Supporting Information for:

Engineering high-capacity hydrogen storage in pristine $Ca_{12}O_{12}$ nanocages via cooperative adsorption

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S1. Benchmarking

This section details the protocol used to benchmark our computational approach. Geometry optimizations were first performed at the B3LYP-D3/6-31G(d,p) level. Single-point energies were then calculated using the more extensive 6-311++G(d,p) basis set with several DFT functionals (B3LYP-D3, BP86-D3, M06-D3, PBE0-D3, and ωB97X-D). We computed the non-ZPE-corrected adsorption energy (ΔE_{ads}) for the $Ca_{12}O_{12}{\cdot}H_2$ (**O**) system at all these levels and compared them with calculations performed at the DLPNO-CCSD(T)/6-311++G(d,p) level of theory. This configuration was selected because it represents the most stable exohedral adsorption mode and serves as the reference for our multiple H_2 adsorption studies. As summarized in Table S1, ωB97X-D yielded the closest agreement to the high-level reference, followed by M06-D3. Further tests employing ωB97X-D for both geometry optimization and single-point calculations produced results nearly identical to those using B3LYP-D3-optimized geometries. Based on these findings, we have adopted the ωB97X-D/6-311++G(d,p)//B3LYP-D3/6-31G(d,p) level of theory for all calculations in this study.

Table S1. Calculated electronic energies (in atomic units) for the isolated H_2 molecule ($E[H_2]$), pristine $Ca_{12}O_{12}$ nanocage ($E[Ca_{12}O_{12}]$), and the $Ca_{12}O_{12}{\cdot}H_2$ (**O**) complex ($E[Ca_{12}O_{12}{\cdot}H_2$ (**O**)]) together with the corresponding non-ZPE-corrected adsorption energies (ΔE_{ads}, *kJ* mol^{-1}) obtained using various computational methods. The DLPNO-CCSD(T)/6-311++G(d,p) values serve as the high-level reference, while results from B3LYP-D3, BP86-D3, M06-D3, PBE0-D3, and ωB97X-D are compared to assess their performance.

Method	$E[H_2]$	$E[Ca_{12}O_{12}]$	$E[Ca_{12}O_{12}{\cdot}H_2$ (**O**)]	ΔE_{ads}
DLPNO-CCSD(T)	-1.168272	-9027.026842	-9028.197910	-7.3
B3LYP-D3	-1.179571	-9035.910934	-9037.096071	-14.6
BP86-D3	-1.177467	-9036.579738	-9037.763330	-16.1
M06-D3	-1.170558	-9034.989733	-9036.164735	-11.7
PBE0-D3	-1.168149	-9032.538716	-9033.712453	-14.7
ωB97X-D	-1.176085	-9035.410818	-9036.590877	-10.4

S2. Additional Data

Table S2. Summary of key structural, energetic, and electronic properties of all the investigated systems. *n*: total number of H_2 molecules; *E*: DFT energy (a.u.); *H*: enthalpy (a.u.); ΔE_{ads}: adsorption energy (kJ mol^{-1}); ΔH_{ads}: adsorption enthalpy (kJ mol^{-1}); ΔH_{ads}^{norm}: normalized adsorption enthalpy (kJ mol^{-1}); *wt%*: hydrogen weight percentage; E_g: HOMO–LUMO DFT energy gap. Energies are obtained at the ωB97X-D/6-311++G(d,p)//B3LYP-D3/6-31G(d,p) level of theory. For cluster labels, see the main text.

Structure	*n*	*E*	*H*	ΔE_{ads}	ΔH_{ads}	ΔH_{ads}^{norm}	*wt%*	E_g
$Be_{12}O_{12}$	0	-1081.431102	-1081.415073	-	-	-	0.00	11.319
$Mg_{12}O_{12}$	0	-3305.057214	-3305.030419	-	-	-	0.00	8.705
$Ca_{12}O_{12}$	0	-9035.363389	-9035.330472	-	-	-	0.00	7.475
$Be_{12}O_{12}{\cdot}H_2$	1	-1082.598700	1082.579685	-4.4	-5.3	-	0.67	11.305
$Mg_{12}O_{12}{\cdot}H_2$ (**M**)	1	-3306.225706	-3306.195798	-6.8	-7.3	-	0.42	8.718
$Mg_{12}O_{12}{\cdot}H_2$ (**O**)	1	-3306.223682	-3306.194395	-1.5	-3.6	-	0.42	8.731
$Ca_{12}O_{12}{\cdot}H_2$ (**M**)	1	-9036.529626	-9036.493262	-0.9	-0.5	-	0.30	7.476
$Ca_{12}O_{12}{\cdot}H_2$ (**O**)	1	-9036.529997	-9036.494726	-1.8	-4.3	0.0	0.30	7.500
(H_2@$Ca_{12}O_{12}$)	1	-9036.532731	-9036.496572	-9.0	-9.2	-4.8	0.30	7.497
$Ca_{12}O_{12}{\cdot}2H_2$	2	-9037.696778	-9037.659459	-4.1	-9.9	-1.3	0.60	7.532
($2H_2$@$Ca_{12}O_{12}$)	2	-9037.673378	-9037.636964	57.3	49.2	57.8	0.60	7.334
$Ca_{12}O_{12}{\cdot}3H_2$	3	-9038.863603	-9038.823971	-6.5	-14.9	-1.9	0.89	7.564
$Ca_{12}O_{12}{\cdot}4H_2$	4	-9040.030464	-9039.988703	-9.0	-20.5	-3.2	1.18	7.600
$Ca_{12}O_{12}{\cdot}5H_2$	5	-9041.197087	-9041.153140	-10.9	-25.3	-3.7	1.48	7.633
$Ca_{12}O_{12}{\cdot}6H_2$	6	-9042.364167	-9042.318011	-13.9	-31.2	-5.3	1.77	7.689
$Ca_{12}O_{12}{\cdot}7H_2$	7	-9043.530923	-9043.482610	-16.2	-36.5	-6.2	2.05	7.714
$Ca_{12}O_{12}{\cdot}8H_2$	8	-9044.698117	-9044.647607	-19.5	-42.7	-8.2	2.34	7.748
$Ca_{12}O_{12}{\cdot}9H_2$	9	-9045.864884	-9045.812153	-21.8	-47.8	-8.9	2.63	7.775
$Ca_{12}O_{12}{\cdot}10H_2$	10	-9047.032214	-9046.977414	-25.5	-54.8	-11.6	2.91	7.807
$Ca_{12}O_{12}{\cdot}11H_2$	11	-9048.198665	-9048.141730	-26.9	-59.3	-11.7	3.19	7.835
$Ca_{12}O_{12}{\cdot}12H_2$	12	-9049.365444	-9049.306471	-29.2	-64.9	-13.0	3.47	7.883
(H_2@$Ca_{12}O_{12}$) ·$12H_2$	13	-9050.535466	-9050.473231	-40.0	-75.8	-19.6	3.75	7.877
$Ca_{12}O_{12}{\cdot}13H_2$	13	-9050.532010	-9050.470744	-30.9	-69.3	-13.1	3.75	7.894
(H_2@$Ca_{12}O_{12}$) ·$13H_2$	14	-9051.701704	-9051.638750	-40.8	-83.4	-22.9	4.03	7.891
$Ca_{12}O_{12}{\cdot}14H_2$	14	-9051.698501	-9051.634876	-32.4	-73.3	-12.7	4.03	7.901
$Ca_{12}O_{12}{\cdot}15H_2$	15	-9052.864957	-9052.799163	-33.9	-77.7	-12.8	4.30	7.914
$Ca_{12}O_{12}{\cdot}16H_2$	16	-9054.030881	-9053.962860	-33.9	-80.5	-11.4	4.57	7.923
$Ca_{12}O_{12}{\cdot}17H_2$	17	-9055.197111	-9055.126917	-34.7	-84.3	-10.8	4.85	7.951
$Ca_{12}O_{12}{\cdot}18H_2$	18	-9056.363450	-9056.290815	-35.9	-87.7	-9.9	5.12	7.973
$Ca_{12}O_{12}{\cdot}19H_2$	19	-9057.529631	-9057.454782	-36.6	-91.3	-9.2	5.39	7.980
$Ca_{12}O_{12}{\cdot}20H_2$	20	-9058.695260	-9058.618593	-35.8	-94.5	-8.0	5.65	7.985
$Ca_{12}O_{12}{\cdot}21H_2$	21	-9059.861521	-9059.782618	-36.7	-98.2	-7.4	5.92	8.021
$Ca_{12}O_{12}{\cdot}22H_2$	22	-9061.027879	-9060.946730	-37.9	-102.1	-7.0	6.18	8.025
$Ca_{12}O_{12}{\cdot}23H_2$	23	-9062.193578	-9062.110352	-37.4	-104.8	-5.4	6.45	8.044
$Ca_{12}O_{12}{\cdot}24H_2$	24	-9063.361165	-9063.275175	-41.8	-110.6	-6.9	6.71	8.067
(H_2@$Ca_{12}O_{12}$) ·$24H_2$	25	-9064.530438	-9064.441460	-50.6	-120.3	-12.2	6.97	8.046
$Ca_{12}O_{12}{\cdot}25H_2$	25	-9064.527427	-9064.438869	-42.7	-113.5	-5.4	6.97	8.058
$Ca_{12}O_{12}{\cdot}26H_2$	26	-9065.693717	-9065.602291	-43.7	-115.6	-3.2	7.23	8.048
$Ca_{12}O_{12}{\cdot}27H_2$	27	-9066.859982	-9066.767876	-44.6	-123.4	-6.7	7.48	7.959
$Ca_{12}O_{12}{\cdot}28H_2$	28	-9068.026359	-9067.931631	-45.8	-126.4	-5.4	7.74	8.056
$Ca_{12}O_{12}{\cdot}29H_2$	29	-9069.190928	-9069.094339	-42.3	-126.7	-1.3	7.99	8.055
$Ca_{12}O_{12}{\cdot}30H_2$	30	-9070.358890	-9070.259575	-47.7	-133.6	-3.9	8.25	8.051

$Ca_{12}O_{12}{\cdot}31H_2$	31	-9071.524552	-9071.421409	-47.0	-131.6	2.4	8.50	8.050
$Ca_{12}O_{12}{\cdot}32H_2$	32	-9072.692705	-9072.587478	-52.9	-140.7	-2.3	8.75	8.044
$(H_2@Ca_{12}O_{12})\cdot32H_2$	33	-9073.861560	-9073.751360	-60.7	-144.0	-1.4	9.00	8.010
$Ca_{12}O_{12}{\cdot}33H_2$	33	-9073.855484	-9073.749392	-44.7	-138.8	3.8	9.00	8.059
$(H_2@Ca_{12}O_{12})\cdot33H_2$	34	-9075.024741	-9074.915759	-53.5	-148.7	-1.7	9.24	8.051
$Ca_{12}O_{12}{\cdot}34H_2$	34	-9075.023868	-9074.912487	-51.2	-140.1	6.9	9.24	8.030
$(H_2@Ca_{12}O_{12})\cdot34H_2$	35	-9076.189738	-9076.079197	-51.1	-150.9	0.4	9.49	8.056
$Ca_{12}O_{12}{\cdot}35H_2$	35	-9076.189934	-9076.077592	-51.6	-146.7	4.6	9.49	8.020
$Ca_{12}O_{12}{\cdot}36H_2$	36	-9077.352493	-9077.239289	-42.8	-144.3	11.3	9.73	8.053
$Ca_{12}O_{12}{\cdot}37H_2$	37	-9078.517024	-9078.402806	-39.2	-146.7	13.3	9.98	8.074
$Ca_{12}O_{12}{\cdot}38H_2$	38	-9079.683955	-9079.567976	-41.9	-153.4	10.9	10.22	8.053
$Ca_{12}O_{12}{\cdot}39H_2$	39	-9080.852807	-9080.729699	-49.6	-151.1	17.5	10.46	8.030
$Ca_{12}O_{12}{\cdot}40H_2$	40	-9082.018006	-9081.896805	-47.7	-162.9	10.0	10.70	8.049
$Ca_{12}O_{12}{\cdot}41H_2$	41	-9083.182962	-9083.058259	-45.2	-159.9	17.4	10.94	8.056
$Ca_{12}O_{12}{\cdot}42H_2$	42	-9084.350472	-9084.222729	-49.4	-164.8	16.8	11.17	8.022
$Ca_{12}O_{12}{\cdot}43H_2$	43	-9085.513782	-9085.385084	-42.6	-164.1	21.8	11.41	8.056
$Ca_{12}O_{12}{\cdot}44H_2$	44	-9086.682062	-9086.549248	-48.8	-168.2	22.0	11.64	8.033
$Ca_{12}O_{12}{\cdot}45H_2$	45	-9087.847934	-9087.712423	-48.7	-169.7	24.8	11.88	8.035
$Ca_{12}O_{12}{\cdot}46H_2$	46	-9089.013335	-9088.875224	-47.3	-170.2	28.7	12.11	8.031
$Ca_{12}O_{12}{\cdot}47H_2$	47	-9090.178195	-9090.038975	-44.6	-173.2	30.0	12.34	8.056
$Ca_{12}O_{12}{\cdot}48H_2$	48	-9091.344376	-9091.202627	-45.3	-175.9	31.6	12.57	8.050

