Supporting information for paper:

"Global optimization of ~ 1nm MoS_2 and $CaCO_3$ nanoparticles"

Jiří Hostaš[1,*], Alain Tchagang[2], Maicon Pierre Lourenço[3], Andreas M. Köster[4], Dennis R. Salahub[1]

[1] Department of Chemistry, CMS - Centre for Molecular Simulation, IQST - Institute for Quantum Science and Technology, Quantum Alberta, University of Calgary, 2500 University Drive NW, Calgary, AB, T2N 1N4, Canada.

[2] Digital Technologies Research Centre, National Research Council of Canada, 1200 Montréal Road, Ottawa, ON, K1A 0R6 Canada.

[3] Departamento de Química e Física – Centro de Ciências Exatas, Naturais e da Saúde – CCENS – Universidade Federal do Espírito Santo, 29500-000, Alegre, Espírito Santo, Brasil.

[4] Departamento de Química, Cinvestav, Avenida Instituto Politécnico Nacional 2508, A.P. 14-740, CDMX, C.P. 07360, México

* Address correspondence to: jiri.hostas1@ucalgary.ca

Table 1: Optimized xyz coordinates for MoS_2 clusters in Å and their energies in Hartree. (Optimization/Single Point energy method: PBE-D/DZVP/GEN-A2*, fine grid)

12
Mo_3S_9: -4495.657477
Mo 0.000000 0.000000 0.000000
S 0.000000 0.000000 2.371597
S 2.371823 0.000000 -0.003634
Mo 1.546712 -1.597350 1.543916
S 3.166251 -1.846654 3.164718
S -0.662210 2.106916 -0.659428
S -1.983306 -1.240508 0.393983
Mo -0.205538 -2.691779 -0.205088
S -0.231493 -3.049645 2.139649
S 0.387698 -1.240037 -1.984561
S 2.139648 -3.047566 -0.236673
S -1.174747 -4.550779 -1.162421

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$(MoS_2)_8$, Starting Crystal geometry: -6758.551781
S 1.511609 3.637048 -1.667381
S 1.554843 3.654616 1.637775
Mo -0.000298 4.389187 -0.000165
S -1.511739 3.636839 1.667208
Mo -3.092083 4.303099 0.037831
S -4.725703 3.741361 1.594885
S -4.781061 3.763833 -1.471352
S -1.555185 3.654273 -1.638047
Mo -4.936587 1.944654 0.041956
S -1.602344 -1.841140 -1.568463
Mo -3.204396 -0.995210 0.007699
Mo 0.000001 -0.976098 -0.000177
S 1.588506 -1.937592 -1.522149
S -1.588401 -1.937712 1.521817
S -0.007646 0.849432 -1.558699
S 0.007606 0.849354 1.558428
S 1.602180 -1.841057 1.568380
Mo 3.204152 -0.994972 -0.007761
Mo 1.540253 1.844587 -0.011123
Mo -1.540380 1.844452 0.010964
S 3.231133 0.942132 1.446444
S -3.231310 0.941967 -1.446430
S -3.207940 0.921125 1.486902
S 3.207985 0.921409 -1.486887

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$(MoS_2)_8$, Minimum 1: -6758.775532

Mo	0.000000	0.000000	0.000000
S	0.000000	0.000000	2.631523
S	2.356512	0.000000	1.173926
S	-1.881762	1.296406	0.035322
S	0.564406	-2.177561	-1.077197
S	0.869353	1.297325	-1.668331
Mo	0.088950	2.657365	0.145373
S	-1.213428	-2.179168	0.023654
Mo	0.846337	-2.108669	1.364444
Mo	1.422081	2.062480	2.296829
Mo	2.097412	-1.282291	3.388385
S	2.322760	3.483065	0.298900
S	0.250076	-2.884032	3.451874
S	2.981401	-2.881612	1.761055
S	-0.767904	3.482622	2.214342
S	1.009669	2.531237	4.781126
Mo	2.343196	4.140795	3.780725
S	1.158228	6.370137	3.879546
Mo	2.855029	0.880062	4.618136
S	2.954174	6.371513	2.766759
Mo	1.201332	4.748314	1.941099
S	3.830869	2.528256	3.035860
S	4.394709	-0.568553	3.835161
S	1.468596	-0.569944	5.644202

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$(MoS_2)_8$, Minimum 2: -6759.024117

