

Electronic Supplementary Information

Unveiling the Mg(II) Promoted [3+2] Cycloaddition Reaction of Mesitronitrile Oxide to Baylis-Hillman Adduct from the Molecular Electron Density Theory Perspective

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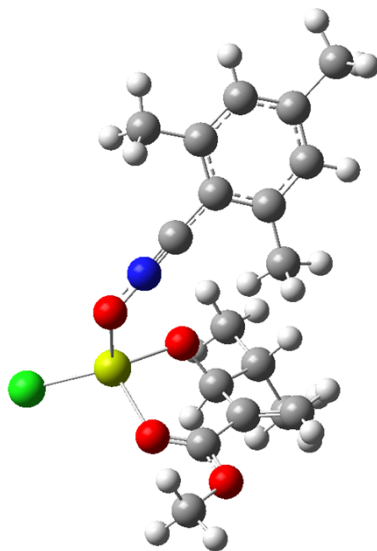


Figure S1. ω B97X-D/6-311G(d,p) optimized geometries of MC-Mg

Table S1. ω B97X-D/6-311G(d,p) total electronic energies, in a.u., in the gas phase and toluene, of the stationary points involved in the *zw-type* 32CA reaction of MNO **9** with BHA **10**.

	gas phase	toluene
MNO 9	-517.540861	-517.544284
BHA 10	-538.922886	-538.926314
TS-o-I	-1056.453708	-1056.458795
TS-o-II	-1056.446798	-1056.453036
TS-m-I	-1056.445111	-1056.450280
TS-m-II	-1056.448570	-1056.452850
11	-1056.531794	-1056.537374
12	-1056.530424	-1056.535908
18	-1056.520022	-1056.525846
19	-1056.524436	-1056.530133

Table S2. ω B97X-D/6-311G(d,p) enthalpies, H in a.u., entropies, S in kcal·mol⁻¹K⁻¹, and Gibbs free energies, G in a.u., computed in toluene at 80 °C, of the stationary points involved in the *zw-type* 32CA reaction of MNO **9** with BHA **10**.

	H	S	G
MNO 9	-517.339863	120.2	-517.407493
BHA 10	-538.693107	119.5	-538.760354
TS-o-I	-1056.020355	191.0	-1056.127852
TS-o-II	-1056.014925	195.0	-1056.124674
TS-m-I	-1056.011953	186.9	-1056.117116
TS-m-II	-1056.014308	187.7	-1056.119946
11	-1056.095676	189.2	-1056.202163
12	-1056.094158	188.2	-1056.200062
18	-1056.083317	180.2	-1056.184750
19	-1056.087656	182.3	-1056.190241

Table S3. ω B97X-D/6-311G(d,p) total electronic energies, in a.u., in the gas phase and toluene, of the stationary points involved in the Mg(II)-promoted *zw-type* 32CA reaction of MNO **9** with BHA **10**.

	Gas phase	DCM
MNO 9	-517.540861	-517.547007
17	-1198.748648	-1198.781181
MC-Mg	-1716.329156	-1716.355255
TS-o-I-Mg	-1716.276377	-1716.313151
TS-o-II-Mg	-1716.293852	-1716.321133
TS-m-I-Mg	-1716.271934	-1716.306541
TS-m-II-Mg	-1716.294236	-1716.318767
20	-1716.355843	-1716.394622
21	-1716.372323	-1716.404258
22	-1716.351318	-1716.386410
23	-1716.371082	-1716.396808

Table S4. ω B97X-D/6-311G(d,p) enthalpies, H in a.u., entropies, S in kcal·mol⁻¹K⁻¹, and Gibbs free energies, G in a.u., computed in DCM at r.t., of the stationary points involved in the Mg(II)-promoted *zw-type* 32CA reaction of MNO **9** with BHA **10**.

	H	S	G
MNO 9	-517.347098	111.6	-517.400127
17	-1198.559321	126.1	-1198.619212
MC-Mg	-1715.932176	188.4	-1716.021708
TS-o-I-Mg	-1715.891276	188.6	-1715.980871
TS-o-II-Mg	-1715.900129	182.3	-1715.986735
TS-m-I-Mg	-1715.884243	184.5	-1715.971888
TS-m-II-Mg	-1715.896150	179.7	-1715.981550
20	-1715.969406	176.4	-1716.053228
21	-1715.979484	179.9	-1716.064981
22	-1715.959770	178.6	-1716.044620
23	-1715.970117	180.6	-1716.055915

ω B97X-D/6-311G(d,p) gas phase Cartesian coordinates of the stationary points involved in the *zw-type* 32CA reaction of MNO **9** with BHA **10**.

