	1.6	1.7	1.3	1.5
110	-0.715	0.0	0.0	-0.1	-0.1	-0.1	0.0	0.1	-0.1	0.0	0.1	0.1	0.2	0.0	-0.1	-0.1	0.1	1.0	-0.3
111	0.343	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.3	-0.2	-0.3	-0.4	-0.4	-0.5	-0.4	-0.4	-0.5	-0.6	-1.3	-0.2
112	0.297	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	-0.1	-0.1	-0.1	-0.1	0.0	0.0	-0.1	0.0	-0.1	-0.1

(D) CM charges for the $Mg_cMg_nNa_p$ system.

Index	**C_{is}**	**$(C_{cs}-C_{is})*10^{-2}$ along the reaction coordinate ----------\>|**													
1	0.330	0.0	0.1	0.1	0.1	0.1	0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.5
2	-0.588	0.0	0.1	0.1	0.2	0.2	0.3	0.3	0.4	0.5	0.5	0.6	0.7	0.7	0.8
3	0.379	0.0	0.1	0.1	0.2	0.3	0.3	0.4	0.4	0.4	0.5	0.5	0.8	0.7	0.8
4	0.412	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.3	0.4	0.3	0.4
5	-0.591	0.0	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.3	0.4	0.4	-0.2	0.0	0.0
6	0.374	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.1	0.3	0.3
7	0.325	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1

8	-0.580	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.5	0.4	0.4
9	0.379	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.2	1.0	1.1	1.1
10	0.327	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.2	0.3	0.4	0.5	0.1	0.2	0.2
11	0.090	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	0.5	0.3	0.3
12	-0.246	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	0.5	0.4	0.3
13	0.087	0.0	0.1	0.1	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	1.2	1.3	1.3
14	0.116	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.1	-0.3	-0.4
15	0.275	-0.1	0.0	0.0	-0.1	-0.1	0.0	0.0	-0.1	-0.1	0.0	0.1	1.9	2.0	2.0
16	-0.411	0.0	-0.4	-0.6	-0.4	-0.5	-0.7	-0.9	-1.1	-1.3	-1.7	-2.0	0.3	-0.7	-1.0
17	-0.428	0.1	0.3	0.4	0.4	0.4	0.5	0.7	0.9	1.2	1.3	1.6	2.4	3.4	3.6
18	0.099	0.0	0.1	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	0.2	0.2	0.2
19	-0.252	0.0	-0.1	-0.1	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	0.1	0.1	0.1
20	0.076	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.1
21	0.101	0.0	0.1	0.1	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	0.5	0.7	0.7
22	0.286	0.0	0.1	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	0.5	0.6	0.5
23	-0.395	-0.2	0.0	0.2	0.2	0.3	0.4	0.6	0.6	0.9	1.1	1.4	-0.9	0.3	0.6
24	-0.438	0.0	-0.1	-0.2	-0.4	-0.5	-0.6	-0.7	-0.9	-1.2	-1.4	-1.7	0.2	-1.1	-1.3
25	0.321	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	0.2	0.1	0.1
26	-0.590	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	0.1	-0.1	-0.2
27	0.382	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.6	-0.7	-0.7
28	0.416	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.2	-0.2
29	-0.594	0.0	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.2
30	0.358	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	0.2	0.1	0.1
31	0.358	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.9	-1.0	-1.0
32	-0.569	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.2	-0.8	-0.7	-0.7
33	0.327	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.3	-0.3	-0.3
34	0.317	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1
35	0.089	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.2	-0.3	-0.3
36	-0.246	0.0	0.0	-0.1	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.3	-0.4	-0.4
37	0.110	0.0	0.0	-0.1	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.3	-0.4	-0.4
38	0.089	0.0	0.0	-0.1	-0.1	-0.1	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	-0.1	-0.1
39	0.263	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	0.0	-0.2	-0.3
40	-0.450	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	1.2	0.4	0.3
41	-0.417	0.0	-0.1	0.0	0.1	0.2	0.3	0.4	0.4	0.5	0.7	0.9	-0.1	0.6	0.9
42	0.352	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	0.3	0.2	0.2
43	-0.476	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	0.5	0.5	0.4
44	0.499	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5	-0.5	0.2	0.0	-0.1
45	-0.481	-0.1	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.3	-0.4	0.1	0.0	0.0
46	-0.592	0.0	0.0	-0.1	-0.2	-0.2	-0.2	-0.3	-0.4	-0.4	-0.6	-0.7	-0.1	-0.6	-0.8
47	-0.304	0.0	-0.1	-0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.4	0.3
48	-0.053	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	-0.1	-0.1	-0.1	0.2	0.2	0.1
49	0.118	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.1	-0.3	-0.3
50	0.126	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2
51	0.014	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.3	-0.3	-0.7	-1.1	-1.1
52	0.120	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.5	-0.8	-0.8
53	-0.322	0.0	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.3	-0.9	-0.9
54	-0.066	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.5	-0.6	-0.6	-1.0	-1.0
55	0.113	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.4	-0.9	-1.0
56	0.046	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.7	-0.4	-0.9	-1.0
57	0.027	0.0	0.0	0.0	-0.1	-0.2	-0.2	-0.3	-0.4	-0.6	-0.7	-1.0	-1.3	-2.2	-2.3
58	0.124	0.0	0.0	-0.1	-0.1	-0.2	-0.3	-0.4	-0.5	-0.6	-0.8	-1.0	-1.6	-3.4	-3.5
59	-0.164	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.7	-0.8	-1.4	-1.4
60	0.104	0.0	-0.1	-0.2	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-0.7	-0.8	-0.9	-1.4	-1.4
61	0.107	0.0	0.0	0.0	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.4	-0.5	-0.6	-1.2	-1.2
62	-0.292	-0.3	-0.7	-1.1	-1.3	-1.7	-2.3	-2.9	-3.8	-4.7	-5.6	-7.1	-13.2	-22.8	-23.7
63	0.550	-0.1	-0.2	-0.2	-0.2	-0.2	-0.1	0.0	0.1	0.1	0.1	0.1	0.9	2.7	2.4
64	-0.484	0.0	0.2	0.1	-0.2	-0.3	-0.5	-0.9	-1.2	-1.7	-2.1	-2.8	-2.0	1.5	0.5
65	-0.527	-0.6	-1.0	-1.2	-1.2	-1.5	-1.8	-2.1	-2.5	-3.0	-3.4	-3.7	-0.5	2.2	1.0
66	-0.280	0.0	0.1	0.1	0.1	0.0	0.0	-0.1	-0.2	-0.3	-0.4	-0.6	-0.7	0.0	-0.4