Mo	0.000000	0.000000	0.000000
S	0.000000	0.000000	2.131344
S	1.970015	0.000000	-1.022556
S	-1.106583	-1.861047	-0.794985
Mo	-1.760525	-0.099447	-2.211065
S	-3.389615	-0.855816	-3.533827
S	-0.204845	0.382729	-3.839051
Mo	0.568664	-1.413825	-2.530919
S	-1.367665	1.693215	-0.823482
S	2.693507	-1.814561	-3.505450
S	-0.590363	-3.358070	-3.340600
Mo	1.183172	-2.900787	-4.838549
Mo	-1.282878	-1.665939	-4.776730
Mo	-0.667632	-3.153297	-7.084382
Mo	1.660769	-4.467464	-7.404961
S	0.106233	-4.949901	-5.776064
S	3.290041	-3.710859	-6.082940

S	0.490724	-1.208730	-6.274950
Mo	-0.100463	-4.567185	-9.615599
S	1.268525	-6.259802	-8.793099
S	-2.069669	-4.568080	-8.591815
S	-0.102288	-4.567278	-11.746939
S	1.006473	-2.705968	-8.821165
S	-2.792654	-2.751982	-6.110694

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$(MoS_2)_8$, Minimum 3: -6759.030672

Mo	0.000000	0.000000	0.000000
S	0.000000	0.000000	2.133622
S	2.032058	0.000000	-0.939291
S	-1.374682	-1.650555	-0.877208
S	-0.954068	1.928248	-0.798878
Mo	0.724078	1.406854	-2.471972
Mo	-1.550485	0.165619	-2.308056
S	0.024366	-0.369130	-3.890938
S	-3.046385	1.322787	-3.490946
S	-0.215938	3.440046	-3.351378
Mo	-0.799214	1.687271	-4.898262
Mo	1.492845	2.953337	-4.826942
S	2.947964	1.872588	-3.492916
S	1.066801	1.287843	-6.369186
S	1.415532	4.795239	-6.117919
Mo	-0.111947	3.189584	-7.255365
S	-2.053471	3.506081	-5.918429
Mo	-2.362379	1.931066	-7.560198
S	-0.482768	1.537137	-8.992765
Mo	-1.569323	3.392652	-9.794734
S	-1.467907	3.450013	-11.925179
S	-3.737465	3.085199	-9.027782
S	-0.534993	5.086564	-8.759279
S	-2.233956	0.017759	-6.420534

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$(MoS_2)_{16}$ – Starting Crystal geometry

Mo	-1.575000	6.365287	-3.075000
Mo	-3.150001	9.093267	-3.075000
Mo	-4.725000	11.821247	-3.075000
Mo	1.575000	6.365287	-3.075000
Mo	0.000000	9.093267	-3.075000
Mo	-1.575000	11.821247	-3.075000
Mo	-3.150001	14.549227	-3.075000
Mo	4.725000	6.365287	-3.075000
Mo	3.150000	9.093267	-3.075000

Mo 1.575000 11.821247 -3.075000
Mo 0.000000 14.549227 -3.075000
Mo 6.300000 9.093267 -3.075000
Mo 4.725000 11.821247 -3.075000
Mo 3.150001 14.549227 -3.075000
Mo 7.875000 11.821247 -3.075000
Mo 6.300000 14.549227 -3.075000
S -3.150000 7.274614 -4.661700
S -4.725000 10.002594 -4.661700
S 0.000000 7.274614 -4.661700
S -1.575000 10.002594 -4.661700
S -3.150000 12.730574 -4.661700
S 3.150000 7.274614 -4.661700
S 1.575000 10.002594 -4.661700
S 0.000000 12.730574 -4.661700
S -1.575000 15.458553 -4.661700
S 6.300001 7.274614 -4.661700
S 4.725000 10.002594 -4.661700
S 3.150001 12.730574 -4.661700
S 1.575001 15.458553 -4.661700
S 7.875000 10.002594 -4.661700
S 6.300000 12.730574 -4.661700
S 4.725000 15.458553 -4.661700
S -3.150000 7.274614 -1.488300
S -4.725000 10.002594 -1.488300
S 0.000000 7.274614 -1.488300
S -1.575000 10.002594 -1.488300
S -3.150000 12.730574 -1.488300
S 3.150000 7.274614 -1.488300
S 1.575000 10.002594 -1.488300
S 0.000000 12.730574 -1.488300
S -1.575000 15.458553 -1.488300
S 6.300001 7.274614 -1.488300
S 4.725000 10.002594 -1.488300
S 3.150001 12.730574 -1.488300
S 1.575001 15.458553 -1.488300
S 7.875000 10.002594 -1.488300
S 6.300000 12.730574 -1.488300
S 4.725000 15.458553 -1.488300

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$(MoS_2)_{16}$ Minimum 1: -13517.912510
Mo 0.000000 0.000000 0.000000
S 0.000000 0.000000 2.291432
S 2.400642 0.000000 0.142274
Mo 2.058062 0.008561 -2.153454