MNO 9

8	-1.339826	0.373711	1.709563
7	-0.218805	0.220405	1.302436
6	0.861188	0.072815	0.910576
6	2.194281	-0.109692	0.426720
6	2.766234	-1.393219	0.448804
6	2.909388	0.997671	-0.059014
6	4.062594	-1.543892	-0.024713
6	4.203118	0.794292	-0.521699
6	4.795747	-0.465690	-0.515221
1	4.514871	-2.530944	-0.009238
1	4.765041	1.644380	-0.896513
6	2.283556	2.364605	-0.070367
1	2.970912	3.106788	-0.478206
1	2.003296	2.676258	0.939954
1	1.372003	2.373544	-0.674910
6	6.187400	-0.665613	-1.052731
1	6.709520	-1.460469	-0.515916
1	6.779685	0.248029	-0.972575
1	6.153705	-0.947594	-2.109858
6	1.987799	-2.566082	0.976634
1	1.068460	-2.716456	0.403306
1	1.695347	-2.406352	2.018439
1	2.576673	-3.482624	0.923978

BHA 10

6	-0.099771	0.588005	0.142415
6	-0.058693	1.917157	0.147018
1	0.882559	2.439518	0.281867
1	-0.953179	2.513566	0.018883
6	-1.393745	-0.138805	-0.007335
8	-1.517213	-1.330872	0.169210
8	-2.414492	0.646319	-0.353757
6	-3.683470	0.000374	-0.472655
1	-4.384206	0.783789	-0.751037
1	-3.971780	-0.453702	0.476598
1	-3.647221	-0.773193	-1.241122
6	1.132123	-0.282746	0.315886
1	1.968460	0.381005	0.562246
8	0.991622	-1.142231	1.428713
1	0.221498	-1.691409	1.246620
6	1.507700	-1.056415	-0.965798
1	0.692410	-1.760952	-1.169107
6	1.659816	-0.123799	-2.167532

1	2.415541	0.644740	-1.967875
1	0.726276	0.385313	-2.417772
1	1.983699	-0.685239	-3.047560
6	2.788720	-1.855505	-0.729719
1	3.016374	-2.486645	-1.592896
1	2.695904	-2.489455	0.152550
1	3.638588	-1.181318	-0.573825

TS-o-I

6	1.803994	0.140630	-0.153408
8	1.103933	0.566677	2.081146
6	0.569073	-0.014631	-0.720654
7	-0.085476	0.452912	1.797212
6	-0.794144	0.216750	0.854120
1	0.122895	0.803252	-1.271855
1	0.232929	-1.017335	-0.963596
6	2.447483	1.474929	-0.084736
8	3.610020	1.664911	0.168634
8	1.583464	2.473960	-0.346455
6	2.124184	3.788830	-0.245008
1	2.951544	3.921678	-0.944158
1	2.482374	3.975649	0.768780
1	1.306334	4.463689	-0.489592
6	2.632373	-1.060135	0.262276
1	3.472080	-0.696501	0.866168
8	1.836968	-1.966192	1.013661
1	1.597863	-1.494300	1.816750
6	3.199142	-1.837718	-0.933402
1	2.337163	-2.255371	-1.470208
6	3.977461	-0.929438	-1.885280
1	4.427498	-1.520675	-2.686972
1	4.776925	-0.403289	-1.356114
1	3.334263	-0.176428	-2.348090
6	4.071127	-2.992956	-0.442530
1	4.412246	-3.602793	-1.283720
1	3.521331	-3.629542	0.251208
1	4.957910	-2.608263	0.073060
6	-2.148339	0.010046	0.404223
6	-2.880066	1.099957	-0.092525
6	-2.666976	-1.294049	0.390265
6	-4.155539	0.861053	-0.586709
6	-3.947197	-1.481932	-0.116255
6	-4.704066	-0.420023	-0.605746
1	-4.735305	1.693596	-0.973770
1	-4.363105	-2.484763	-0.135198
6	-1.870243	-2.446199	0.939749
1	-1.916683	-2.446357	2.033652

1	-0.812522	-2.387932	0.669616
1	-2.268873	-3.398820	0.588092
6	-6.098580	-0.647315	-1.124498
1	-6.829587	-0.528066	-0.318603
1	-6.213190	-1.655031	-1.528561
1	-6.352311	0.068429	-1.909082
6	-2.303237	2.489106	-0.058430
1	-2.889471	3.170640	-0.676445
1	-1.265671	2.507148	-0.402255
1	-2.302102	2.874724	0.965796

