Table 1S. Optimization geometries for the C60/Mg^{2+} and C60/Mg complexes.

	C60/Mg^{2+}			C60/Mg		
Atom(s)	X	Y	Z	X	Y	Z
C	-3.044	-1.081	0.945	-3.005	-0.958	-1.073
C	-3.044	0.313	1.403	-2.999	-1.418	0.302
C	-3.043	1.362	0.464	-3.008	-0.499	1.340
C	-3.043	1.062	-0.972	-3.022	0.921	1.051
C	-3.044	-0.276	-1.411	-3.027	1.361	-0.265
C	-3.045	-1.370	-0.433	-3.018	0.400	-1.350
C	-2.244	-1.852	1.862	-2.160	-1.848	-1.845
C	-1.732	-0.940	2.866	-1.632	-2.856	-0.948
C	-2.243	0.389	2.598	-2.152	-2.591	0.379
C	-1.432	1.505	2.770	-1.349	-2.793	1.491
C	-2.242	2.541	0.673	-2.170	-0.711	2.503
C	-2.242	2.058	-1.635	-2.193	1.587	2.035
C	-1.431	1.648	-2.688	-1.403	2.663	1.660
C	-1.431	0.268	-3.142	-1.408	3.123	0.285
C	-2.243	-0.686	-2.536	-2.202	2.487	-0.656
C	-1.732	-2.011	-2.249	-1.683	2.221	-1.983
C	-2.244	-2.443	-0.964	-2.187	0.932	-2.412
C	-1.433	-3.151	-0.083	-1.379	0.082	-3.149
C	-1.433	-2.853	1.339	-1.365	-1.339	-2.860
C	-0.429	-1.088	3.314	-0.333	-3.312	-1.105
C	0.407	-2.150	2.791	0.499	-2.780	-2.166
C	-0.084	-3.021	1.831	-0.006	-1.816	-3.025
C	0.751	-3.421	0.716	0.820	-0.690	-3.416
C	-0.084	-3.502	-0.466	-0.029	0.482	-3.493
C	0.408	-3.089	-1.695	0.453	1.715	-3.083
C	-0.428	-2.326	-2.600	-0.392	2.604	-2.311
C	0.409	-1.342	-3.258	0.438	3.270	-1.327
C	-0.082	-0.075	-3.532	-0.058	3.524	-0.058
C	-1.730	2.954	-0.618	-1.665	0.579	2.932
C	2.560	1.835	-1.830	2.608	1.847	1.845
C	1.765	2.856	-1.337	1.813	1.339	2.860
C	1.765	3.153	0.080	1.827	-0.082	3.150
C	2.560	2.415	0.941	2.636	-0.931	2.411
C	3.397	1.351	0.425	3.467	-0.400	1.350
C	3.396	-0.310	-1.383	3.448	1.418	-0.302
C	2.559	-0.394	-2.562	2.600	2.590	-0.379
C	2.042	0.932	-2.841	2.080	2.856	0.948
C	0.754	1.090	-3.320	0.781	3.312	1.105
C	-0.081	2.154	-2.800	-0.050	2.780	2.167
C	0.410	3.012	-1.828	0.454	1.816	3.025