S	0.551250	-1.665185	-1.663186
S	2.660791	2.301497	-2.028340
Mo	2.287924	2.236901	-4.372108
S	1.066067	2.883343	-6.242092
S	2.930652	4.471776	-4.371037
S	0.658631	0.543841	-4.010981
Mo	0.570960	4.637856	-4.711126
S	0.806476	6.980016	-4.423169
Mo	-1.512027	6.767281	-4.411306
S	-1.089023	5.399282	-6.243770
S	-1.413264	7.152641	-2.080280
S	-3.447099	5.453451	-4.055941
Mo	-3.773573	7.034776	-2.316941
S	-3.628416	7.325146	0.033673
Mo	-5.980532	7.154373	-0.152741
S	-6.051384	7.558842	2.136386
S	-7.961334	6.016737	0.298059
S	-5.673405	5.656002	-1.956171
Mo	-6.585832	5.236466	2.065259
S	-6.429847	5.209141	4.440711
Mo	-6.588178	2.941207	3.951929
S	-8.306389	3.651959	2.555327
S	-6.325933	1.134993	2.433457
Mo	-4.640013	0.462112	3.963727
S	-2.404025	0.138170	4.419812
S	-4.326033	-1.328537	2.520540
S	-4.276180	2.764234	4.476899
Mo	-2.432740	0.061436	2.004153
S	-1.848901	-1.537797	0.470435
S	-3.943933	0.978099	0.353152
Mo	-4.420989	2.598453	2.059971
Mo	-2.092602	2.430481	-0.135205
S	-3.616790	3.202303	-1.821254
S	-1.712194	4.791910	0.066115
S	-1.556238	0.739311	-1.752750
S	-2.026342	2.471339	2.264409
S	0.300755	2.398461	0.080195
Mo	0.247713	2.230023	-2.314628
Mo	-4.093954	4.943482	-0.226295
Mo	-1.858508	4.758777	-2.338158
S	-5.930863	3.520589	0.405279
S	0.543907	4.632924	-2.235629
S	-4.125539	4.997990	2.183657
S	-1.248201	3.119684	-3.997197

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$(MoS_2)_{16}$ Minimum 2: -13518.231110

Mo	0.000000	0.000000	0.000000
S	0.000000	0.000000	2.215175
S	2.394901	0.000000	0.203936
S	-1.908511	1.174044	-0.617241
Mo	-1.958482	-0.976091	-1.458509
S	-3.880090	-1.889665	-0.790771
S	0.360398	-1.344930	-1.958551
Mo	-0.376486	-2.827435	-0.209863
S	-2.392317	-3.944357	0.457512
Mo	-1.026334	-5.867236	-0.048214
S	-0.991473	-7.556794	-1.769590
S	-3.060157	-7.005237	0.585209
Mo	-3.318201	-7.202441	-1.757592
S	-4.713747	-5.141197	-2.027651
S	-5.173117	-8.513606	-1.588198
S	-0.339484	-4.493074	-1.911744
Mo	-2.615858	-3.851522	-1.883623
S	-3.368736	-5.536264	-3.575998
S	-2.337910	-2.263703	-3.493014
Mo	-1.709107	-8.901302	0.083468
Mo	-3.395136	-10.179620	-1.652261
S	-2.708483	-9.049654	-3.448003
S	-2.971886	-12.412731	-2.061307
Mo	-2.008143	-11.742285	-0.055426
S	0.161549	-12.122753	-0.289108
S	-1.634652	-12.227605	2.268827
S	-3.647364	-10.172997	0.735132
S	1.379982	-6.374659	0.019608
Mo	1.328517	-4.758741	1.762829
Mo	3.041773	-3.776123	3.618215
S	3.686861	-5.258130	1.793886
S	1.706585	-2.156279	4.273616
S	3.380857	-5.202964	5.390122
Mo	2.944564	-6.563434	3.578421
S	4.494980	-8.272179	3.580937
Mo	2.466576	-9.284061	3.190892
S	1.005094	-7.658957	4.269540
S	2.707066	-10.712161	1.535952
Mo	0.709901	-7.693074	1.877048
S	-0.690048	-5.840728	2.388743
S	1.986049	-3.294009	-0.031558
Mo	1.878949	-1.686251	1.710854
S	4.076894	-2.023412	2.304143
S	-0.120847	-2.877164	2.190754

S	-1.275510	-8.924885	2.458839
Mo	0.120991	-10.758742	1.894110
S	0.924762	-10.947861	4.042315
S	0.670179	-9.313628	0.089188

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$(MoS_2)_{16}$ Minimum 3: -13518.398824