TS-o-II

6	-1.759492	0.062420	-0.163838
8	-1.043537	0.604069	2.041051
6	-0.522458	-0.186939	-0.700431
7	0.136752	0.396805	1.786251
6	0.841438	0.068259	0.866310
1	-0.241420	-1.216046	-0.903278
1	-0.029307	0.572124	-1.295027
6	-2.315445	1.441633	-0.221360
8	-3.480471	1.730133	-0.160438
8	-1.343205	2.364596	-0.382832
6	-1.788218	3.717693	-0.415103
1	-0.891302	4.319701	-0.548498
1	-2.285001	3.977626	0.521113
1	-2.482643	3.878188	-1.241662
6	-2.670165	-1.084930	0.235832
1	-2.021439	-1.979572	0.281512
8	-3.305979	-0.885962	1.472373
1	-2.648975	-0.515907	2.068016
6	-3.771407	-1.373635	-0.802587
1	-4.428894	-0.500329	-0.796976
6	-3.205767	-1.569427	-2.207880
1	-4.005565	-1.843122	-2.900673
1	-2.463780	-2.376839	-2.225162
1	-2.727360	-0.665564	-2.592103
6	-4.573951	-2.599558	-0.366217
1	-5.408342	-2.774372	-1.051133
1	-4.970254	-2.466221	0.640135
1	-3.943061	-3.496560	-0.371349
6	2.207365	-0.112316	0.434580
6	2.775000	-1.395986	0.450642
6	2.914748	0.996188	-0.056608
6	4.071998	-1.546540	-0.021097
6	4.209299	0.794657	-0.520012
6	4.801347	-0.465675	-0.513331
1	4.527185	-2.532167	-0.005916
1	4.771228	1.644092	-0.896299

6	2.297958	2.368274	-0.043171
1	2.885299	3.065217	-0.642645
1	2.253353	2.753514	0.980344
1	1.271378	2.356884	-0.418176
6	6.191137	-0.664977	-1.055439
1	6.715752	-1.458809	-0.519801
1	6.782699	0.249342	-0.979751
1	6.151858	-0.948834	-2.111801
6	2.001662	-2.567852	0.990008
1	1.049844	-2.693180	0.465954
1	1.766350	-2.424410	2.048228
1	2.570375	-3.492823	0.888169

TS-m-I

6	-1.623973	0.537478	0.236907
8	-1.215227	1.216083	2.864954
6	-2.331126	1.279436	1.164983
7	-0.167630	0.678412	2.497176
6	0.275643	0.191415	1.481623
1	-2.298163	2.358913	1.142920
1	-3.159231	0.813630	1.683021
6	-0.854568	1.190885	-0.847098
8	-0.330759	0.606559	-1.763684
8	-0.786634	2.532928	-0.719722
6	-0.069015	3.203060	-1.753847
1	-0.560327	3.056376	-2.717212
1	0.953897	2.827629	-1.819455
1	-0.074495	4.256168	-1.480223
6	-2.039580	-0.904339	-0.028984
1	-1.243714	-1.379755	-0.617832
6	-3.357239	-1.036016	-0.812686
1	-4.142206	-0.654963	-0.147041
6	-3.378850	-0.222035	-2.105654
1	-4.317383	-0.398238	-2.637794
1	-2.552907	-0.503224	-2.764073
1	-3.305939	0.852024	-1.915212
6	-3.641885	-2.511162	-1.100897
1	-4.614794	-2.628722	-1.585987
1	-3.638599	-3.098640	-0.182482
1	-2.881301	-2.920098	-1.775639
6	1.482761	-0.220380	0.811997
6	1.739388	-1.577481	0.548621
6	2.377837	0.781393	0.387561
6	2.870651	-1.901603	-0.188366
6	3.492218	0.404117	-0.348121
6	3.744258	-0.927891	-0.663945
1	3.079741	-2.946822	-0.394147
1	4.186398	1.170029	-0.680265

6	2.183576	2.219070	0.786344
1	2.457682	2.354050	1.837572
1	1.147103	2.541514	0.683215
1	2.816076	2.876731	0.187969
6	4.928944	-1.306210	-1.509960
1	5.750712	-0.598319	-1.384444
1	4.651384	-1.308579	-2.568706
1	5.293211	-2.304994	-1.261257
6	0.858052	-2.670790	1.088257
1	-0.098230	-2.728030	0.565151
1	0.645433	-2.512856	2.149257
1	1.348504	-3.639735	0.987432
8	-2.255362	-1.602027	1.189486
1	-1.508148	-1.434988	1.766311