S3. Cartesian Coordinates

All coordinates are given in Å. All geometries were optimized using the B3LYP-D3/6-31G(d,p) level of theory, and the reported energies include ZPE corrections computed at this level.

$Be_{12}O_{12}$, ωB97XD/6-31++G(d,p)

Energy: -1081.431102 E_h

O	-1.193259000	0.000000000	2.240179000
O	1.193259000	0.000000000	2.240179000
O	0.000000000	2.240179000	1.193259000
O	0.000000000	2.240179000	-1.193259000
O	2.240179000	1.193259000	0.000000000
O	2.240179000	-1.193259000	0.000000000
O	1.193259000	0.000000000	-2.240179000
O	0.000000000	-2.240179000	-1.193259000
O	-1.193259000	0.000000000	-2.240179000
O	-2.240179000	-1.193259000	0.000000000
O	0.000000000	-2.240179000	1.193259000
O	-2.240179000	1.193259000	0.000000000
Be	0.000000000	-1.023031000	2.101930000
Be	-2.101930000	0.000000000	1.023031000
Be	2.101930000	0.000000000	1.023031000
Be	0.000000000	1.023031000	2.101930000
Be	-1.023031000	2.101930000	0.000000000
Be	1.023031000	2.101930000	0.000000000
Be	2.101930000	0.000000000	-1.023031000
Be	0.000000000	1.023031000	-2.101930000
Be	-2.101930000	0.000000000	-1.023031000
Be	0.000000000	-1.023031000	-2.101930000
Be	-1.023031000	-2.101930000	0.000000000
Be	1.023031000	-2.101930000	0.000000000

$Mg_{12}O_{12}$, ωB97X-D/6-31++G(d,p)

Energy: -3305.057214 E_h

O	0.000000000	2.761185000	1.410601000
O	0.000000000	2.761185000	-1.410601000
O	-2.761185000	1.410601000	0.000000000
O	-2.761185000	-1.410601000	0.000000000
O	-1.410601000	0.000000000	-2.761185000
O	1.410601000	0.000000000	-2.761185000
O	0.000000000	-2.761185000	-1.410601000
O	2.761185000	-1.410601000	0.000000000
O	0.000000000	-2.761185000	1.410601000
O	1.410601000	0.000000000	2.761185000
O	2.761185000	1.410601000	0.000000000
O	-1.410601000	0.000000000	2.761185000
Mg	0.000000000	1.329221000	2.636834000
Mg	-1.329221000	2.636834000	0.000000000
Mg	-2.636834000	0.000000000	-1.329221000
Mg	-2.636834000	0.000000000	1.329221000
Mg	0.000000000	-1.329221000	2.636834000
Mg	-1.329221000	-2.636834000	0.000000000
Mg	0.000000000	-1.329221000	-2.636834000
Mg	1.329221000	-2.636834000	0.000000000
Mg	2.636834000	0.000000000	1.329221000
Mg	2.636834000	0.000000000	-1.329221000
Mg	0.000000000	1.329221000	-2.636834000
Mg	1.329221000	2.636834000	0.000000000

$Ca_{12}O_{12}$, ωB97XD/6-31++G(d,p)

Energy: -9035.363389 E_h

O	-3.181363000	-1.593360000	0.000000000
O	-3.181363000	1.593360000	0.000000000
O	-1.593360000	0.000000000	-3.181363000
O	1.593360000	0.000000000	-3.181363000
O	0.000000000	3.181363000	-1.593360000
O	0.000000000	3.181363000	1.593360000
O	3.181363000	1.593360000	0.000000000
O	1.593360000	0.000000000	3.181363000
O	3.181363000	-1.593360000	0.000000000
O	0.000000000	-3.181363000	1.593360000
O	-1.593360000	0.000000000	3.181363000
O	0.000000000	-3.181363000	-1.593360000
Ca	0.000000000	1.608044000	3.159162000
Ca	1.608044000	3.159162000	0.000000000
Ca	-1.608044000	3.159162000	0.000000000
Ca	3.159162000	0.000000000	1.608044000
Ca	3.159162000	0.000000000	-1.608044000
Ca	0.000000000	1.608044000	-3.159162000
Ca	0.000000000	-1.608044000	-3.159162000
Ca	1.608044000	-3.159162000	0.000000000
Ca	-3.159162000	0.000000000	-1.608044000
Ca	-1.608044000	-3.159162000	0.000000000
Ca	-3.159162000	0.000000000	1.608044000
Ca	0.000000000	-1.608044000	3.159162000

$Be_{12}O_{12}\cdot H_2$ (M), ωB97XD/6-31++G(d,p)

Energy: -1082.598700 E_h

O	0.098072000	0.004704000	2.535859000
O	-2.023136000	0.002772000	1.442660000
O	-0.483939000	-2.239060000	1.064791000
O	0.609278000	-2.241438000	-1.056099000
O	-1.931071000	-1.195666000	-1.023488000
O	-1.930964000	1.192036000	-1.027913000
O	0.028580000	-0.004702000	-2.534942000
O	0.609477000	2.237451000	-1.064409000
O	2.151776000	-0.002776000	-1.445271000
O	2.054951000	1.195255000	1.023367000
O	-0.483737000	2.243049000	1.056476000
O	2.054844000	-1.191627000	1.027796000
Be	-0.899810000	1.024420000	1.861497000
Be	1.463074000	0.003410000	1.871187000
Be	-2.318629000	0.000000000	-0.055684000
Be	-0.899902000	-1.017415000	1.865286000
Be	0.971674000	-2.100999000	0.472502000
Be	-0.847605000	-2.098268000	-0.464303000
Be	-1.333601000	-0.003391000	-1.861072000
Be	1.026300000	-1.026173000	-1.865523000
Be	2.400530000	-0.000006000	0.053029000
Be	1.026391000	1.019157000	-1.869319000
Be	0.971863000	2.102658000	0.464703000
Be	-0.847418000	2.096611000	-0.472084000
H	-4.414209000	0.000880000	0.376319000
H	-4.470305000	-0.000874000	-0.367821000

$Mg_{12}O_{12}{\cdot}H_2$ (M), ωB97XD/6-31++G(d,p)

Energy: -3306.225706 E_h

O	-0.113090000	0.373262000	3.071290000
O	-2.559118000	0.206938000	1.673378000
O	-0.663901000	-2.595207000	1.547058000
O	0.745390000	-2.889012000	-0.878922000
O	-2.351699000	-1.563622000	-1.197742000
O	-2.347161000	1.236971000	-1.537589000
O	0.203343000	-0.373563000	-3.071356000
O	0.753944000	2.592491000	-1.544604000
O	2.649152000	-0.207616000	-1.675952000
O	2.439937000	1.563509000	1.198910000
O	-0.655353000	2.891858000	0.880768000
O	2.435614000	-1.237010000	1.538998000
Mg	1.664257000	0.295803000	2.449082000
Mg	-1.275208000	-1.041581000	2.422395000
Mg	-1.111298000	-2.693747000	-0.340731000
Mg	1.192349000	-2.539018000	0.978488000
Mg	2.993956000	0.015831000	0.163885000
Mg	1.361565000	-1.597312000	-2.106034000
Mg	-1.572568000	-0.295182000	-2.442139000
Mg	1.365114000	1.042260000	-2.425811000
Mg	1.200371000	2.696876000	0.342366000
Mg	-1.103247000	2.536010000	-0.975953000
Mg	-2.927496000	-0.016429000	-0.166559000
Mg	-1.271737000	1.595259000	2.102866000
H	-5.201090000	0.056874000	0.340414000
H	-5.288084000	-0.034106000	-0.396568000

$Mg_{12}O_{12}{\cdot}H_2$ (O), ωB97XD/6-31++G(d,p)

Energy: -3306.223682 E_h

O	-1.342808000	-2.458274000	-1.283226000
O	1.411232000	-2.127781000	-1.796007000
O	0.639973000	-2.676812000	1.450225000
O	0.651911000	-0.334118000	3.021516000
O	3.048772000	-0.445171000	0.638729000
O	2.435839000	1.092049000	-1.645617000
O	1.436338000	2.458520000	1.281065000
O	-0.547260000	2.678112000	-1.449693000
O	-1.317746000	2.126679000	1.794684000
O	-2.960693000	0.446343000	-0.640450000
O	-0.559133000	0.334115000	-3.018783000
O	-2.340785000	-1.092007000	1.641107000
Mg	-2.535187000	-1.414269000	-0.263116000
Mg	0.322547000	-2.914315000	-0.392721000
Mg	1.917135000	-1.282048000	1.893008000
Mg	-0.678931000	-1.593189000	2.376451000
Mg	-2.522363000	0.794349000	1.222999000
Mg	0.347121000	1.464008000	2.544881000
Mg	2.627718000	1.412684000	0.260512000
Mg	-0.229114000	2.915772000	0.393196000
Mg	-1.823484000	1.283239000	-1.891845000
Mg	0.772174000	1.593811000	-2.375896000
Mg	2.614293000	-0.794939000	-1.221758000
Mg	-0.252408000	-1.465038000	-2.546520000
H	-5.898506000	-0.116456000	0.193988000
H	-5.260616000	0.102443000	-0.132668000

$Ca_{12}O_{12}\cdot H_2$ (M), ωB97XD/6-31++G(d,p)

Energy: -9036.529626 E_h

O	-2.805509000	-1.383710000	-1.759373000
O	-2.872566000	-1.620533000	1.418253000
O	-2.947975000	2.043777000	0.090972000
O	-0.144972000	3.551188000	0.262047000
O	-0.860694000	1.163940000	3.262840000
O	0.652105000	-1.636017000	3.084103000
O	2.726674000	1.386559000	1.759915000
O	2.873604000	-2.047625000	-0.091298000
O	2.793661000	1.623833000	-1.418801000
O	0.785549000	-1.163325000	-3.260696000
O	0.068579000	-3.549966000	-0.262072000
O	-0.727327000	1.636887000	-3.086331000
Ca	1.426734000	-2.897525000	1.429080000
Ca	1.312159000	0.525424000	3.238234000
Ca	-1.519487000	-0.993429000	3.063161000
Ca	3.495981000	0.076904000	0.079431000
Ca	1.980705000	2.908893000	0.258938000
Ca	-1.568538000	2.656666000	1.779288000
Ca	-1.501256000	2.895688000	-1.428998000
Ca	1.444644000	0.995143000	-3.065913000
Ca	-3.581321000	-0.077245000	-0.080040000
Ca	-1.387017000	-0.524282000	-3.235434000
Ca	-2.056032000	-2.905115000	-0.258599000
Ca	1.494056000	-2.658440000	-1.779763000
H	6.408651000	-0.419488000	0.005298000
H	6.449755000	0.325784000	0.010465000