Mo	0.000000	0.000000	0.000000
S	0.000000	0.000000	2.127533
S	2.026287	0.000000	-0.899565
S	-1.028771	1.821812	-0.786417
S	-1.155696	-1.741740	-0.904629
Mo	0.703481	-1.434888	-2.549586
S	-0.404049	-3.172340	-3.599447
S	0.172153	0.466244	-3.824307
Mo	-1.664617	0.116158	-2.425818
S	-3.203340	-1.421008	-3.339926
Mo	-3.438779	0.493666	-4.774573
S	-3.070242	1.979392	-3.116294
S	-1.786412	0.585390	-6.367225
Mo	-1.297921	-1.168223	-4.841158
S	-2.263420	-3.073900	-6.092396
Mo	-2.905243	-1.368076	-7.510529
S	-4.867898	1.977143	-5.991668
Mo	-5.582924	0.559370	-7.741133
S	-6.848441	2.274664	-8.682617
Mo	-7.389701	0.417859	-9.899274
S	-9.461728	0.395687	-10.400428
S	-5.988730	0.134066	-11.626944
S	-6.907040	-1.342549	-8.535534
S	-3.658645	0.633413	-8.963174
Mo	-4.872876	-1.119268	-9.834744
S	-3.467065	-1.742682	-11.690618
Mo	-2.472273	-2.754852	-9.902226
S	-1.090530	-1.094355	-9.048135
S	-0.808965	-3.708389	-11.757541
Mo	0.133885	-4.549190	-9.956832
S	1.574816	-2.957927	-9.079024
S	1.403675	-6.315335	-9.402798
S	-1.882472	-4.866586	-8.850030
Mo	-0.521625	-3.075926	-7.847660
Mo	2.049619	-4.768147	-7.513243
S	0.237390	-4.829997	-6.220284
S	3.350772	-6.627592	-6.776159
Mo	3.762513	-4.947692	-5.299908
S	3.462343	-3.063180	-6.601943

S	2.102273	-5.274082	-3.697748
Mo	3.304281	-3.449330	-2.852832
S	2.217351	-3.168820	-0.953976
Mo	1.708171	-3.228445	-4.948752
S	2.812311	-1.388464	-3.798102
S	5.342249	-4.086082	-3.715915
S	-4.955223	-1.009186	-5.966614
S	-4.351036	-3.042053	-8.536378
S	0.640158	-1.504853	-6.325910

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$(MoS_2)_{16}$ Minimum 4: -13518.440275

Mo	0.000000	0.000000	0.000000
S	0.000000	0.000000	2.231632
S	1.978071	0.000000	-0.783009
S	-1.158624	-1.879368	-0.589346
S	-1.203083	1.663622	-0.868604
Mo	-1.956457	-1.403739	1.724557
S	-3.360130	0.450444	1.535876
S	-3.140943	-3.440516	1.287855
Mo	-4.576741	-1.530342	0.911626
S	-4.211258	-1.955214	-1.461398
Mo	-5.744038	-0.171794	-1.451931
S	-4.207966	1.465174	-1.879905
Mo	-2.890658	-0.130046	-0.683597
S	-6.463765	0.088054	0.640390
S	-5.412268	-1.284030	3.250500
Mo	-3.801487	-2.809280	3.451454
S	-1.892565	-1.737695	4.083430
S	-4.058478	-3.365945	5.973776
Mo	-5.934671	-4.386483	5.291599
S	-7.278558	-6.115149	5.865409
S	-7.507625	-2.706621	5.352552
S	-5.100846	-4.885010	3.189674
Mo	-8.784898	-4.620496	4.645362
Mo	-6.980435	-3.319092	3.061986
S	-8.278102	-5.180241	2.453259
S	-8.380394	-1.426674	2.473805
Mo	-8.239937	-1.730861	0.085665
S	-9.445520	-3.642125	-0.347186
S	-9.707594	0.190489	-0.046821
Mo	-8.841019	-0.327641	-2.134416
S	-10.601345	-1.298434	-2.999181
S	-7.238328	-2.005762	-2.131797
S	-7.384242	1.257413	-2.750317
S	-10.583088	-6.356061	4.948637

Mo	-11.586889	-4.738053	3.777982
Mo	-9.839729	-3.315912	2.109089
S	-10.424587	-2.890901	4.467008
S	-13.677309	-3.980189	3.724208
S	-11.559312	-1.516571	1.939346
Mo	-12.774115	-3.375281	1.414961
S	-11.275839	-5.273634	1.566715
S	-12.468773	-3.773644	-0.962546
Mo	-14.006127	-2.092841	-0.813669
S	-15.527022	-2.302276	-2.285735
S	-14.893032	-2.359483	1.261686
S	-12.881241	-0.183549	-0.900174
Mo	-11.054640	-1.842737	-0.322211
S	-6.378011	-3.229732	0.684246