TS-m-II

6	1.714834	0.220097	0.356206
8	1.241195	0.810975	2.975534
6	2.480510	0.595158	1.448631
7	0.121145	0.635107	2.481635
1	2.835942	1.611710	1.537777
1	3.043378	-0.159924	1.982021
6	1.387189	1.210652	-0.685323
8	0.864723	0.935612	-1.748563
6	1.722482	-1.234610	-0.109955
1	1.830003	-1.860913	0.784610
8	0.501973	-1.624673	-0.704976
1	0.303581	-0.957052	-1.373118
6	2.899144	-1.563128	-1.062719
1	2.736175	-0.977572	-1.975793
6	4.266434	-1.195250	-0.487695
1	5.059242	-1.507453	-1.172534
1	4.439121	-1.704250	0.467723
1	4.373939	-0.121106	-0.322463
6	2.860349	-3.047382	-1.429733
1	3.625872	-3.282524	-2.174232
1	1.885443	-3.325306	-1.829759
1	3.054238	-3.665564	-0.545319
6	-0.367987	0.366021	1.415765
6	-1.602971	0.088690	0.728006
6	-2.229932	1.096179	-0.016316
6	-2.163065	-1.204083	0.820626
6	-3.409646	0.786858	-0.689697
6	-3.342735	-1.456199	0.143012
6	-3.974593	-0.478394	-0.628735
1	-3.898314	1.563370	-1.270752
1	-3.784397	-2.445983	0.209198
6	-1.707504	2.505236	-0.068992

1	-0.714577	2.599464	0.370047
1	-2.377697	3.172179	0.481299
1	-1.666720	2.854209	-1.103154
6	-1.494216	-2.282425	1.621788
1	-1.221960	-1.930296	2.619817
1	-0.582890	-2.592429	1.105896
1	-2.148631	-3.148707	1.728556
6	-5.237106	-0.806656	-1.378536
1	-5.692436	0.087882	-1.806796
1	-5.969757	-1.283162	-0.722042
1	-5.027744	-1.503116	-2.195879
8	1.726092	2.471484	-0.369663
6	1.522573	3.447026	-1.389527
1	1.869698	4.387315	-0.966907
1	2.098092	3.193109	-2.281263
1	0.467967	3.516445	-1.657873

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6	1.696563	0.078209	0.407264
8	1.162156	0.337722	1.744669
6	0.461909	-0.231717	-0.434894
7	-0.228568	0.319471	1.722418
6	-0.637163	0.018489	0.557292
1	0.359274	0.410760	-1.309133
1	0.440440	-1.274207	-0.759953
6	2.409638	1.391590	0.084903
8	3.532542	1.649173	0.420941
8	1.606491	2.254390	-0.545928
6	2.151936	3.557479	-0.767808
1	3.049726	3.493351	-1.384123
1	2.402727	4.028417	0.183487
1	1.373458	4.117752	-1.280121
6	2.669775	-1.104386	0.568801
1	3.523255	-0.738181	1.153626
8	1.990870	-2.133035	1.263299
1	1.685751	-1.749985	2.090311
6	3.181535	-1.719494	-0.737937
1	2.328872	-2.240221	-1.190274
6	3.710425	-0.694628	-1.741806
1	4.097946	-1.209825	-2.624178
1	4.519510	-0.099445	-1.311510
1	2.932058	-0.006801	-2.087614
6	4.250568	-2.766473	-0.419767
1	4.546534	-3.303404	-1.324866
1	3.880192	-3.489142	0.308047
1	5.143879	-2.286642	-0.006158
6	-2.078936	-0.070359	0.233178
6	-2.819235	1.108778	0.067721

6	-2.673304	-1.322770	0.053887
6	-4.162107	1.008522	-0.273927
6	-4.024508	-1.378106	-0.280771
6	-4.783474	-0.226438	-0.448512
1	-4.741680	1.917931	-0.405438
1	-4.493655	-2.349341	-0.411022
6	-1.884060	-2.600025	0.200319
1	-2.511916	-3.397492	0.602145
1	-1.022078	-2.482619	0.859598
1	-1.510837	-2.937270	-0.772622
6	-6.250343	-0.305096	-0.781106
1	-6.542579	0.488317	-1.472989
1	-6.856960	-0.193542	0.123063
1	-6.504913	-1.264759	-1.235343
6	-2.176435	2.457305	0.269034
1	-2.830418	3.255880	-0.085363
1	-1.221262	2.529696	-0.258736
1	-1.964284	2.627583	1.327564