C	0.410	3.492	0.467	0.477	-0.482	3.493
C	-0.082	3.096	1.701	-0.005	-1.715	3.083
C	0.754	2.330	2.604	0.840	-2.604	2.310
C	2.042	1.993	2.229	2.131	-2.221	1.982
C	2.558	0.666	2.506	2.651	-2.486	0.655
C	3.396	0.271	1.391	3.476	-1.361	0.264
C	3.395	-1.045	0.959	3.471	-0.921	-1.050
C	3.396	-1.342	-0.459	3.457	0.499	-1.340
C	1.764	-1.508	-2.771	1.797	2.793	-1.491
C	1.763	-2.588	-1.805	1.807	1.832	-2.576
C	2.557	-2.505	-0.674	2.618	0.711	-2.502
C	2.040	-2.928	0.613	2.113	-0.579	-2.931
C	2.557	-2.024	1.622	2.641	-1.587	-2.034
C	1.763	-1.647	2.691	1.852	-2.663	-1.660
C	1.763	-0.271	3.143	1.857	-3.123	-0.285
C	0.408	0.076	3.523	0.506	-3.524	0.058
C	-0.083	1.348	3.266	0.010	-3.270	1.327
C	-0.426	3.415	-0.714	-0.371	0.690	3.416
C	-1.431	2.588	1.802	-1.358	-1.832	2.576
C	3.397	1.067	-0.931	3.453	0.958	1.073
Mg	-4.930	0.000	0.000	-6.725	0.000	0.000

Table 2S. Optimization geometries for the Cone/Mg^{2+} and Cone/Mg complexes.

	Cone/Mg^{2+}			Cone/Mg		
	X	Y	Z	X	Y	Z
C	4.680	4.633	-1.096	0.82	-6.540	-1.127
C	3.456	5.251	-0.899	2.05	-5.941	-0.932
C	3.120	6.531	-1.488	3.28	-6.453	-1.518
C	0.766	6.239	-0.899	4.48	-4.405	-0.932
C	1.851	6.997	-1.488	4.42	-5.731	-1.518
C	-0.567	6.561	-1.096	5.55	-3.549	-1.127
C	7.227	0.402	-1.488	-4.08	-5.979	-1.519
C	6.171	1.200	-0.899	-2.80	-5.629	-0.933
C	6.065	2.567	-1.096	-1.65	-6.380	-1.128
C	3.953	2.649	0.130	-0.30	-4.753	0.091
C	4.932	3.305	-0.665	-0.38	-5.929	-0.697
C	2.734	3.320	0.433	0.97	-4.188	0.391
C	2.436	4.567	-0.163	2.13	-4.712	-0.200
C	0.066	4.300	0.432	3.36	-2.671	0.392
C	1.100	5.057	-0.163	3.34	-3.949	-0.200
C	-1.298	4.578	0.130	4.42	-1.760	0.091
C	-1.619	5.711	-0.665	5.52	-2.195	-0.697
C	-3.926	4.909	-0.900	6.28	0.121	-0.933
C	-2.960	5.883	-1.097	6.47	-1.235	-1.128
C	-5.247	4.985	-1.488	7.15	1.128	-1.519
C	6.062	-1.664	-0.899	-5.01	-3.793	-0.933
C	7.176	-0.949	-1.487	-5.12	-5.116	-1.519
C	5.096	-0.906	-0.163	-3.82	-3.488	-0.200
C	5.150	0.516	-0.163	-2.72	-4.399	-0.200
C	3.124	0.598	1.203	-1.42	-2.827	1.150
C	4.110	1.266	0.433	-1.49	-4.029	0.391
C	2.038	1.365	1.704	-0.15	-2.416	1.659
C	1.741	2.662	1.203	1.05	-2.987	1.150
C	-0.669	2.360	1.703	2.25	-0.895	1.659
C	0.397	3.156	1.203	2.24	-2.231	1.150
C	-1.994	2.478	1.203	3.16	0.078	1.150
C	-2.313	3.626	0.432	4.28	-0.371	0.391
C	-4.470	2.609	-0.163	4.78	1.958	-0.201
C	-3.590	3.728	-0.164	5.14	0.575	-0.200
C	-5.697	2.656	-0.899	5.57	2.906	-0.933
C	-6.083	3.923	-1.488	6.81	2.436	-1.519
C	4.667	-3.669	-0.664	-5.75	-1.470	-0.697
C	5.853	-3.020	-1.095	-5.96	-2.808	-1.128
C	3.741	-2.941	0.131	-4.61	-1.178	0.091
C	4.003	-1.574	0.433	-3.68	-2.217	0.391