$Ca_{12}O_{12}\cdot H_2$ (O), ωB97XD/6-31++G(d,p)

Energy: -9036.529997 E_h

O	1.867496000	1.313928000	-2.705024000
O	-1.190536000	2.198810000	-2.548777000
O	0.967373000	3.383175000	0.471794000
O	0.593446000	1.625199000	3.103377000
O	-2.681732000	2.135017000	1.050611000
O	-3.496017000	-0.372557000	-0.739757000
O	-1.936009000	-1.313263000	2.706310000
O	-1.034578000	-3.383632000	-0.471888000
O	1.122482000	-2.196565000	2.550204000
O	2.611400000	-2.132689000	-1.049550000
O	-0.662178000	-1.624788000	-3.102824000
O	3.428974000	0.372184000	0.744258000
Ca	-2.387280000	-2.041609000	-1.696168000
Ca	-3.255654000	-0.012627000	1.482998000
Ca	-2.878876000	1.762765000	-1.174417000
Ca	-0.816282000	-3.008245000	1.705368000
Ca	0.006999000	-0.476956000	3.513696000
Ca	-0.770908000	2.930733000	1.852206000
Ca	2.317590000	2.044268000	1.698921000
Ca	2.809738000	-1.767428000	1.173809000
Ca	0.748289000	3.011216000	-1.706785000
Ca	3.190279000	0.008886000	-1.492624000
Ca	-0.077129000	0.477613000	-3.510481000
Ca	0.701583000	-2.931451000	-1.853803000
H	5.424776000	0.082558000	0.215503000
H	6.087260000	-0.064397000	-0.139743000

(H_2@$Ca_{12}O_{12}$), ωB97XD/6-31++G(d,p)

Energy: -9036.532731 E_h

O	3.203085000	0.679056000	-1.401104000
O	3.111733000	-1.443634000	0.970983000
O	1.147984000	-2.540731000	-2.226713000
O	-1.996108000	-2.123699000	-1.980203000
O	-0.305743000	-3.294245000	1.311239000
O	0.114777000	-0.950379000	3.431189000
O	-3.203045000	-0.679104000	1.401019000
O	-1.148044000	2.540778000	2.226676000
O	-3.111645000	1.443564000	-0.971019000
O	0.305898000	3.294239000	-1.311123000
O	1.996043000	2.123481000	1.980391000
O	-0.114870000	0.950381000	-3.431199000
Ca	0.373746000	1.248897000	3.294463000
Ca	-1.686921000	-1.912521000	2.454891000
Ca	1.498033000	-2.289781000	2.240288000
Ca	-2.902168000	1.561652000	1.280434000
Ca	-3.375138000	-0.800730000	-0.851854000
Ca	-0.471387000	-3.399807000	-0.898567000
Ca	-0.373910000	-1.248908000	-3.294425000
Ca	-1.497929000	2.289795000	-2.240191000
Ca	2.902279000	-1.561738000	-1.280496000
Ca	1.686939000	1.912498000	-2.454944000
Ca	3.375037000	0.800644000	0.851803000
Ca	0.471461000	3.399906000	0.898695000
H	0.271895000	0.204205000	0.154661000
H	-0.273254000	-0.199996000	-0.157659000

$Ca_{12}O_{12}\cdot 2H_2$, ωB97XD/6-31++G(d,p)

Energy: -9037.696778 E_h

O	-1.454821000	3.098070000	0.992939000
O	1.625548000	3.171793000	0.179581000
O	-0.773705000	2.158899000	-2.721044000
O	-0.857866000	-0.970463000	-3.313588000
O	2.666193000	0.373341000	-2.322882000
O	3.484983000	-0.208197000	0.700069000
O	1.455130000	-3.081534000	-0.991762000
O	0.775106000	-2.142553000	2.723174000
O	-1.624350000	-3.155890000	-0.174878000
O	-2.666161000	-0.357873000	2.325561000
O	0.855781000	0.986531000	3.318335000
O	-3.486415000	0.231541000	-0.695691000
Ca	2.362572000	-0.536626000	2.590349000
Ca	3.012130000	-1.505143000	-1.111006000
Ca	3.098990000	1.665802000	-0.518594000
Ca	0.328831000	-3.397060000	0.946379000
Ca	-0.496854000	-2.799710000	-2.105659000
Ca	0.745518000	0.625933000	-3.407272000
Ca	-2.363136000	0.554690000	-2.586622000
Ca	-3.101144000	-1.654899000	0.524738000
Ca	-0.326573000	3.412875000	-0.944243000
Ca	-3.009031000	1.517825000	1.109141000
Ca	0.495455000	2.814793000	2.109154000
Ca	-0.745959000	-0.611798000	3.410253000
H	-5.442278000	-0.367403000	-0.286896000
H	-6.079175000	-0.713336000	-0.037528000
H	6.075649000	-0.853745000	-0.260001000
H	5.434443000	-0.628485000	0.093562000

($2H_2@Ca_{12}O_{12}$), ωB97XD/6-31++G(d,p)

Energy: -9037.673378 E_h

O	-3.066561000	1.762028000	0.069296000
O	-0.403334000	3.527846000	0.036868000
O	-0.922322000	1.394185000	-3.129428000
O	0.812234000	-1.275768000	-3.146536000
O	2.705844000	1.773689000	-1.634863000
O	2.664264000	1.652906000	1.549969000
O	3.166708000	-1.840909000	-0.109659000
O	0.934847000	-1.360645000	3.151390000
O	0.391655000	-3.459721000	-0.050018000
O	-2.699139000	-1.782559000	1.614066000
O	-0.802113000	1.306177000	3.206458000
O	-2.777358000	-1.758007000	-1.575928000
Ca	1.415542000	0.848036000	3.213511000
Ca	3.586159000	0.355464000	-0.091887000
Ca	1.772287000	3.044385000	-0.007362000
Ca	1.785786000	-2.616665000	1.526078000
Ca	1.743601000	-2.655496000	-1.680551000
Ca	1.297660000	0.934790000	-3.142516000
Ca	-1.406254000	-0.824757000	-3.064344000
Ca	-1.804962000	-3.087817000	-0.013487000
Ca	-1.781778000	2.706634000	-1.561904000
Ca	-3.621432000	-0.419620000	0.052839000
Ca	-1.695670000	2.634270000	1.669448000
Ca	-1.286388000	-0.910696000	3.096332000
H	1.142106000	0.281483000	0.462824000
H	0.985387000	-0.202403000	-0.083974000
H	-0.933768000	-0.200363000	-0.098132000
H	-1.322560000	0.436946000	-0.056759000

$Ca_{12}O_{12}\cdot 3H_2$, ωB97XD/6-31++G(d,p)

Energy: -9038.863603 E_h

O	1.204129000	1.492690000	2.987074000
O	-1.741954000	0.279318000	3.095954000
O	1.058676000	-2.367426000	2.466780000
O	1.333225000	-3.293131000	-0.569052000
O	-2.338050000	-2.642157000	0.591297000
O	-3.527667000	0.160485000	-0.352822000
O	-1.184396000	-1.553755000	-2.968005000
O	-1.038791000	2.304084000	-2.446389000
O	1.760622000	-0.338994000	-3.077811000
O	2.356703000	2.581768000	-0.571938000
O	-1.314812000	3.233731000	0.588959000
O	3.547405000	-0.218673000	0.379339000
Ca	-2.654482000	2.136496000	-0.876087000
Ca	-2.767710000	-1.703810000	-1.421580000
Ca	-3.059099000	-0.781196000	1.656602000
Ca	-0.314602000	0.474631000	-3.475077000
Ca	0.887196000	-2.355762000	-2.531580000
Ca	-0.299586000	-3.425620000	0.995355000
Ca	2.672371000	-2.198522000	0.890756000
Ca	3.078185000	0.721994000	-1.641295000
Ca	0.333604000	-0.537346000	3.491001000
Ca	2.787717000	1.638082000	1.438367000
Ca	-0.866279000	2.294476000	2.552987000
Ca	0.323251000	3.368703000	-0.986940000
H	5.457077000	0.483701000	-0.127261000
H	6.066214000	0.819852000	-0.445776000
H	-5.898401000	-1.271433000	-0.987636000
H	-5.343231000	-0.788462000	-0.776451000
H	-1.843456000	5.840608000	-0.429855000

H	-1.770250000	5.169674000	-0.070306000

$Ca_{12}O_{12}\cdot 4H_2$, ωB97XD/6-31++G(d,p)

Energy: -9040.030464 E_h

O	-0.373556000	-1.968946000	2.956109000
O	1.358585000	0.693846000	3.218103000
O	-2.378936000	1.315509000	2.309534000
O	-2.868871000	1.937985000	-0.777245000
O	0.412885000	3.467449000	0.652028000
O	3.048236000	1.842029000	-0.107640000
O	0.374362000	1.966931000	-2.941224000
O	2.381414000	-1.317204000	-2.294655000
O	-1.354574000	-0.697669000	-3.203808000
O	-0.410490000	-3.470427000	-0.637245000
O	2.871060000	-1.942613000	0.791671000
O	-3.045550000	-1.846476000	0.127385000
Ca	3.483115000	-0.277204000	-0.616541000
Ca	1.462630000	2.973952000	-1.289147000
Ca	1.965426000	2.316095000	1.828950000
Ca	0.841155000	-0.194181000	-3.435595000
Ca	-1.813029000	1.453266000	-2.672271000
Ca	-1.733381000	2.970300000	0.907368000
Ca	-3.480515000	0.273706000	0.632291000
Ca	-1.962098000	-2.323180000	-1.819784000
Ca	-0.837929000	0.193067000	3.449658000
Ca	-1.462633000	-2.971141000	1.300753000
Ca	1.814441000	-1.457849000	2.686061000
Ca	1.735524000	-2.973146000	-0.894127000
H	-4.188002000	-3.471043000	-0.536720000
H	-4.476203000	-4.075434000	-0.907461000
H	4.253730000	4.383668000	-0.518629000

H	4.045645000	3.663994000	-0.362154000
H	4.666650000	-3.974819000	-0.059797000
H	4.270443000	-3.406758000	0.266171000
H	-4.670592000	3.965065000	0.073921000
H	-4.272316000	3.398292000	-0.251727000

$Ca_{12}O_{12}\cdot 5H_2$, ωB97XD/6-31++G(d,p)

Energy: -9041.197087 E_h

O	-0.872307000	-2.627658000	-2.305025000
O	-1.593225000	0.346723000	-3.196931000
O	2.222917000	-0.298936000	-2.773921000
O	3.444792000	0.809746000	-0.049387000
O	0.691553000	3.084528000	-1.611766000
O	-2.167384000	2.805503000	-0.228568000
O	0.835852000	2.586705000	2.247974000
O	-2.257483000	0.256967000	2.713338000
O	1.556000000	-0.389557000	3.136601000
O	-0.724451000	-3.129648000	1.555729000
O	-3.480679000	-0.857854000	-0.008850000
O	2.130497000	-2.853826000	0.164681000
Ca	-3.215656000	1.202433000	0.898732000
Ca	-0.111575000	3.504499000	0.459037000
Ca	-1.339978000	2.357262000	-2.293482000
Ca	-0.253921000	0.947521000	3.376784000
Ca	2.641963000	1.222004000	1.981788000
Ca	2.455363000	1.759896000	-1.866128000
Ca	3.177579000	-1.249058000	-0.960241000
Ca	1.306217000	-2.404916000	2.241206000
Ca	0.218634000	-0.993402000	-3.433091000
Ca	0.078303000	-3.541747000	-0.518606000
Ca	-2.666780000	-1.273168000	-2.036718000