12

6	1.664822	0.100505	-0.100835
8	1.183272	-0.240984	-1.420152
6	0.407841	0.168854	0.772975
7	-0.201866	-0.341215	-1.420343
6	-0.652589	-0.135401	-0.249939
1	0.416311	-0.557922	1.586792
1	0.241691	1.151008	1.218488
6	2.308600	1.483724	-0.275225
8	3.478648	1.734081	-0.125498
8	1.405609	2.386083	-0.644896
6	1.899375	3.698589	-0.923675
1	1.026762	4.284901	-1.200729
1	2.615066	3.665066	-1.745951
1	2.383713	4.119332	-0.041326
6	2.734611	-0.908022	0.369475
1	3.519365	-0.923525	-0.400052
8	3.248441	-0.428475	1.599459
1	3.792685	0.335539	1.390177
6	2.273941	-2.353431	0.604643
1	1.519654	-2.337461	1.401376
6	1.674679	-3.031867	-0.629279
1	1.500513	-4.089280	-0.410971
1	2.363602	-2.974114	-1.477111
1	0.729632	-2.595049	-0.944636
6	3.463013	-3.172401	1.117388
1	3.144014	-4.189054	1.361488
1	3.903975	-2.719719	2.004516
1	4.237227	-3.242912	0.345191

6	-2.102193	-0.163761	0.055673
6	-2.688043	-1.333600	0.551250
6	-2.856454	1.003746	-0.108408
6	-4.038835	-1.314451	0.883463
6	-4.204220	0.981019	0.235380
6	-4.812304	-0.167477	0.733067
1	-4.499223	-2.219659	1.268937
1	-4.794746	1.884281	0.111299
6	-2.226248	2.252065	-0.670577
1	-2.922869	3.091116	-0.632313
1	-1.927298	2.095488	-1.710195
1	-1.320899	2.530406	-0.123898
6	-6.280282	-0.178678	1.069880
1	-6.497721	-0.883269	1.875492
1	-6.872645	-0.478208	0.199544
1	-6.624601	0.810486	1.379183
6	-1.883966	-2.600510	0.689316
1	-2.459263	-3.375732	1.197585
1	-0.962052	-2.440849	1.255822
1	-1.592341	-2.980513	-0.293333

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6	-1.227507	0.121199	0.517217
8	-1.298205	-0.271418	2.845632
6	-2.068058	0.316591	1.780029
7	0.002966	-0.421801	2.439510
6	0.124935	-0.192770	1.190879
1	-2.228308	1.370206	2.009748
1	-3.018274	-0.212959	1.741752
6	-1.062145	1.323915	-0.397421
8	-0.470100	1.280459	-1.441355
8	-1.629862	2.437273	0.082068
6	-1.537168	3.586251	-0.761498
1	-2.022668	3.389984	-1.719135
1	-0.493411	3.848860	-0.938566
1	-2.047465	4.383991	-0.227371
6	-1.691638	-1.117335	-0.317819
1	-0.938385	-1.268574	-1.104000
6	-3.086244	-1.031962	-0.968562
1	-3.805862	-1.078243	-0.142977
6	-3.377597	0.225909	-1.786574
1	-4.358189	0.125363	-2.258576
1	-2.636185	0.374649	-2.575068
1	-3.413114	1.127492	-1.170248
6	-3.294207	-2.277090	-1.836976
1	-4.318315	-2.310733	-2.217696
1	-3.105090	-3.187856	-1.269482
1	-2.617538	-2.257040	-2.698301

6	1.463359	-0.222448	0.536584
6	2.041976	-1.430329	0.109479
6	2.164146	0.979487	0.375100
6	3.279631	-1.398501	-0.520642
6	3.403879	0.964279	-0.259528
6	3.971614	-0.209329	-0.730862
1	3.725186	-2.334178	-0.845837
1	3.940195	1.901774	-0.377994
6	1.645362	2.303069	0.878639
1	2.421828	2.817971	1.449006
1	0.777198	2.199670	1.529263
1	1.372917	2.946335	0.037383
6	5.293359	-0.204287	-1.451283
1	5.139777	-0.211838	-2.534929
1	5.887208	-1.085171	-1.196661
1	5.877601	0.684568	-1.204884
6	1.386452	-2.766306	0.349050
1	0.519401	-2.921686	-0.298548
1	1.067939	-2.863805	1.390685
1	2.088203	-3.576113	0.145539
8	-1.782605	-2.244763	0.530660
1	-0.970129	-2.344525	1.029400