67	-0.034	0.0	0.0	0.1	0.2	0.2	0.2	0.2	0.2	0.2	0.1	0.1	-0.4	-0.3	-0.6
68	0.125	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.6	0.5
69	0.126	0.0	0.0	0.1	0.0	0.0	0.0	-0.1	-0.1	-0.2	-0.3	-0.4	-0.1	-0.3	-0.4
70	0.005	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.0
71	0.117	-0.1	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	0.3	0.3	0.3
72	-0.271	0.0	0.0	0.1	0.1	0.2	0.2	0.3	0.3	0.4	0.4	0.5	0.2	0.3	0.3
73	-0.063	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2
74	0.116	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.3	0.3
75	0.040	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0
76	-0.001	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.3	-0.3	-0.4	-0.2	-0.3	-0.4
77	0.116	0.0	0.0	-0.1	0.0	-0.1	-0.1	-0.1	-0.2	-0.3	-0.3	-0.4	-0.6	-0.7	-0.8
78	-0.176	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	0.2	0.2	0.2
79	0.097	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.1	0.0	0.1	0.0
80	0.105	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.3	0.3
81	-0.477	-0.1	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-0.3	-0.3	-0.3	0.8	0.7	0.7
82	0.305	0.0	0.0	-0.1	0.0	-0.1	-0.1	0.0	0.0	0.0	0.0	0.1	0.8	0.7	0.8
83	-0.434	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.2	0.6	1.1	1.1
84	0.390	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.3	1.3	1.6	1.6
85	0.523	0.1	0.1	0.1	0.3	0.3	0.4	0.4	0.5	0.6	0.8	0.9	0.5	0.8	0.9
86	-0.449	0.1	0.1	0.2	0.1	0.2	0.3	0.4	0.5	0.6	0.8	1.1	-2.0	-1.1	-0.7
87	-0.634	0.0	-0.2	-0.2	0.2	0.3	0.4	0.5	0.6	0.7	0.9	1.1	0.7	1.4	1.6
88	-0.352	0.1	0.2	0.2	0.2	0.3	0.3	0.4	0.6	0.7	0.8	1.0	1.9	2.2	2.3
89	0.499	0.0	0.2	0.1	0.0	0.2	0.4	0.7	1.2	1.9	2.6	3.5	5.1	6.8	7.8
90	-0.538	-0.2	-0.2	-0.4	-0.5	-0.5	-0.4	-0.4	-0.2	0.0	0.5	0.9	1.6	3.3	3.9
91	-0.515	0.0	0.0	-0.1	-0.1	-0.1	0.0	0.0	0.0	0.1	0.3	0.5	1.4	2.5	2.9
92	-0.507	0.8	0.8	1.7	2.6	3.3	4.3	5.4	6.9	8.2	9.9	12.0	12.0	16.7	18.3
93	0.735	0.5	1.5	1.3	1.0	1.5	1.4	1.5	1.7	2.0	2.0	1.7	2.2	2.5	2.4
94	0.870	-0.1	0.1	0.0	-0.2	-0.3	-0.4	-0.5	-0.6	-0.7	-1.0	-1.2	3.4	0.8	0.5
95	0.842	0.2	0.1	0.2	0.4	0.5	0.7	0.8	1.0	1.2	1.4	1.5	2.1	2.1	2.2
96	-0.582	-0.1	0.1	0.1	-0.3	-0.2	-0.3	-0.4	-0.3	-0.4	-0.7	-1.4	-12.1	-12.7	-12.2
97	0.328	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	-1.0	-1.0	-0.9
98	0.370	0.0	-0.1	0.0	0.1	0.0	0.1	0.1	0.2	0.1	0.1	0.3	0.1	0.3	0.4
99	-0.636	0.1	-0.3	-0.2	0.0	0.0	0.1	0.2	0.2	0.2	0.4	0.7	-11.4	-11.5	-11.5
100	0.317	0.1	0.0	0.0	0.0	-0.1	-0.1	-0.1	-0.2	-0.2	-0.2	-0.2	-3.5	-3.5	-3.5
101	0.323	0.0	-0.1	0.0	0.0	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	0.0	-2.8	-2.8	-2.7
102	-0.606	0.0	-0.3	-0.3	-0.1	-0.2	-0.2	-0.3	-0.3	-0.4	-0.4	-0.5	-0.7	-0.9	-0.9
103	0.365	0.2	0.0	0.1	0.1	0.1	0.1	0.2	0.3	0.3	0.2	0.1	1.5	1.6	1.5
104	0.369	0.1	-0.3	-0.2	0.0	0.1	0.1	0.1	0.1	0.1	0.2	0.2	-0.3	-0.1	-0.1
105	-0.702	0.2	0.0	0.0	0.1	0.0	0.0	-0.1	-0.1	-0.3	-0.4	-0.6	2.9	3.2	3.4
106	0.355	-0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.6	0.7
107	0.308	-0.1	0.1	0.1	0.0	0.0	-0.1	-0.1	-0.1	0.0	0.0	0.0	4.9	5.4	5.1
108	-0.669	0.3	-0.3	-0.1	0.2	0.0	0.2	0.4	0.4	0.3	0.5	1.0	-0.9	-0.7	-0.7
109	0.345	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.2	0.2	0.2	0.1	0.7	1.0	1.1
110	0.352	-0.1	0.1	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0	-0.2	0.8	1.1	1.0
111	-0.671	-0.4	0.2	0.2	0.1	0.1	0.2	0.0	-0.4	-0.2	-0.3	-0.4	0.6	-0.5	-0.7
112	0.357	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.3	0.3	0.4	0.2	0.5	0.6
113	0.367	-0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.3	0.3	0.3	0.7	1.0	1.1