Table 2: Optimized xyz coordinates for studied $CaCO_3$ clusters in Å and their energies in Hartree. (Optimization/Single Point energy method: PBE-D/DZVP/GEN-A2*, fine grid)

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$(CaCO_3)_1$: -940.881620

Ca	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.280200
O	1.979251	0.000000	1.096801
C	1.334188	-0.000154	2.309766
O	2.054413	-0.000413	3.337439

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$(CaCO_3)_9$ 9-1: -8469.705880

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.294797
O	1.108073	0.000000	-0.705210
O	-1.148800	-0.106198	-0.648657
Ca	0.071150	-1.084105	-2.570661
O	-0.385920	-3.148605	-1.539349
C	-0.747799	-3.818925	-0.489163
O	-1.068120	-3.247290	0.641549
O	-0.749119	-5.135811	-0.556062
O	1.401457	-1.942845	-4.328163
C	1.985432	-2.805183	-3.561064
O	2.197695	-4.039394	-3.853873
O	2.265682	-2.405910	-2.275626
Ca	2.844373	-1.565353	-0.129021
O	4.490558	-1.997027	1.534504
C	4.129078	-0.961277	2.318189
O	4.572910	-0.890993	3.510596

O	3.213256	-0.136773	1.827029
Ca	1.563304	-4.797842	-1.675709
Ca	1.299527	-0.013781	3.416326
O	2.981469	-5.638374	0.106578
C	2.608192	-4.795045	0.991002
O	2.817226	-4.908147	2.271625
O	1.869869	-3.719166	0.587503
Ca	4.152429	-3.359070	3.550456
O	3.051085	-2.974059	5.634445
C	2.283475	-2.090476	5.095455
O	1.869823	-0.998732	5.591634
O	1.942777	-2.338578	3.750375
Ca	0.409352	-3.757045	2.694498
O	-1.505020	-5.016709	3.133715
C	-2.263688	-6.081519	3.616560
O	-2.722123	-5.950331	4.804679
O	-2.530659	-7.006133	2.763588
Ca	-2.689756	-5.316376	1.020917
O	-1.228396	-2.088658	3.394466
C	-1.465875	-1.131364	4.369121
O	-2.189178	-1.483958	5.363692
O	-0.980552	0.042113	4.162047
O	-3.854349	-3.045143	0.622241
C	-4.185715	-3.102329	1.893243
O	-4.139643	-2.022907	2.637091
O	-4.388287	-4.270182	2.458370
Ca	-3.057553	-3.534532	4.460692
Ca	-2.225204	-1.182729	1.348567

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$(CaCO_3)_9$ 9-2: -8469.758099

Ca	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.394760
O	1.895674	0.000000	-1.821142
C	0.904507	0.923024	2.369457
O	0.943292	1.972072	3.098167
O	1.837720	0.816289	1.350292
O	-1.221557	1.414181	-1.528819
Ca	0.217615	1.160590	-3.439611
C	-0.545470	2.509670	-1.195531
O	-0.190897	3.289969	-2.200103
O	-0.159527	2.670445	0.019217
O	0.079967	-1.272910	-2.206092
C	1.375723	-1.164297	-2.328894
Ca	4.052278	0.735833	0.625213
O	5.987284	1.795264	1.806354

O	2.143604	-1.985175	-2.933846
C	5.306037	2.937226	1.772372
O	4.032015	2.889464	1.979088
O	5.944262	4.018034	1.396938
Ca	5.312677	5.695435	-0.326657
O	3.247711	5.766656	1.017322
C	2.512927	5.966253	-0.041912
O	3.038471	6.515786	-1.120727
O	1.305640	5.453761	-0.101165
Ca	1.781929	3.517937	1.416359
O	2.230530	0.776775	-4.730332
C	2.757931	1.955379	-4.448862
O	1.954349	2.946968	-4.173246
Ca	1.776748	4.600545	-2.325658
O	4.057515	2.030646	-4.368345
O	4.167952	4.115499	-2.072554
C	4.039356	3.086438	-1.270946
O	2.880267	2.751724	-0.804554
O	5.118049	2.404099	-0.984362
Ca	6.016506	2.889758	-3.341653
O	8.036239	3.434685	-2.120571
C	7.533400	4.610383	-1.769658
O	6.716230	5.230665	-2.573763
O	7.711066	5.028443	-0.540624
Ca	7.547354	2.557881	0.132136
O	7.228377	0.444628	-0.909158
C	6.240340	0.124180	-1.653288
O	6.191112	0.451320	-2.945551
O	5.175644	-0.515659	-1.172941
Ca	3.922439	-0.385493	-3.276648