C	1.929	-1.516	1.704	-2.34	-0.599	1.659
C	3.070	-0.833	1.203	-2.51	-1.924	1.150
C	0.958	-0.753	2.361	-1.17	-0.299	2.320
C	1.013	0.678	2.361	-0.07	-1.205	2.320
C	-1.218	0.046	2.361	0.77	0.929	2.320
C	-0.332	1.173	2.361	1.12	-0.446	2.320
C	-2.451	0.093	1.704	1.54	1.863	1.658
C	-2.879	1.353	1.203	2.81	1.449	1.150
C	-4.756	0.181	0.131	3.04	3.665	0.090
C	-4.070	1.392	0.433	3.58	2.378	0.391
C	-5.933	0.225	-0.664	3.79	4.572	-0.698
C	-6.416	1.488	-1.095	5.09	4.186	-1.129
C	3.048	-5.498	-0.899	-6.21	0.925	-0.934
C	4.316	-4.975	-1.095	-6.58	-0.395	-1.128
C	2.083	-4.738	-0.163	-5.02	1.230	-0.201
C	2.474	-3.518	0.433	-4.29	0.181	0.391
C	1.534	-2.787	1.203	-3.13	0.483	1.150
C	-0.846	-2.303	1.704	-1.29	2.046	1.658
C	-0.420	-1.144	2.361	-0.64	1.021	2.320
C	-2.176	-2.320	1.203	-0.50	3.126	1.149
C	-2.973	-1.131	1.204	0.90	3.035	1.149
C	-4.655	-2.263	-0.163	1.04	5.067	-0.201
C	-4.164	-1.079	0.433	1.67	3.958	0.390
C	-5.883	-2.217	-0.899	1.82	6.016	-0.934
C	-6.510	-0.997	-1.095	3.17	5.777	-1.129
C	2.616	-6.749	-1.488	-6.94	2.035	-1.519
C	-0.260	-4.293	0.432	-3.24	2.817	0.390
C	0.157	-3.177	1.203	-2.60	1.798	1.149
C	-1.641	-4.467	0.130	-2.54	4.024	0.090
C	-2.581	-3.440	0.433	-1.15	4.140	0.390
C	-4.287	-4.597	-0.899	-1.04	6.200	-0.935
C	-3.863	-3.445	-0.163	-0.38	5.159	-0.202
C	-5.611	-4.573	-1.488	-0.21	7.236	-1.520
C	-6.363	-3.450	-1.487	1.13	7.149	-1.520
C	0.291	-6.279	-0.900	-5.15	3.596	-0.934
C	0.714	-5.126	-0.163	-4.49	2.556	-0.201
C	-1.063	-6.499	-1.097	-4.51	4.804	-1.130
C	-2.047	-5.572	-0.666	-3.17	5.020	-0.699
C	-3.398	-5.641	-1.097	-2.40	6.136	-1.130
C	1.315	-7.117	-1.488	-6.44	3.290	-1.520
C	1.615	7.939	-1.974	5.31	-6.118	-2.003
H	3.909	7.096	-1.974	3.25	-7.425	-2.003
H	5.442	5.144	-1.679	0.76	-7.457	-1.711

H	6.827	3.078	-1.679	-1.71	-7.297	-1.711
H	8.050	0.917	-1.974	-4.17	-6.947	-2.004
H	7.957	-1.525	-1.974	-6.05	-5.386	-2.004
H	6.574	-3.587	-1.679	-6.85	-3.035	-1.712
H	5.037	-5.542	-1.679	-7.47	-0.622	-1.712
H	3.360	-7.372	-1.974	-7.89	1.824	-2.004
H	1.008	-8.038	-1.975	-6.99	4.095	-2.005
H	-1.380	-7.360	-1.680	-5.00	5.580	-1.713
H	-3.714	-6.502	-1.680	-2.89	6.912	-1.713
H	-5.973	-5.473	-1.974	-0.70	8.074	-2.005
H	-7.334	-3.443	-1.973	1.73	7.917	-2.005
H	-7.427	-0.962	-1.678	3.76	6.483	-1.712
H	-7.333	1.523	-1.679	5.67	4.893	-1.712
H	-7.052	3.989	-1.974	7.46	3.165	-2.004
H	-5.541	5.910	-1.975	8.06	0.797	-2.004
H	-3.210	6.765	-1.680	7.32	-1.574	-1.711
H	-0.817	7.444	-1.680	6.40	-3.889	-1.711
Mg	0.000	0.001	4.271	-0.00	0.013	5.870