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6	1.261589	0.057442	0.463465
8	1.301281	0.840493	2.707266
6	2.143148	0.267302	1.701933
7	-0.010592	0.691168	2.338080
1	2.976692	0.946724	1.548331
1	2.510828	-0.694000	2.074165
6	1.390256	1.129371	-0.613889
8	0.968792	0.993363	-1.738337
6	1.451405	-1.341612	-0.198697
1	1.437475	-2.066587	0.623553
8	0.358338	-1.677284	-1.018442
1	0.249473	-0.958352	-1.651487
6	2.762654	-1.531766	-0.997890
1	2.644692	-0.953301	-1.921249
6	4.037285	-1.052977	-0.302900
1	4.903938	-1.286645	-0.926163
1	4.184930	-1.553375	0.659466
1	4.046007	0.026505	-0.134504
6	2.890067	-3.007656	-1.380362
1	3.726162	-3.158377	-2.068148
1	1.977202	-3.363589	-1.858452
1	3.074143	-3.620703	-0.490885
6	-0.112414	0.256095	1.144956
6	-1.468391	0.082118	0.554076

6	-2.099037	1.155590	-0.082911
6	-2.136662	-1.146175	0.698512
6	-3.374681	0.968261	-0.616472
6	-3.407470	-1.285051	0.160499
6	-4.040078	-0.243232	-0.515083
1	-3.861886	1.804907	-1.109492
1	-3.924900	-2.233267	0.276788
6	-1.465955	2.519154	-0.209349
1	-0.680703	2.680765	0.530438
1	-2.217598	3.298373	-0.067457
1	-1.037396	2.647264	-1.207446
6	-1.502799	-2.310551	1.410759
1	-0.942769	-1.988541	2.290696
1	-0.817696	-2.823972	0.731592
1	-2.261935	-3.024662	1.734623
6	-5.410574	-0.438037	-1.107761
1	-5.841837	0.509969	-1.435045
1	-6.092434	-0.889674	-0.382463
1	-5.366416	-1.103791	-1.975050
8	1.985872	2.237526	-0.186755
6	2.092691	3.303801	-1.135760
1	2.644881	4.089971	-0.627556
1	2.624819	2.967738	-2.026208
1	1.099571	3.654822	-1.418303

ω B97X-D/6-311G(d,p) gas phase cartesian coordinates of the stationary points involved in the Mg(II)-promoted *zw*-type 32CA reaction of MNO **9** with BHA **10**.

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6	-2.008841	0.152212	-0.617490
6	-0.983582	0.048123	-1.464591
1	-0.682943	-0.909099	-1.869795
1	-0.419352	0.917097	-1.779133
6	-2.345929	1.518598	-0.132517
8	-3.444240	1.874879	0.303987
8	-1.357352	2.382644	-0.188988
6	-1.641697	3.732498	0.211307
1	-0.709441	4.272060	0.069771
1	-1.948731	3.757196	1.256591
1	-2.432438	4.152550	-0.410375
6	-2.859710	-1.008453	-0.067891
1	-2.560993	-1.075194	0.999373
8	-4.212520	-0.768706	-0.180440
6	-2.508004	-2.379220	-0.686574
1	-1.418228	-2.506320	-0.667674
6	-3.117726	-3.478797	0.184130
1	-2.924919	-4.467351	-0.241364
1	-4.198312	-3.334828	0.254284
1	-2.703479	-3.460368	1.196897
6	-3.018881	-2.499700	-2.123037
1	-2.754751	-3.473441	-2.544875
1	-2.615611	-1.726183	-2.781651
1	-4.105858	-2.401076	-2.128578
12	-5.153856	0.768953	0.234470
17	-7.107422	1.771288	0.560461

MC-Mg

6	2.216340	-1.379899	-0.979423
8	0.459212	2.503456	-0.142274
6	1.723099	-2.279690	-1.828456
7	-0.631285	1.928725	-0.176873
6	-1.650791	1.402956	-0.201614
1	1.864925	-2.187532	-2.898270
1	1.156746	-3.132211	-1.472947
6	2.955596	-0.212641	-1.531052
8	3.119457	0.849551	-0.937529
8	3.459382	-0.391367	-2.735832
6	4.153380	0.722934	-3.315222
1	4.999884	1.005350	-2.689524
1	3.480837	1.574864	-3.419457
1	4.490179	0.374909	-4.288037
6	2.004976	-1.328835	0.538185