Ca	-2.486870000	-1.803958000	1.807661000
H	2.778594000	-4.543583000	1.217739000
H	2.914147000	-5.084153000	1.742585000
H	-2.366166000	5.632055000	-0.548702000
H	-2.437352000	4.873467000	-0.483372000
H	-5.748364000	-1.604667000	1.559579000
H	-5.224328000	-1.384912000	1.048302000
H	5.717304000	1.552625000	-1.611723000
H	5.191620000	1.333753000	-1.101761000
H	2.701134000	3.475462000	4.183733000
H	2.119181000	3.341091000	3.703764000

$Ca_{12}O_{12}\cdot 6H_2$, ωB97XD/6-31++G(d,p)

Energy: -9042.364167 E_h

O	3.319054000	-0.795283000	-0.992975000
O	0.992412000	-1.770891000	-2.940100000
O	1.252145000	2.098367000	-2.583082000
O	-0.897626000	3.389069000	-0.617016000
O	-2.241317000	0.393507000	-2.736710000
O	-2.409069000	-2.355686000	-1.135622000
O	-3.309029000	0.790266000	0.982697000
O	-1.242816000	-2.104633000	2.573056000
O	-0.982167000	1.763617000	2.930764000
O	2.250879000	-0.398957000	2.728154000
O	0.909671000	-3.395233000	0.609669000
O	2.425757000	2.347870000	1.122812000
Ca	-1.352017000	-3.226511000	0.614587000
Ca	-3.409349000	-0.320599000	-0.938389000
Ca	-1.223278000	-1.617343000	-2.924199000
Ca	-2.221899000	-0.122387000	2.764131000

Ca	-2.040043000	2.661310000	1.146217000
Ca	-1.006524000	2.230300000	-2.576224000
Ca	1.363973000	3.219654000	-0.624251000
Ca	1.232956000	1.611866000	2.921077000
Ca	2.230945000	0.116187000	-2.774450000
Ca	3.414267000	0.317319000	0.927953000
Ca	2.050429000	-2.666719000	-1.154156000
Ca	1.015873000	-2.235679000	2.568798000
H	3.556239000	3.175036000	2.674123000
H	3.855770000	3.382559000	3.347338000
H	-4.899494000	-2.786813000	-2.445314000
H	-4.214149000	-2.795870000	-2.105576000
H	1.238285000	-5.400704000	2.605533000
H	1.163190000	-4.966970000	1.979702000
H	-1.222606000	5.398455000	-2.609530000
H	-1.148785000	4.963096000	-1.984682000
H	-5.117716000	1.309922000	3.119064000
H	-4.724697000	1.212312000	2.470064000
H	4.735040000	-1.218451000	-2.478720000
H	5.129108000	-1.316617000	-3.127022000

$Ca_{12}O_{12}\cdot 7H_2$, ωB97XD/6-31++G(d,p)

Energy: -9043.530923 E_h

O	0.506646000	-3.397324000	-0.891060000
O	-0.626668000	-1.486384000	-3.175439000
O	2.920739000	-0.510567000	-1.902224000
O	2.954838000	1.930260000	0.149914000
O	0.320363000	2.259992000	-2.712016000
O	-2.657274000	1.542568000	-1.831303000
O	-0.582138000	3.392431000	0.908301000
O	-2.998937000	0.508626000	1.911359000

O	0.551347000	1.479817000	3.190858000
O	-0.396051000	-2.265975000	2.730433000
O	-3.026052000	-1.940269000	-0.129507000
O	2.581935000	-1.555688000	1.843862000
Ca	-3.566421000	0.257779000	-0.262405000
Ca	-1.143238000	3.129375000	-1.225378000
Ca	-1.169370000	0.663196000	-3.301600000
Ca	-1.520316000	2.061364000	2.488602000
Ca	1.499494000	2.777924000	1.601298000
Ca	2.350785000	1.676930000	-2.031823000
Ca	3.496938000	-0.264631000	0.285667000
Ca	1.092058000	-0.668599000	3.323345000
Ca	1.447006000	-2.068340000	-2.483387000
Ca	1.068752000	-3.131651000	1.243270000
Ca	-1.565860000	-2.782361000	-1.577841000
Ca	-2.425836000	-1.675762000	2.052828000
H	3.278226000	-2.427884000	3.623675000
H	3.380862000	-2.671561000	4.341415000
H	-3.471570000	3.803895000	-3.368715000
H	-3.363730000	3.143036000	-2.999466000
H	-5.348920000	-2.812145000	1.275056000
H	-4.785921000	-2.625309000	0.792420000
H	5.128581000	2.972283000	-1.377105000
H	4.624092000	2.737234000	-0.852730000
H	0.279927000	5.544326000	2.550208000
H	-0.060781000	5.044340000	2.081153000
H	0.886371000	-4.850398000	-2.356834000
H	1.063918000	-5.240093000	-2.990600000
H	5.727943000	-0.937847000	-1.765219000
H	4.991179000	-0.844277000	-1.950221000

$Ca_{12}O_{12}\cdot 8H_2$, ωB97XD/6-31++G(d,p)

Energy: -9044.698117 E_h

O	0.631345000	-3.404754000	-0.849726000
O	-0.169376000	-1.461132000	-3.242938000
O	3.184771000	-0.519809000	-1.507604000
O	2.943393000	1.899337000	0.554607000
O	0.718162000	2.279321000	-2.627944000
O	-2.354776000	1.573726000	-2.156881000
O	-0.648719000	3.389123000	0.842652000
O	-3.198076000	0.507451000	1.496339000
O	0.155753000	1.445971000	3.235028000
O	-0.731237000	-2.292031000	2.622006000
O	-2.956107000	-1.916535000	-0.560287000
O	2.342509000	-1.594702000	2.141632000
Ca	-3.481187000	0.276763000	-0.748965000
Ca	-0.928485000	3.154899000	-1.349675000
Ca	-0.686312000	0.690902000	-3.415820000
Ca	-1.797625000	2.051914000	2.270019000
Ca	1.315168000	2.753164000	1.801902000
Ca	2.633370000	1.671434000	-1.688682000
Ca	3.469746000	-0.293921000	0.737843000
Ca	0.673143000	-0.704716000	3.413106000
Ca	1.787910000	-2.064992000	-2.284143000
Ca	0.915665000	-3.163554000	1.341791000
Ca	-1.323160000	-2.767268000	-1.804226000
Ca	-2.645918000	-1.683159000	1.682712000
H	2.817499000	-2.481737000	3.985196000
H	2.837148000	-2.735150000	4.706512000
H	-2.969802000	3.903915000	-3.669004000
H	-2.910947000	3.221091000	-3.328460000
H	-5.154634000	-3.262781000	0.649961000

H	-4.626733000	-2.941570000	0.199339000
H	5.143764000	3.244875000	-0.653338000
H	4.615596000	2.923858000	-0.202912000
H	-0.091832000	5.509775000	2.668400000
H	-0.339009000	5.020333000	2.135415000
H	1.223207000	-4.834292000	-2.275776000
H	1.494773000	-5.207381000	-2.885575000
H	6.013224000	-0.368415000	-1.126350000
H	5.290443000	-0.428164000	-1.367473000
H	-5.303685000	0.410302000	1.356135000
H	-6.026462000	0.348299000	1.115622000

$Ca_{12}O_{12}\cdot 9H_2$, ωB97XD/6-31++G(d,p)

Energy: -9045.864884 E_h

O	0.802977000	-2.778837000	-2.097271000
O	-0.019930000	-0.062734000	-3.541859000
O	3.236740000	0.206503000	-1.438566000
O	2.841789000	1.579258000	1.412891000
O	0.697279000	3.151064000	-1.439478000
O	-2.353786000	2.219057000	-1.424421000
O	-0.819217000	2.710425000	2.119206000
O	-3.251623000	-0.264180000	1.457607000
O	0.008240000	-0.002981000	3.565176000
O	-0.709565000	-3.209457000	1.466051000
O	-2.854629000	-1.643871000	-1.389608000
O	2.341935000	-2.285596000	1.435155000
Ca	-3.452886000	0.429564000	-0.701269000
Ca	-1.026120000	3.382003000	0.011474000
Ca	-0.623224000	1.963978000	-2.865748000
Ca	-1.943391000	0.878774000	2.843102000
Ca	1.145077000	1.805862000	2.828968000

Ca	2.616529000	2.271295000	-0.744113000
Ca	3.438763000	-0.493082000	0.718519000
Ca	0.602366000	-2.031733000	2.884574000
Ca	1.935505000	-0.941360000	-2.826619000
Ca	1.008716000	-3.443311000	0.014537000
Ca	-1.151922000	-1.871644000	-2.797816000
Ca	-2.626324000	-2.331466000	0.769895000
H	2.786648000	-3.867679000	2.754496000
H	2.789606000	-4.406619000	3.296403000
H	-3.111830000	4.960956000	-1.654534000
H	-3.017982000	4.203229000	-1.695818000
H	-5.161182000	-3.229108000	-0.863521000
H	-4.596760000	-2.791209000	-1.136610000
H	5.154528000	3.155366000	0.881524000
H	4.589638000	2.719752000	1.157244000
H	-0.412421000	3.956892000	4.653555000
H	-0.621452000	3.708766000	3.961182000
H	1.535431000	-3.497929000	-3.933430000
H	1.857227000	-3.583870000	-4.621920000
H	6.034013000	-0.001932000	-0.930712000
H	5.326559000	0.096961000	-1.203883000
H	-5.340659000	-0.175142000	1.215065000
H	-6.048189000	-0.084117000	0.939203000
H	0.327689000	4.570425000	-2.951245000
H	0.085663000	4.938451000	-3.576149000

$Ca_{12}O_{12}\cdot 10H_2$, ωB97XD/6-31++G(d,p)

Energy: -9047.032214 E_h

O	1.404004000	3.280629000	0.468574000
O	0.213973000	1.846532000	3.053398000
O	3.236836000	-0.018212000	1.467215000

O	2.444617000	-2.540444000	-0.317748000
O	0.235069000	-2.053452000	2.861392000
O	-2.607332000	-0.727456000	2.289295000
O	-1.387571000	-3.195203000	-0.473605000
O	-3.226044000	0.101337000	-1.466169000
O	-0.209733000	-1.761656000	-3.067150000
O	-0.225459000	2.130413000	-2.867398000
O	-2.434124000	2.626560000	0.314266000
O	2.617237000	0.813657000	-2.287206000
Ca	-3.424719000	0.634704000	0.736833000
Ca	-1.589845000	-2.667239000	1.673878000
Ca	-0.770360000	-0.099039000	3.458851000
Ca	-2.235451000	-1.796393000	-2.056738000
Ca	0.643981000	-3.145604000	-1.472516000
Ca	2.227552000	-2.000223000	1.883562000
Ca	3.436524000	-0.548649000	-0.736688000
Ca	0.770988000	0.191252000	-3.467736000
Ca	2.243251000	1.879716000	2.057656000
Ca	1.596527000	2.742975000	-1.678237000
Ca	-0.629295000	3.222856000	1.468896000
Ca	-2.215352000	2.083404000	-1.887352000
H	3.224327000	1.312677000	-4.232634000
H	3.270464000	1.447836000	-4.984296000
H	-3.743966000	-2.774107000	3.919225000
H	-3.534878000	-2.135980000	3.553385000
H	-4.425086000	4.124233000	-1.073497000
H	-3.943246000	3.792398000	-0.580939000
H	4.446347000	-4.032997000	1.065503000
H	3.962251000	-3.703102000	0.574110000
H	-3.049214000	-4.816833000	-2.133386000
H	-2.580925000	-4.508234000	-1.613760000