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$(CaCO_3)_9$ 9-3: -8469.763136

Ca	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.557964
Ca	2.381590	0.000000	3.022327
O	0.928994	-2.013355	3.100904
O	0.067687	0.903882	-2.290927
C	0.940242	0.995817	-3.271024
O	4.083840	-1.371696	2.243721
C	3.936778	-2.113498	1.214657
O	4.454580	-1.783922	0.033046
O	3.282071	-3.270523	1.262834
O	1.373872	-1.970221	-0.776706
Ca	0.824929	-3.649240	0.870562
O	-1.160645	-3.619868	-0.831305

C	-1.676794	-2.648812	-1.524212
O	-2.242568	-2.934164	-2.692509
O	-1.561820	-1.370045	-1.243693
C	0.031245	-1.316889	2.448092
O	-0.710504	-1.892062	1.544628
Ca	-1.225874	-0.852446	-3.621764
O	2.174174	1.346491	-3.128011
O	2.237138	0.669547	0.601209
O	0.523491	0.587002	-4.476772
Ca	-0.589538	-4.678642	-3.082795
O	0.723416	-4.530365	-5.179447
C	0.570004	-3.222071	-5.319933
O	1.598252	-2.515582	-5.702248
O	-0.564857	-2.694671	-4.963903
Ca	2.679512	-0.478654	-4.913332
O	4.361522	-2.242350	-4.975112
C	4.721729	-2.036592	-3.718633
O	2.211986	-1.287460	-2.733068
C	1.645712	-2.208715	-2.025209
Ca	3.001954	-4.222081	-4.357313
O	3.120078	-5.667774	-2.395670
C	1.994227	-5.797656	-1.683603
O	0.926395	-6.271227	-2.217251
O	2.039571	-5.367236	-0.436707
O	1.411541	-3.369699	-2.575941
O	4.808492	-3.106040	-2.952139
Ca	4.092143	-4.000788	-0.878703
O	4.852993	-0.822128	-3.288873
Ca	3.687130	0.142055	-1.323380
O	3.897482	2.121542	0.035829
C	3.094740	1.709228	0.943174
O	3.065227	2.108383	2.169366

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$(CaCO_3)_9$ 9-4: -8469.788976

Ca	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.339336
O	2.313836	0.000000	0.450383
O	0.148787	-0.551505	-2.313312
C	0.662692	-1.600780	-2.885335
O	1.700106	-2.253685	-2.414671
O	0.018512	-2.125438	-3.909735
O	-2.293171	-0.492060	-0.540988
C	-2.925682	-1.525170	-0.046859
O	-2.704664	-2.000903	1.147964
O	-3.732581	-2.194615	-0.855844

O	0.393884	-2.349924	0.448679
C	-0.038066	-3.390243	-0.204447
O	0.506357	-4.546412	-0.002189
O	-1.006049	-3.306943	-1.078776
Ca	3.040502	-2.277666	-0.359854
O	3.200218	-3.034176	1.953874
C	2.438975	-2.539870	2.925507
O	2.699388	-1.426843	3.487987
Ca	2.316646	0.760439	2.824743
O	1.390305	-3.277801	3.282105
Ca	-0.817492	-2.328054	2.777452
O	3.974467	1.361145	1.185091
C	3.636928	0.401171	0.392797
O	4.413188	-0.276342	-0.367632
O	0.380492	1.296424	4.161660
C	-0.296303	0.325237	3.653835
O	-1.135316	-0.429463	4.258318
O	-1.588460	-4.612866	2.255229
C	-1.183421	-5.764090	1.775919
O	-0.050570	-6.324841	2.076157
O	-1.937467	-6.335706	0.847097
Ca	2.032876	-5.131464	1.838184
Ca	-0.041553	-6.881900	-0.591984
O	-1.116210	-6.077859	-2.562140
C	-2.134611	-5.222104	-2.693890
O	-3.193633	-5.323940	-1.977112
O	-1.951391	-4.232772	-3.547837
Ca	-3.099628	-4.318650	0.168399
O	3.254522	-4.723212	-0.675061
C	2.559318	-5.779505	-0.947392
O	1.939977	-5.965211	-2.092409
Ca	0.546318	-4.383544	-3.194616
Ca	-2.126257	-1.911873	-2.706772
O	2.339311	-6.685157	0.002175

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$(CaCO_3)_{10}$ 10-1: -9410.853971

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.307346
O	1.143241	0.000000	-0.648181
O	-1.126753	-0.198765	-0.648135
Ca	0.137337	-1.697113	-2.136535
O	1.868325	-2.748935	-0.842286
C	1.809368	-3.951118	-0.282863
O	1.449763	-4.990401	-0.937749
O	2.098530	-3.996467	1.007617