(E) Atom identities of QM atoms (Fig. S2) for $Na_cMg_nMg_p$. Amber atom names, residue names, and residue numbers (crystallographic numbering is used) are given. Me_n = 93, Me_c = 94, and Me_p = 95. Note that atom 94 is Mg for the $Mg_cMg_nMg_p$ and Mg_cMg_n systems. For the Mg_cMg_n system, the first water index begins at 95.

Index	Name	ResID	Index	Name	ResID	Index	Name	ResID
1	CD	ARG-183	39	CG	ASP-256	77	H3'	DC3-362
2	NE	ARG-183	40	OD1	ASP-256	78	C2'	DC3-362
3	HE	ARG-183	41	OD2	ASP-256	79	H2'	DC3-362
4	CZ	ARG-183	42	C3'	DG -360	80	H2''	DC3-362
5	NH1	ARG-183	43	O3'	DG -360	81	O3'	DC3-362
6	HH11	ARG-183	44	P	DC -361	82	HO3'	DC3-362
7	HH12	ARG-183	45	OP1	DC -361	83	O21	PPV-369
8	NH2	ARG-183	46	OP2	DC -361	84	H21	PPV-369
9	HH21	ARG-183	47	O5'	DC -361	85	P1	PPV-369
10	HH22	ARG-183	48	C5'	DC -361	86	O11	PPV-369
11	CA	ASP-190	49	H5'	DC -361	87	O31	PPV-369
12	CB	ASP-190	50	H5''	DC -361	88	OPP	PPV-369
13	HB2	ASP-190	51	C4'	DC -361	89	P2	PPV-369
14	HB3	ASP-190	52	H4'	DC -361	90	O22	PPV-369
15	CG	ASP-190	53	O4'	DC -361	91	O32	PPV-369
16	OD1	ASP-190	54	C1'	DC -361	92	O12	PPV-369
17	OD2	ASP-190	55	H1'	DC -361	93	Mg	Mg -370
18	CA	ASP-192	56	N1	DC -361	94	Na	Na -371
19	CB	ASP-192	57	C3'	DC -361	95	Mg	Mg -372
20	HB2	ASP-192	58	H3'	DC -361	96	O	WAT-W01
21	HB3	ASP-192	59	C2'	DC -361	97	H1	WAT-W01
22	CG	ASP-192	60	H2'	DC -361	98	H2	WAT-W01
23	OD1	ASP-192	61	H2''	DC -361	99	O	WAT-W02