H	2.410873000	4.658681000	1.686655000
H	2.805864000	5.012859000	2.238067000
H	6.014391000	-0.486103000	1.017831000
H	5.312116000	-0.334663000	1.279879000
H	-5.300969000	0.426813000	-1.282243000
H	-6.002934000	0.582247000	-1.021907000
H	-0.129594000	-2.351176000	4.914254000
H	-0.340272000	-2.270539000	5.645015000
H	0.083027000	-4.325195000	-4.283872000
H	-0.046369000	-3.595629000	-4.094504000

$Ca_{12}O_{12}\cdot 11H_2$, ωB97XD/6-31++G(d,p)

Energy: -9048.198665 E_h

O	-2.398091000	1.450002000	-2.244154000
O	-0.001148000	-0.169976000	-3.576137000
O	-2.327947000	-2.346667000	-1.347736000
O	-1.142948000	-2.967851000	1.546117000
O	1.523425000	-2.945047000	-1.296343000
O	3.254631000	-0.274188000	-1.435665000
O	2.391940000	-1.444068000	2.185047000
O	2.323365000	2.355815000	1.283537000
O	-0.000120000	0.186804000	3.519010000
O	-1.524316000	2.953880000	1.247790000
O	1.134004000	2.981963000	-1.607651000
O	-3.261794000	0.285738000	1.369838000
Ca	2.937906000	1.843103000	-0.847312000
Ca	2.990298000	-1.932967000	0.099176000
Ca	1.768950000	-1.275095000	-2.824072000
Ca	2.069820000	0.730293000	2.776909000
Ca	0.310757000	-1.981102000	2.905130000
Ca	-0.514335000	-3.465719000	-0.583412000

Ca	-2.946853000	-1.832772000	0.781767000
Ca	-1.771952000	1.293871000	2.765976000
Ca	-2.068039000	-0.722212000	-2.842296000
Ca	-2.996302000	1.934912000	-0.158582000
Ca	-0.314458000	1.983204000	-2.966232000
Ca	0.509431000	3.477690000	0.523536000
H	-4.521020000	1.115503000	2.844908000
H	-4.800284000	1.483176000	3.454347000
H	5.586008000	-1.914330000	-1.650904000
H	5.028701000	-1.393447000	-1.697809000
H	1.792844000	5.730472000	-1.226791000
H	1.668315000	5.014751000	-1.465308000
H	-1.806844000	-5.717563000	1.171961000
H	-1.680722000	-5.001440000	1.408048000
H	3.831678000	-1.078975000	4.622409000
H	3.499750000	-1.313907000	3.975096000
H	-3.379075000	1.458516000	-4.105749000
H	-3.663899000	1.299166000	-4.797090000
H	-4.558603000	-4.012230000	-0.729981000
H	-3.965072000	-3.634717000	-1.030081000
H	3.958534000	3.648811000	0.962526000
H	4.549963000	4.028370000	0.661227000
H	2.658159000	-3.889023000	-2.793158000
H	3.056751000	-4.052476000	-3.425116000
H	0.360028000	-1.282803000	5.939929000
H	0.248630000	-0.770677000	5.383412000
H	-3.221325000	4.187031000	1.406119000
H	-3.914985000	4.500423000	1.331034000

$Ca_{12}O_{12}\cdot 12H_2$, ωB97XD/6-31++G(d,p)

Energy: -9049.365444 E_h

O	3.383429000	0.213830000	-1.073354000
O	1.169157000	0.082606000	-3.360913000
O	0.933666000	3.245550000	-1.107600000
O	-1.334739000	3.104886000	1.128688000
O	-2.314418000	1.459012000	-2.269185000
O	-2.109522000	-1.721827000	-2.295262000
O	-3.384671000	-0.219744000	1.073934000
O	-0.939944000	-3.245571000	1.102122000
O	-1.168550000	-0.076220000	3.360385000
O	2.303812000	-1.458779000	2.278416000
O	1.338550000	-3.103399000	-1.123434000
O	2.118934000	1.723295000	2.285802000
Ca	-0.920964000	-3.227828000	-1.174649000
Ca	-3.361812000	-0.206910000	-1.148517000
Ca	-1.047390000	-0.055764000	-3.402018000
Ca	-2.169787000	-1.760488000	2.203034000
Ca	-2.368197000	1.466685000	2.217937000
Ca	-1.325377000	3.103428000	-1.149156000
Ca	0.925335000	3.228151000	1.169090000
Ca	1.048765000	0.053090000	3.403329000
Ca	2.161708000	1.760515000	-2.210788000
Ca	3.361047000	0.210479000	1.148837000
Ca	2.376103000	-1.465987000	-2.210003000
Ca	1.318341000	-3.102657000	1.154532000
H	2.999213000	1.828209000	4.201403000
H	3.192560000	1.708275000	4.931252000
H	-4.724389000	-1.810667000	-3.433068000
H	-3.992483000	-1.896090000	-3.229113000
H	2.161657000	-5.717413000	-0.327129000

H	1.962465000	-5.067715000	-0.677494000
H	-2.164752000	5.715428000	0.329948000
H	-1.963205000	5.067239000	0.681867000
H	-5.305798000	0.730530000	2.955873000
H	-4.898084000	0.381092000	2.411425000
H	4.815287000	1.011742000	-2.398775000
H	5.177486000	1.411779000	-2.940524000
H	1.521572000	5.920020000	-0.293893000
H	1.378240000	5.259228000	-0.650330000
H	-1.377863000	-5.261804000	0.645475000
H	-1.517964000	-5.924018000	0.290563000
H	-3.185105000	1.499309000	-4.186944000
H	-3.362945000	1.375020000	-4.920188000
H	-3.024165000	-1.276981000	5.165922000
H	-2.495249000	-0.865596000	4.798429000
H	4.208460000	-1.453815000	3.189081000
H	4.930128000	-1.299480000	3.388115000
H	2.583391000	-0.537981000	-4.796987000
H	3.160469000	-0.879694000	-5.164268000

(H_2@$Ca_{12}O_{12}$)·12H_2 , ωB97XD/6-31++G(d,p)

Energy: -9050.535466 E_h

O	-3.085295000	0.004279000	-1.697007000
O	-0.487321000	-0.015226000	-3.535459000
O	-0.896670000	-3.186611000	-1.311562000
O	0.883015000	-3.180798000	1.334603000
O	2.628209000	-1.604211000	-1.785659000
O	2.626632000	1.579657000	-1.809780000
O	3.085309000	0.003711000	1.696972000
O	0.903091000	3.186783000	1.307148000
O	0.487274000	0.008606000	3.535569000

O	-2.620059000	1.603883000	1.798337000
O	-0.889430000	3.181036000	-1.330220000
O	-2.634751000	-1.580030000	1.797126000
Ca	1.337302000	3.158840000	-0.926477000
Ca	3.553439000	-0.010620000	-0.473257000
Ca	1.694671000	-0.014192000	-3.119595000
Ca	1.794173000	1.623861000	2.607323000
Ca	1.778469000	-1.611306000	2.623844000
Ca	1.328369000	-3.171345000	-0.896925000
Ca	-1.341919000	-3.159410000	0.919855000
Ca	-1.694691000	0.015670000	3.119643000
Ca	-1.785606000	-1.622989000	-2.612395000
Ca	-3.553399000	0.007858000	0.473247000
Ca	-1.787096000	1.612279000	-2.618773000
Ca	-1.323758000	3.170810000	0.903518000
H	-3.851170000	-1.663881000	3.520995000
H	-4.169154000	-1.544692000	4.205919000
H	5.415118000	1.541542000	-2.404862000
H	4.661884000	1.662571000	-2.349224000
H	-1.787935000	5.810806000	-0.683646000
H	-1.536699000	5.159843000	-0.996404000
H	1.788653000	-5.808021000	0.691369000
H	1.534837000	-5.157846000	1.003794000
H	4.603402000	-1.080223000	3.863599000
H	4.315238000	-0.704851000	3.263452000
H	-4.318206000	-0.710273000	-3.258311000
H	-4.607953000	-1.088789000	-3.855723000
H	-1.810597000	-5.806217000	-0.649178000
H	-1.554789000	-5.159117000	-0.966323000
H	1.556427000	5.161101000	0.958823000
H	1.809579000	5.809015000	0.641317000

H	3.844084000	-1.705153000	-3.508894000
H	4.162442000	-1.592069000	-4.194687000
H	2.045333000	1.102149000	5.663739000
H	1.567802000	0.723071000	5.202304000
H	-4.654944000	1.699034000	2.336945000
H	-5.408675000	1.581476000	2.393357000
H	-1.564185000	0.692440000	-5.207511000
H	-2.039871000	1.070421000	-5.671741000
H	-0.365314000	0.003444000	-0.075986000
H	0.365577000	0.006473000	0.076137000

$Ca_{12}O_{12}\cdot 13H_2$, ωB97XD/6-31++G(d,p)

Energy: -9050.532010 E_h

O	-0.706145000	3.317394000	1.043297000
O	1.947524000	2.018131000	2.234425000
O	1.995695000	2.460543000	-1.634737000
O	1.398311000	-0.200258000	-3.283677000
O	3.501552000	-0.747326000	-0.045771000
O	1.843266000	-1.869516000	2.432193000
O	0.765644000	-3.327520000	-1.027551000
O	-1.927383000	-2.456933000	1.644048000
O	-1.872814000	-2.005033000	-2.225936000
O	-3.453695000	0.740506000	0.047330000
O	-1.339328000	0.207865000	3.288868000
O	-1.777602000	1.883493000	-2.417726000
Ca	-0.284665000	-1.783399000	3.066527000
Ca	2.366692000	-2.661627000	0.362881000
Ca	2.961834000	0.053927000	2.016020000
Ca	-1.400683000	-3.233693000	-0.369474000
Ca	0.293629000	-2.084192000	-2.875407000
Ca	3.036979000	0.462374000	-1.850121000

Ca	0.349562000	1.793192000	-3.056359000
Ca	-2.901853000	-0.051533000	-2.014218000
Ca	1.471166000	3.230217000	0.381341000
Ca	-2.300326000	2.663425000	-0.357676000
Ca	-0.233618000	2.092384000	2.885725000
Ca	-2.974663000	-0.463858000	1.856701000
H	-3.543894000	2.167524000	-3.550270000
H	-4.226880000	2.090849000	-3.883706000
H	3.883789000	-3.825063000	2.832684000
H	3.339816000	-3.289513000	2.873978000
H	-3.640464000	-0.326877000	4.901921000
H	-2.961181000	-0.146070000	4.602154000
H	3.700515000	0.328400000	-4.893438000
H	3.020266000	0.149432000	-4.594408000
H	0.766868000	-5.141021000	-3.229966000
H	0.801562000	-4.775681000	-2.559136000
H	-0.071331000	5.307712000	1.325721000
H	0.335585000	5.954407000	1.355825000
H	2.440402000	3.849745000	-4.086349000
H	2.442728000	3.553199000	-3.381584000
H	-2.379444000	-3.543805000	3.396165000
H	-2.379738000	-3.837576000	4.101967000
H	5.349633000	-0.846424000	0.966754000
H	5.908104000	-0.805011000	1.487306000
H	-3.008344000	-4.587876000	-2.660904000
H	-2.761211000	-3.864702000	-2.681319000
H	-5.286422000	-0.434584000	-0.411559000
H	-5.815139000	-0.903715000	-0.686070000
H	1.984078000	3.461154000	3.772830000
H	1.796681000	3.947415000	4.332374000
H	-5.382370000	2.822135000	-0.415434000