Table 3S. Optimization geometries for the Tube/Mg^{2+} and Tube/Mg complexes.

	Tube/Mg^{2+}			Tube/Mg		
	X	Y	Z	X	Y	Z
C	1.214	1.103	2.157	0.065	0.015	0.016
C	1.587	-0.127	1.508	0.100	-0.009	1.523
C	1.183	1.147	3.578	1.237	0.014	-0.692
C	1.682	0.015	4.323	2.550	0.115	0.046
C	1.118	1.270	6.401	3.759	0.279	-2.078
C	1.771	0.073	5.742	3.718	0.313	-0.605
C	1.100	1.271	7.811	4.951	0.452	-2.704
C	1.779	0.110	8.500	6.155	0.706	-1.886
C	1.190	1.224	10.650	7.404	0.790	-4.016
C	1.675	0.084	9.928	7.344	0.853	-2.520
C	1.203	1.190	12.063	8.646	0.955	-4.620
C	1.695	-0.010	12.723	9.837	1.206	-3.778
C	1.156	0.984	14.879	11.161	1.410	-5.811
C	1.750	-0.070	14.126	11.079	1.389	-4.377
C	-1.173	1.150	2.126	-0.786	1.856	-1.365
C	0.038	1.472	1.436	-1.160	0.715	-0.531
C	-1.167	1.180	3.545	0.460	1.995	-1.829
C	0.002	1.666	4.256	1.320	0.813	-1.955
C	-1.226	1.272	6.402	2.964	2.360	-2.953
C	-0.032	1.694	5.673	2.527	0.898	-2.703
C	-1.226	1.288	7.816	4.174	2.552	-3.578
C	-0.034	1.738	8.534	4.951	1.280	-3.985
C	-1.183	1.237	10.681	6.698	2.854	-4.869
C	0.001	1.690	9.946	6.263	1.520	-4.533
C	-1.181	1.210	12.084	7.948	3.024	-5.494
C	0.023	1.609	12.797	8.750	1.835	-5.768
C	-1.093	1.002	14.895	10.528	3.277	-6.604
C	0.033	1.594	14.217	9.988	1.965	-6.426
C	-1.179	-1.226	2.224	0.085	2.434	0.876
C	-1.536	-0.073	1.462	-1.139	2.229	0.002
C	-1.197	-1.156	3.626	1.271	2.833	0.322
C	-1.656	0.049	4.290	1.387	2.927	-1.165
C	-1.277	-1.087	6.442	3.801	3.395	-0.990
C	-1.690	0.096	5.713	2.624	3.160	-1.768
C	-1.286	-1.066	7.818	5.038	3.602	-1.633
C	-1.704	0.129	8.527	5.110	3.536	-3.066
C	-1.240	-1.121	10.638	7.511	3.979	-2.935
C	-1.674	0.107	9.948	6.339	3.721	-3.733
C	-1.223	-1.156	12.007	8.750	4.168	-3.539
C	-1.686	0.014	12.752	8.874	4.029	-4.977