Ca	0.147261	-5.765699	-2.826023
O	0.719289	-7.799105	-3.901748
C	0.604694	-8.541328	-2.859085
O	1.045351	-9.747325	-2.756186
O	0.010141	-7.978958	-1.745827
Ca	0.901499	-10.018970	-0.422875
O	2.567674	-9.308767	1.186902
C	1.878781	-8.421729	1.783251
O	2.106713	-7.960344	2.989858
O	0.753503	-7.930861	1.195939
O	-1.496667	-9.956354	-0.042293
C	-1.333376	-9.975221	1.256126
O	-2.001984	-9.118827	1.993626
O	-0.362494	-10.690753	1.786888
O	-0.055022	-3.506163	-3.751310
C	-1.366970	-3.507089	-3.615262
O	-2.043184	-4.614701	-3.696457
O	-1.957639	-2.395395	-3.216450
Ca	-3.368747	-3.720689	-1.739230
Ca	-1.405932	-7.477135	0.170498
Ca	-0.186001	-8.994173	3.610861
O	-1.079314	-7.944130	5.526769
C	-1.394014	-6.849066	4.925155
O	-2.187318	-5.949573	5.375237
O	-0.856966	-6.651459	3.657997
Ca	-2.062073	-4.478746	3.505622
O	-3.599653	-3.199005	2.158529
C	-3.992188	-3.361330	0.914760
O	-4.258227	-4.516997	0.399703
O	-3.984177	-2.280699	0.130504
Ca	1.116511	-5.701972	2.480307
O	0.363703	-3.953191	3.876026
C	0.254535	-2.693504	3.528186
O	1.283517	-1.931890	3.406628
O	-0.979611	-2.263754	3.279579
Ca	2.006319	-1.478173	1.258161
Ca	-2.084885	-1.333670	1.391896
O	-1.565980	-5.293252	-0.960888
C	-1.214601	-4.528960	0.068451
O	-1.166537	-3.242194	-0.102668
O	-1.003727	-5.119139	1.211171

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$(CaCO_3)_{10}$ 10-2: -9410.874451

Ca	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.321132

O	2.269932	0.000000	-0.522998
C	0.071296	-1.062045	3.037090
C	2.961357	-1.082132	-0.595510
O	3.877237	-1.381657	0.308676
O	1.174575	-1.365252	3.710834
O	-0.934304	-1.919445	3.143352
O	2.765819	-1.971346	-1.568027
Ca	3.284487	-1.968911	2.635677
O	5.334989	-3.197465	2.742179
C	5.573101	-4.408715	2.379257
O	5.752385	-5.393451	3.243986
O	5.582159	-4.750089	1.095976
Ca	4.040903	-3.763787	-0.458945
Ca	4.196741	-5.788554	5.041638
O	2.176946	-3.532427	1.148212
C	0.925179	-3.493984	0.828006
O	0.148986	-4.527924	0.873481
O	0.395777	-2.361354	0.394564
Ca	0.657503	-3.161392	-2.008174
O	2.181116	-4.936450	-1.736546
C	2.360408	-6.017862	-0.974376
O	1.398498	-6.789758	-0.652135
O	3.601438	-6.186486	-0.533296
Ca	4.548836	-6.949660	1.551696
O	2.875347	-5.656664	2.640013
C	2.161095	-4.883685	3.380667
O	0.891962	-5.146066	3.528837
O	2.680838	-3.896262	4.063447
Ca	0.113715	-3.315410	4.894493
O	0.838049	-4.730700	6.679167
C	2.091334	-5.163939	6.702474
O	3.116171	-4.426750	6.912805
O	2.270986	-6.444095	6.354501
Ca	0.179431	-6.815675	5.248581
O	1.533296	-8.162049	3.839106
C	2.686755	-8.222279	3.230093
O	3.834798	-7.955566	3.818087
O	2.682938	-8.445328	1.931990
Ca	0.671417	-6.854668	1.666437
Ca	-1.919018	-3.157904	1.219480
O	-2.438121	-4.931163	2.623941
C	-1.801675	-5.622016	3.507175
O	-1.298512	-6.814427	3.220963
O	-1.584782	-5.150865	4.727225
O	-0.790825	-1.179888	-2.032164
C	-1.660189	-1.814119	-1.261484

O	-1.813456	-3.105292	-1.383804
O	-2.206753	-1.166694	-0.255958

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$(CaCO_3)_{10}$ 10-3: -9410.886553