H	-4.994886000	2.180847000	-0.272435000

(H_2@$Ca_{12}O_{12}$)·13H_2 , ωB97XD/6-31++G(d,p)

Energy: -9051.701704 E_h

O	3.417277000	-0.097315000	0.975856000
O	1.315719000	0.480270000	3.297152000
O	0.938876000	-3.028750000	1.637923000
O	-1.394643000	-3.222238000	-0.525290000
O	-2.231999000	-0.979167000	2.555860000
O	-1.973456000	2.144417000	2.015445000
O	-3.365460000	0.099343000	-0.971700000
O	-0.884745000	3.031064000	-1.626555000
O	-1.249397000	-0.475791000	-3.283846000
O	2.289014000	0.982970000	-2.563647000
O	1.458493000	3.224942000	0.526265000
O	2.042667000	-2.139664000	-2.001170000
Ca	-0.795663000	3.405554000	0.615615000
Ca	-3.313422000	0.489000000	1.220406000
Ca	-0.895370000	0.676236000	3.361169000
Ca	-2.170763000	1.401664000	-2.410894000
Ca	-2.428894000	-1.772364000	-1.848101000
Ca	-1.313446000	-2.817347000	1.712439000
Ca	0.860744000	-3.400105000	-0.604375000
Ca	0.961691000	-0.668752000	-3.359421000
Ca	2.225541000	-1.394995000	2.415970000
Ca	3.371925000	-0.489326000	-1.208617000
Ca	2.498787000	1.777274000	1.849547000
Ca	1.367080000	2.815963000	-1.709890000
H	2.826442000	-2.635828000	-3.900058000
H	2.990052000	-2.662844000	-4.646252000
H	-4.537160000	2.534787000	3.215169000

H	-3.812500000	2.554559000	2.972372000
H	2.393876000	5.596376000	-0.755564000
H	2.169665000	5.036901000	-0.285032000
H	-2.320046000	-5.606036000	0.744885000
H	-2.098292000	-5.043088000	0.277706000
H	-5.252766000	1.175102000	-2.868200000
H	-4.873922000	0.822522000	-2.308794000
H	4.904879000	-0.687224000	2.358010000
H	5.289106000	-0.994102000	2.942968000
H	1.441065000	-5.815958000	1.281431000
H	1.323773000	-5.100009000	1.522689000
H	-1.256620000	5.107882000	-1.515430000
H	-1.367847000	5.825282000	-1.276330000
H	-3.036199000	-0.671501000	4.488931000
H	-3.183715000	-0.417891000	5.194568000
H	-3.388061000	-0.742988000	-5.195123000
H	-2.773754000	-0.691696000	-4.746746000
H	4.147834000	0.749221000	-3.533086000
H	4.855807000	0.534386000	-3.726903000
H	2.800460000	1.304188000	4.550473000
H	3.398592000	1.690230000	4.829447000
H	0.401542000	-0.014669000	-0.056496000
H	-0.330908000	0.028120000	0.081456000
H	-5.769965000	-1.449307000	-0.157660000
H	-5.204338000	-1.043116000	-0.455761000

$Ca_{12}O_{12}\cdot 14H_2$, ωB97XD/6-31++G(d,p)

Energy: -9051.698501 E_h

O	0.390626000	3.419162000	0.914779000
O	2.323290000	1.362909000	2.395794000

O	2.883464000	1.584148000	-1.451483000
O	1.579522000	-0.798387000	-3.114062000
O	3.069087000	-1.858802000	0.329125000
O	0.893078000	-2.258901000	2.621215000
O	-0.288941000	-3.418976000	-0.899687000
O	-2.768003000	-1.580156000	1.461633000
O	-2.196204000	-1.349642000	-2.391399000
O	-2.963342000	1.866066000	-0.326822000
O	-1.464128000	0.809298000	3.118434000
O	-0.776719000	2.269487000	-2.614441000
Ca	-1.125029000	-1.427949000	3.031708000
Ca	1.308465000	-3.269309000	0.638075000
Ca	2.640374000	-0.834921000	2.302369000
Ca	-2.349051000	-2.580225000	-0.485424000
Ca	-0.132378000	-2.179615000	-2.804511000
Ca	3.205986000	-0.654447000	-1.531662000
Ca	1.244529000	1.439816000	-3.021966000
Ca	-2.524657000	0.843835000	-2.310867000
Ca	2.461466000	2.578178000	0.487997000
Ca	-1.197342000	3.275480000	-0.631967000
Ca	0.247392000	2.193235000	2.813125000
Ca	-3.089254000	0.661361000	1.536837000
H	-2.205872000	3.009989000	-3.988635000
H	-2.833326000	3.122644000	-4.409902000
H	2.941951000	-3.044623000	4.444069000
H	2.314774000	-2.951055000	4.016802000
H	-3.946838000	1.131195000	4.502290000
H	-3.222591000	1.063618000	4.268236000
H	4.061363000	-1.107201000	-4.497613000
H	3.336562000	-1.043692000	-4.263540000
H	-0.512322000	-5.267657000	-3.056583000

H	-0.467725000	-4.891759000	-2.392152000
H	1.623266000	5.085706000	1.291188000
H	2.216612000	5.560549000	1.375213000
H	3.976954000	2.684473000	-3.850556000
H	3.819900000	2.423657000	-3.149435000
H	-3.686574000	-2.377583000	3.230733000
H	-3.822740000	-2.616199000	3.941857000
H	4.052514000	-3.641600000	0.906973000
H	4.221315000	-4.351474000	1.133435000
H	-3.876479000	-3.588253000	-3.058027000
H	-3.460956000	-2.949587000	-3.018978000
H	-5.057715000	1.322433000	-0.890120000
H	-5.699935000	1.032526000	-1.168120000
H	2.708997000	2.795749000	3.905527000
H	2.646770000	3.347107000	4.430964000
H	-4.049571000	4.419372000	-1.104845000
H	-3.908173000	3.701686000	-0.889823000
H	-5.550258000	-2.151333000	0.573084000
H	-4.883774000	-1.997129000	0.898966000

$Ca_{12}O_{12}\cdot 15H_2$, ωB97XD/6-31++G(d,p)

Energy: -9052.864957 E_h

O	0.822000000	-2.085715000	2.792266000
O	2.999439000	-1.982742000	0.467976000
O	2.424506000	1.425550000	2.251655000
O	0.592149000	3.455050000	0.618682000
O	2.969263000	1.314409000	-1.602406000
O	1.528312000	-1.136619000	-3.038462000
O	-0.671079000	2.066143000	-2.796790000
O	-2.274420000	-1.440308000	-2.247866000

O	-2.840240000	1.973441000	-0.461044000
O	-2.818419000	-1.330290000	1.608647000
O	-0.438766000	-3.470394000	-0.613618000
O	-1.376627000	1.127028000	3.040229000
Ca	-0.241785000	-2.404762000	-2.600430000
Ca	1.307860000	1.115766000	-3.144351000
Ca	3.177057000	-0.937657000	-1.483934000
Ca	-2.473346000	0.770952000	-2.357068000
Ca	-1.019179000	3.266427000	-0.896070000
Ca	2.613024000	2.479565000	0.256321000
Ca	0.397463000	2.394382000	2.609213000
Ca	-3.028774000	0.931936000	1.492994000
Ca	2.634752000	-0.781511000	2.352041000
Ca	-1.148565000	-1.123485000	3.144538000
Ca	1.177242000	-3.276909000	0.900148000
Ca	-2.461531000	-2.503450000	-0.246442000
H	-3.109510000	1.522676000	4.207128000
H	-3.824539000	1.628911000	4.452491000
H	3.978746000	-1.713161000	-4.389546000
H	3.260072000	-1.586775000	-4.162054000
H	-2.360858000	-5.555337000	-1.011329000
H	-1.749393000	-5.103829000	-0.935914000
H	2.532924000	5.522612000	0.963377000
H	1.914531000	5.077630000	0.901786000
H	-1.920020000	4.495436000	-3.685356000
H	-1.579432000	3.819404000	-3.587985000
H	2.225217000	-2.749494000	4.220543000
H	2.852324000	-2.845821000	4.647271000
H	2.838929000	3.441608000	4.237842000
H	2.876131000	2.875353000	3.725983000
H	-2.656149000	-2.887647000	-3.784780000

H	-2.583614000	-3.440935000	-4.304249000
H	3.932579000	1.886144000	-3.393565000
H	4.094143000	2.051504000	-4.122218000
H	-4.954606000	2.584509000	-2.324505000
H	-4.472122000	2.524798000	-1.737321000
H	-5.021126000	-1.115462000	1.357342000
H	-5.726434000	-0.862906000	1.241357000
H	3.902535000	-3.766466000	1.165667000
H	4.037796000	-4.466179000	1.440966000
H	-3.842703000	-2.135879000	4.180904000
H	-3.718060000	-1.959237000	3.449759000
H	-5.195716000	-1.940416000	-2.075233000
H	-4.470547000	-1.790069000	-2.236381000
H	-3.587851000	3.915600000	0.305982000
H	-3.686597000	4.623900000	0.558694000

$Ca_{12}O_{12}\cdot16H_2$, ωB97XD/6-31++G(d,p)

Energy: -9054.030881 E_h

O	1.219051000	2.876681000	-1.686891000
O	3.212304000	1.584383000	0.443360000
O	2.409377000	-0.725100000	-2.590120000
O	0.256956000	-2.986506000	-1.953649000
O	2.688453000	-2.223814000	0.995816000
O	1.423465000	-0.402314000	3.284598000
O	-1.079570000	-2.924970000	1.711261000
O	-2.268925000	0.670917000	2.608289000
O	-3.065697000	-1.649883000	-0.431675000
O	-2.544108000	2.166690000	-0.973938000
O	-0.107018000	2.928880000	1.974431000
O	-1.282073000	0.340910000	-3.263799000
Ca	-0.169521000	1.142271000	3.362979000

Ca	0.959226000	-2.457199000	2.456879000
Ca	3.144583000	-0.162948000	1.813193000
Ca	-2.708488000	-1.358727000	1.797847000
Ca	-1.420025000	-3.216232000	-0.518504000
Ca	2.340625000	-2.498059000	-1.180784000
Ca	0.314884000	-1.202855000	-3.347013000
Ca	-3.005990000	0.099776000	-1.798567000
Ca	2.854875000	1.291811000	-1.772262000
Ca	-0.816520000	2.393556000	-2.438401000
Ca	1.573149000	3.157167000	0.541075000
Ca	-2.192270000	2.452978000	1.201724000
H	-2.966252000	0.644099000	-4.517290000
H	-3.672303000	0.727999000	-4.796060000
H	3.832315000	-0.663581000	4.792812000
H	3.118526000	-0.615251000	4.523073000
H	-1.866447000	4.851792000	3.151983000
H	-1.288754000	4.412164000	2.913736000
H	2.031599000	-4.892610000	-3.132720000
H	1.449531000	-4.458765000	-2.894010000
H	-2.356161000	-5.473819000	1.457051000
H	-2.016430000	-4.823314000	1.669006000
H	2.792992000	3.843633000	-2.759297000
H	3.450522000	4.003990000	-3.111027000
H	2.722596000	-1.875128000	-5.185342000
H	2.790197000	-1.555534000	-4.494329000
H	-2.611055000	1.534224000	4.536724000
H	-2.522457000	1.857144000	5.221764000
H	3.483282000	-3.587297000	2.402427000
H	3.588590000	-4.053090000	2.999095000
H	-5.272160000	-2.871249000	0.992135000
H	-4.771834000	-2.595649000	0.488330000