24	OD2	ASP-192	62	O3'	DC -361	100	H1	WAT-W02
25	CD	ARG-254	63	P	DC3-362	101	H2	WAT-W02
26	NE	ARG-254	64	OP1	DC3-362	102	O	WAT-W03
27	HE	ARG-254	65	OP2	DC3-362	103	H1	WAT-W03
28	CZ	ARG-254	66	O5'	DC3-362	104	H2	WAT-W03
29	NH1	ARG-254	67	C5'	DC3-362	105	O	WAT-W04
30	HH11	ARG-254	68	H5'	DC3-362	106	H1	WAT-W04
31	HH12	ARG-254	69	H5''	DC3-362	107	H2	WAT-W04
32	NH2	ARG-254	70	C4'	DC3-362	108	O	WAT-W05
33	HH21	ARG-254	71	H4'	DC3-362	109	H1	WAT-W05
34	HH22	ARG-254	72	O4'	DC3-362	110	H2	WAT-W05
35	CA	ASP-256	73	C1'	DC3-362	111	O	WAT-W06
36	CB	ASP-256	74	H1'	DC3-362	112	H1	WAT-W06
37	HB2	ASP-256	75	N1	DC3-362	113	H2	WAT-W06
38	HB3	ASP-256	76	C3'	DC3-362			

Figure S1: Optimization of the unconstrained $Na_cMg_nMg_p$ system at P_α–O_β = 1.7 Å yielded a configuration similar to the one used in the start of the calculations (open triangle).

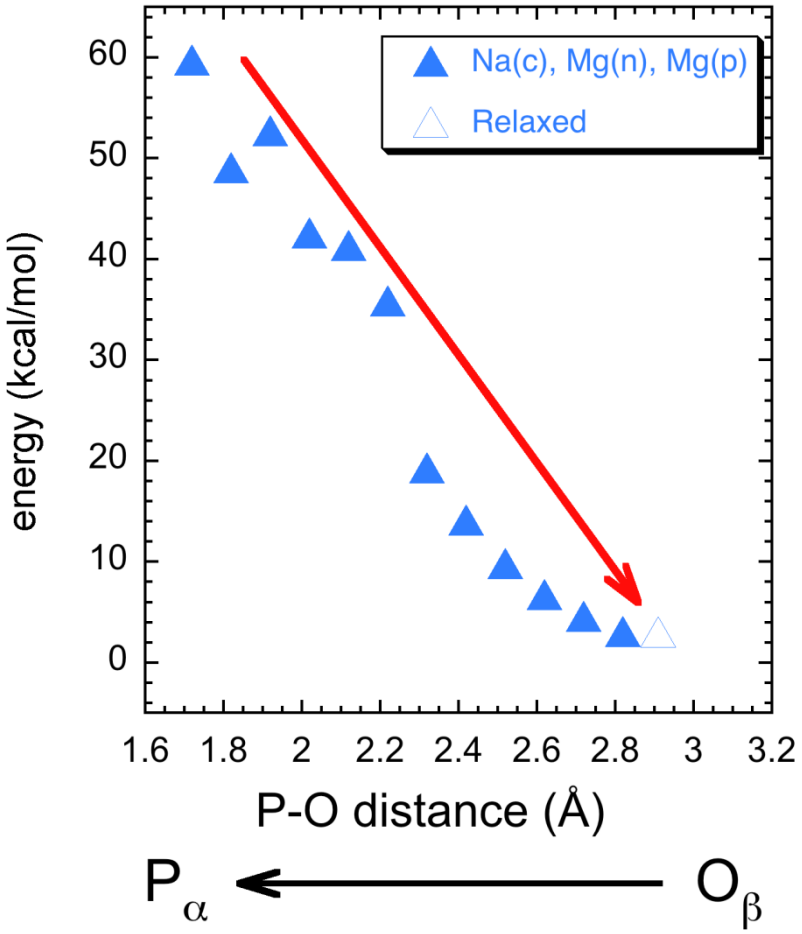

Figure S2: Charge variations (the difference between the charge at current state and the charge at initial state) of the QM atoms as a function of the reaction coordinate for the systems studied. The reaction coordinate of the P_α-O_β distance (Å) is given outside the y-axis. Tick marks for the charge variation (given on the inside of the y-axis) are spaced at 0.25e where "e" is the electron charge. The atom identities (given as atom numbers on the x-axis) are tabulated in Table S1*E* and the charges calculated using the CM5 charge method (35).