1	3.017830	-1.192312	0.978616
8	1.184096	-0.247943	0.816522
6	1.485156	-2.645916	1.145405
1	0.585288	-2.949083	0.595048
6	2.525941	-3.764818	1.059029
1	2.129971	-4.694755	1.476482
1	3.416574	-3.498059	1.638043
1	2.846800	-3.965946	0.034237
6	1.076516	-2.407161	2.597656
1	0.681047	-3.325179	3.042465
1	0.322955	-1.622983	2.660710
1	1.940026	-2.088748	3.192023
6	-2.887189	0.691526	-0.210568
6	-4.084968	1.390319	0.010267
6	-2.856617	-0.698700	-0.418435
6	-5.266257	0.662113	0.016792
6	-4.067712	-1.376393	-0.395635
6	-5.276880	-0.717045	-0.183090
1	-6.202633	1.182417	0.190556
1	-4.067136	-2.451786	-0.544112
6	-1.558026	-1.409127	-0.669359
1	-1.231897	-1.248719	-1.702996
1	-1.671992	-2.484189	-0.519482
1	-0.751867	-1.043227	-0.022910
6	-6.570769	-1.484640	-0.189568
1	-6.469316	-2.430711	0.346757
1	-6.870470	-1.718250	-1.215778
1	-7.377228	-0.912802	0.272236
6	-4.078832	2.875783	0.242501
1	-5.090753	3.249861	0.399520
1	-3.649343	3.407412	-0.611483
1	-3.481656	3.133424	1.121908
12	2.043164	1.462851	0.740274
17	3.262200	2.738828	2.138381

TS-o-I-Mg

6	0.000000	0.000000	0.000000
7	0.000000	0.000000	1.200876
8	0.854990	0.000000	2.134963
6	2.768931	0.202028	0.501777
6	2.016610	0.099689	-0.631286
1	1.764902	0.990371	-1.193009
1	2.010777	-0.848290	-1.159534
6	2.991296	1.536925	1.131295
8	3.816426	1.764401	1.976289
8	2.156622	2.474411	0.648863
6	2.275377	3.765701	1.245717
1	3.279092	4.166750	1.097369
1	2.067689	3.709106	2.315298

1	1.536817	4.389552	0.746741
6	3.522424	-0.997662	1.067624
1	3.941547	-0.674317	2.035134
8	2.684006	-2.096070	1.199018
6	4.729359	-1.345953	0.165051
1	4.306070	-1.682802	-0.790583
6	5.647059	-0.149489	-0.087972
1	6.526078	-0.457736	-0.660289
1	5.991452	0.284507	0.855456
1	5.147222	0.641681	-0.654711
6	5.500664	-2.508071	0.785227
1	6.302348	-2.841769	0.120027
1	4.832038	-3.346251	0.981890
1	5.958531	-2.200582	1.732461
6	-0.817187	-0.177682	-1.168693
6	-1.273651	0.939434	-1.881304
6	-1.072981	-1.495033	-1.590750
6	-2.017124	0.712175	-3.032282
6	-1.820253	-1.665621	-2.746553
6	-2.298984	-0.577596	-3.477126
1	-2.383844	1.562544	-3.598520
1	-2.032309	-2.672546	-3.091958
6	-0.565921	-2.669184	-0.798003
1	-0.748207	-3.605311	-1.325829
1	-1.074334	-2.730148	0.170724
1	0.509211	-2.595769	-0.600684
6	-3.126932	-0.800409	-4.713148
1	-3.121727	0.077555	-5.361252
1	-4.166159	-1.008631	-4.440606
1	-2.759764	-1.654396	-5.286136
6	-1.004561	2.334007	-1.386093
1	-1.149194	3.065193	-2.182415
1	0.009060	2.442006	-0.991412
1	-1.691448	2.581876	-0.570800
12	1.263542	-2.026912	2.407559
17	-0.289251	-3.277346	3.391047

TS-o-II-Mg

8	0.000000	0.000000	0.000000
7	0.000000	0.000000	1.250017
6	0.874553	0.000000	2.095610
6	2.613295	0.251669	1.147837
6	2.457866	-0.522674	0.026499
1	3.157200	-0.184259	1.980139
1	2.639899	1.332686	1.056201
6	2.181661	0.073326	-1.305431
8	1.532689	-0.487123	-2.184728
8	2.743645	1.248344	-1.493526
6	2.461135	1.896693	-2.745200