Ca	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.413202
O	2.379619	0.000000	0.647583
C	2.528387	-1.280447	0.374152
O	1.870699	-1.795051	-0.616974
O	3.246019	-1.994190	1.221015
Ca	1.215703	-3.692380	-2.014300
Ca	2.928897	-4.219972	2.011714
O	0.105452	-2.189245	-3.499616
C	-0.747179	-1.232110	-3.275848
O	-0.613677	-0.326152	-2.341676
O	-1.872654	-1.237262	-3.969053
O	3.751257	-5.738411	0.399407
C	2.874578	-5.342081	-0.463863
O	3.050661	-5.226410	-1.721266
O	-2.276937	0.894935	-0.118764
C	-3.421880	0.521143	0.401912
O	-3.543295	0.007547	1.589301
O	-4.493380	0.541308	-0.375598
Ca	-2.013221	-1.312568	2.919073
O	-0.357515	-2.724184	3.911504
C	0.698501	-3.318999	3.536465
O	0.672718	-4.464671	2.865492
O	1.919418	-2.806692	3.746393
Ca	-0.587340	-4.942720	0.873761
O	1.664692	-4.889730	0.059395
O	-2.932189	-4.740129	1.247883
C	-3.900663	-3.929321	1.605567
O	-3.733940	-2.912286	2.396748
O	-5.066374	-4.080353	1.013163
O	-1.256221	-6.284261	-0.999009
C	-1.383710	-5.848456	-2.206146
O	-0.395785	-5.329746	-2.908962
O	-2.592832	-5.795233	-2.757036
Ca	-4.055064	-4.841874	-1.095366
Ca	2.280127	-0.517500	3.055110
O	0.969249	1.117906	4.147356
C	-0.126576	0.648887	3.641207
O	-1.272846	0.635825	4.193189
Ca	-3.169907	-0.026830	-2.321574
O	-5.002800	-1.333885	-3.017371

C	-5.003824	-2.545982	-2.592316
O	-5.656185	-2.903390	-1.500447
O	-4.292439	-3.499839	-3.179188
Ca	-2.019143	-3.672867	-3.832411
Ca	-5.147284	-1.663196	0.528891
O	-1.160679	-2.143329	0.657010
C	-1.825594	-2.518721	-0.401851
O	-1.298187	-3.423605	-1.186252
O	-3.008344	-2.053641	-0.694626

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$(CaCO_3)_{10}$ 10-4: -9410.898097

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.283812
O	1.095847	0.000000	-0.696334
O	-1.157230	0.032569	-0.629805
Ca	2.535529	1.843638	-0.439291
O	3.383212	0.511900	1.386380
C	3.416957	-0.799045	1.582005
O	3.931492	-1.611648	0.733815
O	2.861825	-1.220702	2.715864
O	1.319114	2.741533	1.427479
C	0.009368	2.692439	1.580447
O	-0.815016	2.829533	0.586782
O	-0.460059	2.363204	2.767545
Ca	3.122314	-3.634914	-0.304676
Ca	1.252409	-2.981334	2.967417
Ca	-1.485326	2.177182	-1.676936
Ca	1.405558	0.743342	3.029814
O	0.100254	-1.072344	4.012407
C	-1.100273	-1.546496	3.685215
O	-2.099677	-0.783254	3.443400
O	-1.182235	-2.871261	3.592541
Ca	-1.977798	-4.412569	1.911990
O	-1.204587	-2.637385	0.581421
C	-0.091399	-2.644588	-0.086367
O	1.048456	-2.704687	0.505106
O	-0.168837	-2.613607	-1.408957
O	0.275067	-5.165132	2.181560
C	1.291845	-5.240891	1.344883
O	1.170007	-5.611574	0.112960
O	2.461492	-4.791345	1.779104
Ca	-2.280425	0.919307	1.754259
Ca	-0.170366	-5.052163	-1.878344
Ca	1.133572	-1.040754	-2.894953
O	2.896273	-2.660994	-2.578516

C	2.092319	-3.642126	-2.959392
O	1.098306	-3.409959	-3.768987
O	2.226712	-4.809066	-2.375073
Ca	-2.832587	-1.856891	-1.095469
O	-3.991818	-0.172578	0.238855
C	-3.729379	0.758226	-0.658762
O	-3.475122	1.978735	-0.248373
O	-3.543356	0.433539	-1.916426
O	0.071445	1.155996	-3.429472
C	1.102320	1.750972	-2.861811
O	0.898557	2.812301	-2.115926
O	2.292307	1.200918	-2.901982
O	-2.597227	-4.211189	-2.000758
C	-2.792697	-4.641414	-0.774412
O	-2.023423	-5.599579	-0.300712
O	-3.621175	-4.019618	0.028308