H	-4.769959000	2.126383000	-0.778075000
H	-5.503214000	1.938544000	-0.744156000
H	4.348651000	3.374282000	0.570379000
H	4.575866000	4.101981000	0.613929000
H	-3.346090000	4.120573000	-2.939453000
H	-3.273473000	3.633320000	-2.357902000
H	-5.228275000	1.018810000	2.652881000
H	-4.476636000	0.953977000	2.720573000
H	-3.945909000	-3.019277000	-1.945441000
H	-4.093308000	-3.550625000	-2.465951000
H	0.785306000	5.050942000	-1.545464000
H	0.622463000	5.763564000	-1.344159000

$Ca_{12}O_{12}\cdot 17H_2$, ωB97XD/6-31++G(d,p)

Energy: -9055.197111 E_h

O	0.094751000	3.143352000	-1.658287000
O	2.588207000	2.470484000	0.213174000
O	2.203192000	0.079281000	-2.827823000
O	0.904717000	-2.738698000	-2.107407000
O	3.295810000	-1.329960000	0.632345000
O	1.784910000	-0.004996000	3.111868000
O	-0.002366000	-3.139123000	1.662528000
O	-2.109808000	-0.093272000	2.835369000
O	-2.491977000	-2.492513000	-0.219492000
O	-3.193810000	1.312868000	-0.629093000
O	-0.802727000	2.722512000	2.106079000
O	-1.683691000	-0.007918000	-3.107443000
Ca	-0.182282000	0.980277000	3.411470000
Ca	1.869973000	-2.092006000	2.237991000
Ca	3.195411000	0.769453000	1.503609000
Ca	-2.009700000	-2.146062000	1.977793000

Ca	-0.474501000	-3.480770000	-0.536290000
Ca	2.814364000	-1.658296000	-1.514021000
Ca	0.282306000	-0.994889000	-3.413396000
Ca	-3.103552000	-0.781976000	-1.509260000
Ca	2.110712000	2.126057000	-1.970220000
Ca	-1.770976000	2.077615000	-2.233556000
Ca	0.576484000	3.476530000	0.539852000
Ca	-2.716751000	1.650759000	1.513793000
H	-3.513539000	-0.073122000	-4.206513000
H	-4.239110000	-0.145457000	-4.429692000
H	4.335501000	0.264138000	4.402669000
H	3.610616000	0.151692000	4.191488000
H	-2.909400000	3.955616000	3.606123000
H	-2.260300000	3.728621000	3.273838000
H	3.013094000	-3.928106000	-3.641017000
H	2.363948000	-3.714248000	-3.300180000
H	-0.464300000	-5.949284000	1.370352000
H	-0.317275000	-5.233717000	1.593931000
H	1.259773000	4.637166000	-2.669490000
H	1.820833000	5.020049000	-3.015142000
H	2.558918000	-0.803803000	-5.520938000
H	2.603148000	-0.510774000	-4.816426000
H	-2.478743000	0.568666000	4.838238000
H	-2.414716000	0.881642000	5.530531000
H	4.553626000	-2.516765000	1.904305000
H	4.816885000	-2.965721000	2.461233000
H	-3.983624000	-4.453751000	1.286864000
H	-3.659686000	-3.999105000	0.768226000
H	-5.284138000	0.613581000	-0.287884000
H	-5.924443000	0.213269000	-0.222886000
H	3.152153000	4.505052000	0.428746000

H	3.155263000	5.262197000	0.528370000
H	-4.726791000	2.968043000	-2.435498000
H	-4.459101000	2.515682000	-1.883932000
H	-5.020508000	-0.613166000	3.211629000
H	-4.277626000	-0.465844000	3.194760000
H	-3.385337000	-3.683454000	-1.879353000
H	-3.656509000	-3.972189000	-2.525547000
H	-0.936350000	5.090069000	-1.325300000
H	-1.262542000	5.715048000	-1.046436000
H	6.027458000	-0.299205000	0.130916000
H	5.375391000	-0.672808000	0.234167000

$Ca_{12}O_{12}\cdot 18H_2$, ωB97XD/6-31++G(d,p)

Energy: -9056.363450 E_h

O	0.530884000	3.192277000	-1.451552000
O	2.562422000	2.331232000	0.849126000
O	2.703771000	0.071983000	-2.322941000
O	1.162372000	-2.699393000	-1.994841000
O	3.011963000	-1.513084000	1.222341000
O	1.091292000	-0.210230000	3.409478000
O	-0.499545000	-3.196878000	1.496471000
O	-2.671261000	-0.090913000	2.363670000
O	-2.529271000	-2.360593000	-0.815606000
O	-2.974452000	1.494464000	-1.175403000
O	-1.126466000	2.680130000	2.039871000
O	-1.054893000	0.191591000	-3.361387000
Ca	-0.853654000	0.860696000	3.357607000
Ca	1.262138000	-2.263897000	2.475285000
Ca	2.826037000	0.552289000	2.148943000
Ca	-2.484785000	-2.115693000	1.449885000
Ca	-0.530486000	-3.440392000	-0.765970000

Ca	2.960936000	-1.745439000	-0.988044000
Ca	0.888484000	-0.883537000	-3.318109000
Ca	-2.791528000	-0.569025000	-2.105556000
Ca	2.526918000	2.095459000	-1.401129000
Ca	-1.227396000	2.245187000	-2.429942000
Ca	0.567843000	3.420249000	0.812167000
Ca	-2.929523000	1.732773000	1.033992000
H	-2.639034000	0.158981000	-4.787934000
H	-3.312849000	0.088316000	-5.138902000
H	3.347714000	-0.047814000	5.173369000
H	2.673217000	-0.136097000	4.826562000
H	-3.411044000	4.083899000	3.050181000
H	-2.724388000	3.803343000	2.868676000
H	3.455154000	-4.108902000	-2.974064000
H	2.766128000	-3.828129000	-2.801440000
H	-0.951768000	-5.980992000	0.998603000
H	-0.838580000	-5.278676000	1.276835000
H	1.916218000	4.626723000	-2.249538000
H	2.545421000	4.978619000	-2.496640000
H	3.541428000	-0.894156000	-4.908006000
H	3.466443000	-0.589794000	-4.213085000
H	-3.422058000	0.567901000	4.262084000
H	-3.490862000	0.870875000	4.958145000
H	3.950117000	-2.764202000	2.687836000
H	4.084529000	-3.232396000	3.274202000
H	-4.431417000	-4.226176000	0.302793000
H	-3.979683000	-3.790681000	-0.129512000
H	-5.126358000	0.909386000	-1.242753000
H	-5.793257000	0.553794000	-1.297190000
H	3.154043000	4.340697000	1.182787000
H	3.168396000	5.097567000	1.283866000

H	-4.045987000	3.240560000	-3.210803000
H	-3.912443000	2.767555000	-2.628504000
H	-5.612725000	-0.500044000	2.129232000
H	-4.877184000	-0.381223000	2.266020000
H	-2.858509000	-3.742931000	-2.528801000
H	-2.817752000	-4.222603000	-3.114351000
H	-0.451555000	5.178887000	-1.265508000
H	-0.802432000	5.813109000	-1.042953000
H	5.865180000	-0.669414000	1.207460000
H	5.176519000	-0.985386000	1.206463000
H	5.565840000	0.835460000	-2.125847000
H	4.869331000	0.565812000	-2.255665000

$Ca_{12}O_{12}\cdot 19H_2$, ωB97XD/6-31++G(d,p)

Energy: -9057.529631 E_h

O	-0.479462000	-2.322760000	-2.653651000
O	-2.592552000	-2.445800000	-0.272290000
O	-2.615400000	0.920097000	-2.211186000
O	-1.090572000	3.294932000	-0.712412000
O	-3.060446000	0.903521000	1.659569000
O	-1.218122000	-1.233716000	3.149244000
O	0.446509000	2.249591000	2.720988000
O	2.579841000	-0.971866000	2.278978000
O	2.553471000	2.411553000	0.337674000
O	3.025922000	-0.951026000	-1.585460000
O	1.050434000	-3.337969000	0.782306000
O	1.172621000	1.171996000	-3.072997000
Ca	0.723402000	-2.220017000	2.721222000
Ca	-1.351771000	1.023723000	3.163647000
Ca	-2.913506000	-1.368479000	1.639313000
Ca	2.431207000	1.251510000	2.292101000

Ca	0.563316000	3.407813000	0.768906000
Ca	-2.926834000	2.027658000	-0.255729000
Ca	-0.763063000	2.169953000	-2.661728000
Ca	2.875882000	1.320037000	-1.576437000
Ca	-2.471542000	-1.306129000	-2.218755000
Ca	1.316960000	-1.082530000	-3.085956000
Ca	-0.604177000	-3.464620000	-0.691376000
Ca	2.892265000	-2.085343000	0.324180000
H	2.765230000	1.752120000	-4.373636000
H	3.435630000	1.944210000	-4.681333000
H	-3.488000000	-2.125777000	4.660457000
H	-2.813554000	-1.898942000	4.384067000
H	3.323966000	-4.998907000	1.335901000
H	2.638388000	-4.680830000	1.227227000
H	-3.436611000	4.938425000	-1.083386000
H	-2.738533000	4.637974000	-1.025916000
H	0.950070000	4.974364000	3.426467000
H	0.818076000	4.222656000	3.388874000
H	-1.855911000	-3.368351000	-3.934843000
H	-2.481017000	-3.611242000	-4.296352000
H	-3.373586000	2.795162000	-4.265001000
H	-3.314053000	2.251669000	-3.733919000
H	3.237881000	-2.269225000	3.837976000
H	3.279261000	-2.802311000	4.381941000
H	-4.031790000	1.411444000	3.504055000
H	-4.176723000	1.580299000	4.233129000
H	4.288832000	3.791339000	2.198284000
H	3.881823000	3.528977000	1.610540000
H	5.166474000	-0.386389000	-1.319552000
H	5.824110000	-0.029537000	-1.198461000
H	-3.196332000	-4.442292000	-0.663758000

H	-3.211547000	-5.188049000	-0.827839000
H	4.169288000	-1.591023000	-4.162127000
H	4.015798000	-1.431437000	-3.433201000
H	5.484842000	-0.322583000	2.413705000
H	4.769837000	-0.572472000	2.429787000
H	3.217731000	4.128370000	-0.937604000
H	3.396143000	4.612618000	-1.491984000
H	0.563265000	-4.190185000	-3.281083000
H	0.938015000	-4.846158000	-3.342213000
H	-5.869196000	0.025035000	1.271805000
H	-5.204164000	0.367048000	1.396046000
H	-5.474067000	0.117459000	-2.414643000
H	-4.784522000	0.431753000	-2.404539000
H	-0.017621000	5.341520000	-2.569531000
H	-0.318166000	4.923309000	-2.013226000

$Ca_{12}O_{12}\cdot 20H_2$, ωB97XD/6-31++G(d,p)

Energy: -9058.695260 E_h

O	0.734887000	-2.762395000	2.076057000
O	2.662214000	-2.350754000	-0.435642000
O	2.727697000	0.580356000	2.147020000
O	1.026332000	3.131325000	1.271358000
O	2.853735000	1.336129000	-1.667465000
O	0.954742000	-0.521578000	-3.429521000
O	-0.760207000	2.727045000	-2.159277000
O	-2.758127000	-0.605503000	-2.217542000
O	-2.678534000	2.329216000	0.355206000
O	-2.874690000	-1.369147000	1.586384000
O	-1.039034000	-3.148212000	-1.365460000
O	-0.977379000	0.500640000	3.337539000
Ca	-0.919888000	-1.655835000	-3.062492000