C	-1.107	-1.161	14.827	11.312	4.324	-4.740
C	-1.717	-0.043	14.153	10.140	4.209	-5.596
C	1.223	-1.281	2.274	1.289	0.639	2.065
C	0.028	-1.654	1.559	0.107	1.498	2.062
C	1.203	-1.206	3.670	2.324	0.928	1.277
C	-0.028	-1.662	4.380	2.582	2.346	0.888
C	1.128	-1.128	6.455	4.629	1.396	-0.094
C	-0.071	-1.630	5.738	3.752	2.584	0.240
C	1.128	-1.098	7.811	5.818	1.584	-0.716
C	-0.071	-1.579	8.547	6.250	2.976	-1.076
C	1.201	-1.141	10.613	8.265	1.923	-2.032
C	-0.035	-1.597	9.897	7.442	3.145	-1.708
C	1.197	-1.171	11.984	9.474	2.077	-2.627
C	-0.012	-1.669	12.700	9.913	3.468	-2.946
C	1.130	-1.177	14.807	11.916	2.511	-3.950
C	0.001	-1.717	14.087	11.168	3.651	-3.480
H	1.232	1.007	15.963	12.127	1.443	-6.305
H	1.240	-1.327	15.876	12.968	2.567	-4.210
H	-1.156	1.031	15.980	11.465	3.420	-7.138
H	-1.207	-1.312	15.898	12.276	4.627	-5.135
H	-1.607	-0.119	0.379	-2.098	2.662	0.276
H	0.054	1.498	0.349	-2.122	0.210	-0.566
H	0.044	-1.851	0.491	-0.526	1.680	2.927
H	1.705	-0.178	0.430	-0.535	-0.697	2.076
Mg	3.412	-0.008	7.123	3.080	0.635	-4.766

Table 4S. Optimization geometries for the Sheet/Mg^{2+} and Sheet/Mg complexes.

	Sheet/Mg^{2+}			Sheet/Mg		
	X	Y	Z	X	Y	Z
C	2.840	-0.377	-0.043	-2.452	1.437	-0.127
C	3.691	0.750	-0.049	-3.679	0.738	-0.122
C	3.367	-1.688	-0.049	-2.442	2.849	-0.121
C	2.495	-2.821	-0.052	-1.201	3.555	-0.121
C	1.423	-0.189	-0.038	-1.218	0.714	-0.137
C	1.093	-2.647	-0.038	0.018	2.842	-0.127
C	0.548	-1.327	-0.049	0.009	1.412	-0.136
C	0.221	-3.759	-0.052	1.246	3.539	-0.121
C	-0.875	-1.138	-0.038	1.227	0.698	-0.136
C	-1.746	-2.270	-0.043	2.471	1.405	-0.127
C	-1.196	-3.571	-0.049	2.478	2.817	-0.121
C	-3.145	-2.072	-0.049	3.688	0.690	-0.121
C	3.145	2.071	-0.051	-3.688	-0.690	-0.122
C	1.746	2.270	-0.037	-2.471	-1.405	-0.127
C	0.875	1.138	-0.049	-1.227	-0.698	-0.137
C	-0.548	1.327	-0.038	-0.009	-1.412	-0.136
C	-1.423	0.189	-0.048	1.218	-0.714	-0.137
C	-2.839	0.377	-0.038	2.452	-1.437	-0.127
C	-3.691	-0.751	-0.052	3.679	-0.737	-0.122
C	1.195	3.571	-0.051	-2.478	-2.817	-0.121
C	-0.221	3.760	-0.048	-1.246	-3.539	-0.121
C	-1.093	2.648	-0.043	-0.018	-2.842	-0.127
C	-2.495	2.821	-0.049	1.201	-3.555	-0.121
C	-3.366	1.688	-0.052	2.442	-2.849	-0.121
C	-2.065	-4.693	-0.066	3.715	3.516	-0.113
C	-4.007	-3.200	-0.066	4.921	1.397	-0.113
C	-3.447	-4.482	-0.073	4.909	2.793	-0.111
C	-5.430	-2.974	-0.081	6.145	0.638	-0.108
C	-5.097	-0.559	-0.067	4.903	-1.459	-0.114
C	-5.946	-1.722	-0.081	6.136	-0.716	-0.108
C	-4.774	1.870	-0.066	3.670	-3.564	-0.113
C	-5.604	0.745	-0.073	4.873	-2.855	-0.111
H	-6.682	0.888	-0.089	5.812	-3.405	-0.104
H	-7.022	-1.575	-0.096	7.071	-1.271	-0.102
H	-6.088	-3.837	-0.096	7.086	1.181	-0.102
H	-4.110	-5.343	-0.089	5.855	3.330	-0.104
C	5.097	0.558	-0.066	-4.903	1.459	-0.114
C	5.947	1.722	-0.079	-6.136	0.716	-0.108
C	5.605	-0.745	-0.072	-4.873	2.855	-0.111
C	4.775	-1.870	-0.066	-3.670	3.564	-0.113