1	2.981835	2.849051	-2.696815
1	1.386500	2.043705	-2.853762
1	2.832505	1.292152	-3.572141
6	2.532774	-2.050733	0.116919
1	2.842856	-2.260966	1.161366
8	1.304623	-2.604746	-0.141890
6	3.654559	-2.614492	-0.785560
1	3.366200	-2.409401	-1.823982
6	5.004634	-1.954640	-0.502121
1	5.792769	-2.408881	-1.108065
1	5.283589	-2.081014	0.550400
1	4.998761	-0.881509	-0.718086
6	3.723887	-4.127497	-0.600986
1	4.436823	-4.574043	-1.299619
1	2.742135	-4.573459	-0.761615
1	4.048974	-4.374510	0.416382
6	1.015472	-0.286977	3.506910
6	0.689655	-1.581474	3.956910
6	1.512901	0.693469	4.380076
6	0.876650	-1.861147	5.305670
6	1.673929	0.362120	5.717939
6	1.368796	-0.910658	6.196109
1	0.624853	-2.851286	5.672417
1	2.042398	1.115727	6.407122
6	1.866548	2.071424	3.888385
1	1.884677	2.783279	4.714548
1	1.150939	2.429196	3.144624
1	2.858691	2.078716	3.425763
6	1.588688	-1.258759	7.643144
1	0.872336	-2.008573	7.984083
1	1.496990	-0.378696	8.282539
1	2.592587	-1.670563	7.786678
6	0.118270	-2.618381	3.030385
1	-0.910031	-2.353372	2.762518
1	0.094469	-3.594053	3.517062
1	0.668690	-2.709043	2.088053
12	0.057925	-1.720083	-1.280667
17	-1.794683	-2.248533	-2.419305

TS-m-I-Mg

6	0.663340	0.941748	-0.671401
8	1.694229	-1.493932	-1.489235
6	1.442449	0.639025	-1.766890
7	0.593903	-1.760785	-0.892110
6	-0.254108	-1.046000	-0.407147
1	1.022053	0.586469	-2.762281
1	2.522158	0.718368	-1.707164
6	-0.676687	1.575044	-0.850119
8	-1.290061	2.109976	0.034879

8	-1.141016	1.486532	-2.108926
6	-2.445466	2.032095	-2.316886
1	-2.454297	3.098322	-2.087809
1	-3.173845	1.522549	-1.682726
1	-2.667542	1.865351	-3.368674
6	1.377500	1.149778	0.676085
1	0.589175	1.292447	1.428991
6	2.236105	2.438482	0.683173
1	3.063918	2.262448	-0.019268
6	1.483032	3.692924	0.240737
1	2.125621	4.571909	0.339895
1	0.591783	3.851447	0.853770
1	1.164272	3.638324	-0.804355
6	2.832918	2.630171	2.076544
1	3.541051	3.463466	2.087330
1	3.346459	1.725658	2.402698
1	2.040558	2.854491	2.799619
6	-1.577017	-1.061042	0.152381
6	-1.777110	-0.877581	1.528421
6	-2.662423	-1.197966	-0.742710
6	-3.088462	-0.794797	1.987431
6	-3.944248	-1.108942	-0.229249
6	-4.176580	-0.889079	1.130987
1	-3.257444	-0.650942	3.050092
1	-4.789644	-1.219331	-0.901554
6	-2.436631	-1.489702	-2.201241
1	-3.377061	-1.449424	-2.752317
1	-2.010854	-2.489295	-2.328495
1	-1.740735	-0.778440	-2.649970
6	-5.581765	-0.745203	1.646638
1	-5.943982	0.273337	1.475939
1	-5.635686	-0.942110	2.718529
1	-6.263547	-1.428090	1.135067
6	-0.645719	-0.827972	2.517434
1	-0.690233	-1.712573	3.160019
1	-0.744567	0.048967	3.161536
1	0.340712	-0.794872	2.051353
8	2.160393	0.052707	0.987129
12	3.103306	-1.244105	0.050972
17	5.000486	-2.391580	-0.004365

TS-m-II-Mg

8	0.000000	0.000000	0.000000
7	0.000000	0.000000	1.239102
6	0.781517	0.000000	2.148505
6	2.630771	0.054469	0.636548
6	1.871287	-0.069859	-0.522114
1	1.761681	-1.031428	-1.004054
1	1.756617	0.798039	-1.158265

6	3.216134	-1.143178	1.221982
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1	3.901698	2.053035	-1.701851
1	4.333903	0.346989	-1.502375
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6	1.003129	0.009926	3.565966
6	1.236842	-1.204495	4.241013
6	1.009507	1.243526	4.258273
6	1.543343	-1.159118	5.596471
6	1.314205	1.227199	5.611311
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