C	5.430	2.974	-0.079	-6.145	-0.638	-0.108
C	4.007	3.199	-0.065	-4.921	-1.397	-0.114
C	3.447	4.481	-0.071	-4.909	-2.792	-0.111
C	2.065	4.693	-0.065	-3.715	-3.516	-0.113
C	6.682	-0.888	-0.088	-5.811	3.405	-0.104
H	7.022	1.575	-0.094	-7.071	1.271	-0.102
H	6.088	3.837	-0.094	-7.086	-1.181	-0.102
H	4.110	5.342	-0.086	-5.855	-3.330	-0.104
H	-0.768	5.070	-0.065	-1.251	-4.960	-0.113
C	-2.157	5.226	-0.072	-0.036	-5.648	-0.110
C	-3.032	4.135	-0.066	1.188	-4.976	-0.113
C	-4.464	4.289	-0.080	2.448	-5.672	-0.107
C	-5.290	3.215	-0.080	3.625	-5.003	-0.107
C	-4.875	5.294	-0.095	2.435	-6.759	-0.102
H	-2.572	6.231	-0.087	-0.043	-6.735	-0.104
H	1.482	6.011	-0.078	-3.688	-4.956	-0.107
C	0.139	6.189	-0.079	-2.520	-5.640	-0.107
C	2.147	6.868	-0.093	-4.636	-5.488	-0.102
H	-0.279	7.191	-0.093	-2.521	-6.727	-0.102
H	-6.367	3.354	-0.096	4.566	-5.546	-0.102
H	3.032	-4.135	-0.066	-1.187	4.976	-0.113
C	2.157	-5.226	-0.072	0.036	5.648	-0.110
C	0.767	-5.069	-0.066	1.251	4.960	-0.113
C	-0.139	-6.189	-0.080	2.520	5.640	-0.107
C	-1.482	-6.011	-0.080	3.689	4.956	-0.107
C	0.279	-7.191	-0.095	2.521	6.727	-0.102
H	2.572	-6.230	-0.088	0.043	6.735	-0.104
H	5.291	-3.215	-0.080	-3.625	5.003	-0.107
C	4.464	-4.289	-0.080	-2.448	5.672	-0.107
C	4.875	-5.294	-0.095	-2.434	6.759	-0.102
C	6.367	-3.354	-0.095	-4.566	5.547	-0.102
H	-2.147	-6.869	-0.095	4.636	5.488	-0.102
H	0.000	0.000	1.780	-0.001	-0.001	3.331
Mg						

Table 5S. The frequencies associated with the Mg^{2+} and Mg species and nanostructures.

Nanostructure	ν_1(cm^{-1}) Bending	ν_2(cm^{-1}) Streching
Cone/Mg^{2+}	134.9	310.8
Cone/Mg	19.2	68.0
Tube/Mg^{2+}	53.0	353.2
Tube/Mg	38.0	292.4
Sheet/Mg^{2+}	117.9	418.2
Sheet/Mg	19.7	80.2
C60/Mg^{2+}	150.4	320.6
C60/Mg	12.1	54.5