Ca	1.025466000	1.695624000	-2.980452000
Ca	2.771073000	-0.891364000	-2.111586000
Ca	-2.673043000	1.576943000	-1.793468000
Ca	-0.753861000	3.480221000	-0.014056000
Ca	2.848883000	2.068256000	0.431607000
Ca	0.895799000	1.637923000	2.984638000
Ca	-2.798339000	0.863095000	2.024187000
Ca	2.656297000	-1.598423000	1.711289000
Ca	-1.046751000	-1.715866000	2.900840000
Ca	0.730877000	-3.500766000	-0.073193000
Ca	-2.866631000	-2.099692000	-0.512988000
H	-2.490266000	0.872671000	4.783460000
H	-3.149731000	1.023368000	5.137214000
H	3.141586000	-1.027138000	-5.207964000
H	2.477578000	-0.879169000	-4.860574000
H	-3.292506000	-4.770878000	-2.084598000
H	-2.612769000	-4.445916000	-1.960903000
H	2.563590000	5.381284000	0.071982000
H	2.113062000	4.894374000	0.438460000
H	-1.552507000	5.482647000	-2.322176000
H	-1.354507000	4.752886000	-2.425176000
H	2.217650000	-3.965874000	3.075806000
H	2.867270000	-4.244498000	3.358752000
H	3.081482000	0.192785000	5.073451000
H	3.106528000	0.263260000	4.319100000
H	-3.497675000	-1.550674000	-3.986836000
H	-3.560590000	-1.951522000	-4.632583000
H	3.679043000	2.260436000	-3.413997000
H	3.772173000	2.586557000	-4.096747000
H	-4.658094000	3.840926000	-1.115044000
H	-4.186722000	3.527028000	-0.605596000

H	-5.042732000	-0.829788000	1.597203000
H	-5.709355000	-0.469440000	1.602375000
H	3.300681000	-4.404639000	-0.281988000
H	3.318645000	-5.160908000	-0.193505000
H	-3.791872000	-2.596174000	4.036513000
H	-3.699935000	-2.279924000	3.349460000
H	-5.713055000	-0.610787000	-1.825119000
H	-4.980804000	-0.589488000	-2.017319000
H	-3.021186000	4.103920000	1.664539000
H	-2.966450000	4.735121000	2.080665000
H	-0.231370000	-4.734648000	2.470609000
H	-0.609722000	-5.391055000	2.481125000
H	5.744713000	0.627346000	-1.495620000
H	5.045512000	0.910505000	-1.562932000
H	4.890288000	2.420153000	2.715147000
H	4.365395000	1.868645000	2.699181000
H	1.968352000	4.483873000	3.651343000
H	1.747334000	4.263018000	2.956863000
H	4.837480000	-2.331618000	0.059496000
H	5.512772000	-2.235949000	0.390183000

$Ca_{12}O_{12}\cdot 21H_2$, ωB97XD/6-31++G(d,p)

Energy: -9059.861521 E_h

O	1.256084000	0.404975000	3.308204000
O	3.195464000	-1.000564000	1.200065000
O	2.284809000	2.688785000	0.325052000
O	0.037264000	2.977219000	-1.919999000
O	2.516575000	0.022935000	-2.502951000
O	1.351274000	-2.837668000	-1.700111000
O	-1.270079000	-0.433678000	-3.286566000
O	-2.298543000	-2.719209000	-0.316647000

O	-3.217188000	0.967132000	-1.190437000
O	-2.539691000	-0.056144000	2.515241000
O	-0.059303000	-3.001925000	1.931018000
O	-1.360347000	2.791690000	1.707088000
Ca	-0.181902000	-3.560525000	-0.257985000
Ca	0.787892000	-1.263727000	-3.241783000
Ca	3.069732000	-1.544556000	-0.953532000
Ca	-2.835883000	-1.183165000	-1.835875000
Ca	-1.641080000	1.714288000	-2.641269000
Ca	2.142772000	2.119142000	-1.864762000
Ca	0.168692000	3.536539000	0.281180000
Ca	-3.087490000	1.514416000	0.962755000
Ca	2.825534000	1.151192000	1.842999000
Ca	-0.809222000	1.231715000	3.246855000
Ca	1.620259000	-1.746335000	2.654859000
Ca	-2.165938000	-2.152729000	1.877313000
H	-3.043441000	3.825474000	2.503680000
H	-3.747389000	4.044420000	2.700500000
H	3.805032000	-4.036096000	-2.653480000
H	3.091301000	-3.840065000	-2.473913000
H	-1.739969000	-4.999002000	3.144412000
H	-1.183056000	-4.563539000	2.857597000
H	1.708407000	4.553088000	-3.667244000
H	1.150895000	4.240039000	-3.252056000
H	-2.702896000	0.816476000	-5.429517000
H	-2.324640000	0.360344000	-4.947794000
H	2.054864000	2.109937000	4.485720000
H	2.390728000	2.737470000	4.747307000
H	2.566102000	5.565340000	0.163324000
H	2.639375000	4.808874000	0.211984000
H	-2.611308000	-4.843102000	-0.400741000

H	-2.511230000	-5.598170000	-0.421631000
H	3.257879000	-0.778828000	-4.361565000
H	3.334818000	-1.157320000	-5.017830000
H	-5.350791000	0.221148000	-3.006190000
H	-4.868809000	0.549590000	-2.516915000
H	-4.764686000	-0.263400000	2.473586000
H	-5.503775000	-0.231901000	2.309848000
H	4.137986000	-2.968862000	1.703164000
H	4.317943000	-3.674572000	1.911415000
H	-3.331518000	1.127477000	5.030589000
H	-3.263079000	0.746892000	4.374089000
H	-5.240306000	-2.996736000	0.098858000
H	-4.492347000	-3.007791000	-0.019595000
H	-4.194509000	2.935419000	-1.632291000
H	-4.399997000	3.645638000	-1.795363000
H	2.288978000	-0.463993000	4.979100000
H	2.650678000	-0.944096000	5.447385000
H	5.479861000	0.260603000	-2.304881000
H	4.739322000	0.268959000	-2.464468000
H	5.259239000	2.822175000	0.262288000
H	4.505951000	2.896285000	0.229494000
H	-1.268283000	5.616203000	-1.667855000
H	-0.956385000	4.957876000	-1.879377000
H	4.847315000	-0.602778000	2.549112000
H	5.328848000	-0.284372000	3.044331000
H	0.292912000	-4.456550000	-3.953205000
H	0.612098000	-4.152054000	-3.336594000

$Ca_{12}O_{12}\cdot 22H_2$, ωB97XD/6-31++G(d,p)

Energy: -9061.027879 E_h

O	1.045026000	2.956308000	-1.743525000
O	3.079744000	1.759862000	0.403842000
O	2.372136000	-0.616320000	-2.596544000
O	0.306350000	-2.957599000	-1.925092000
O	2.686140000	-2.059213000	1.015924000
O	1.366890000	-0.237547000	3.280190000
O	-1.045264000	-2.886457000	1.741279000
O	-2.366475000	0.676906000	2.577427000
O	-3.064611000	-1.710837000	-0.428090000
O	-2.697342000	2.111080000	-1.029059000
O	-0.291007000	3.001180000	1.911705000
O	-1.347885000	0.302669000	-3.279409000
Ca	-0.293334000	1.243275000	3.334740000
Ca	0.974250000	-2.332030000	2.482224000
Ca	3.077733000	0.037349000	1.806413000
Ca	-2.742019000	-1.374998000	1.798566000
Ca	-1.369854000	-3.214506000	-0.487466000
Ca	2.371775000	-2.380339000	-1.160961000
Ca	0.296712000	-1.183985000	-3.349142000
Ca	-3.077937000	0.017517000	-1.830943000
Ca	2.736392000	1.434597000	-1.816705000
Ca	-0.972010000	2.385283000	-2.487519000
Ca	1.382310000	3.276830000	0.480589000
Ca	-2.356402000	2.437312000	1.143286000
H	-3.017022000	0.566265000	-4.579776000
H	-3.714531000	0.638932000	-4.879597000
H	3.207094000	1.528343000	4.813427000
H	2.690858000	1.053297000	4.526436000
H	-2.135783000	4.866462000	3.068593000

H	-1.538982000	4.450507000	2.836473000
H	2.226368000	-4.780465000	-3.099518000
H	1.616503000	-4.386736000	-2.869617000
H	-2.196956000	-5.500568000	1.395774000
H	-1.894445000	-4.844322000	1.639245000
H	2.625685000	4.025343000	-2.732357000
H	3.288237000	4.224504000	-3.051610000
H	2.684686000	-1.820465000	-5.203552000
H	2.755964000	-1.486261000	-4.522634000
H	-2.755273000	1.546106000	4.495023000
H	-2.683753000	1.880053000	5.176636000
H	2.933070000	-4.222538000	1.491031000
H	2.861085000	-4.940549000	1.723336000
H	-5.120152000	-3.245078000	0.949641000
H	-4.652868000	-2.892272000	0.464073000
H	-4.920146000	1.971453000	-0.820021000
H	-5.643128000	1.748624000	-0.779707000
H	4.094981000	3.645763000	0.616750000
H	4.255034000	4.387080000	0.688945000
H	-3.579976000	3.956602000	-3.063483000
H	-3.488397000	3.493393000	-2.465259000
H	-5.351072000	0.806106000	2.607128000
H	-4.597657000	0.820636000	2.681074000
H	-4.153241000	-2.670389000	-2.128442000
H	-4.459886000	-2.875311000	-2.790131000
H	0.481056000	5.114224000	-1.644993000
H	0.266992000	5.818822000	-1.466633000
H	5.139750000	-2.127408000	2.580548000
H	4.529026000	-2.265224000	2.148248000
H	5.215980000	-1.487322000	-2.472184000
H	4.533789000	-1.188645000	-2.611547000

H	-1.244510000	-3.984353000	-4.249492000
H	-0.839449000	-3.843910000	-3.624836000
H	5.200022000	1.400789000	-0.188431000
H	5.860866000	1.213919000	-0.507928000
H	2.495774000	-2.115832000	5.178486000
H	2.246582000	-1.516340000	4.780868000
H	-2.246281000	-3.301768000	4.430750000
H	-1.877829000	-3.307833000	3.768442000

$Ca_{12}O_{12}\cdot 23H_2$, ωB97XD/6-31++G(d,p)

Energy: -9062.193578 E_h

O	-1.813179000	2.085929000	-2.267681000
O	-3.447191000	-0.308292000	-0.930167000
O	-2.133800000	2.320929000	1.616218000
O	0.489619000	1.422651000	3.199292000
O	-2.035940000	-1.462447000	2.525839000
O	-1.236699000	-3.352634000	0.084573000
O	1.787175000	-2.127622000	2.215364000
O	2.109774000	-2.355323000	-1.661915000
O	3.412982000	0.276963000	0.891573000
O	2.027779000	1.430465000	-2.571276000
O	-0.512257000	-1.452328000	-3.230031000
O	1.198811000	3.312265000	-0.132688000
Ca	-0.033721000	-3.119346000	-1.776629000
Ca	-0.305025000	-2.870293000	2.104059000
Ca	-2.961627000	-1.937944000	0.501064000
Ca	3.013307000	-1.886653000	0.315331000
Ca	2.182228000	0.040867000	2.785825000
Ca	-1.649187000	0.654156000	3.080808000
Ca	0.006772000	3.088892000	1.728665000
Ca	2.944533000	1.910123000	-0.544088000

Ca	-3.033712000	1.856536000	-0.362958000
Ca	0.280215000	2.826011000	-2.150614000
Ca	-2.213623000	-0.084528000	-2.829053000
Ca	1.624121000	-0.685602000	-3.120443000
H	2.853654000	4.652467000	-0.497499000
H	3.540166000	4.941366000	-0.654663000
H	-2.844795000	-4.986998000	-1.816820000
H	-2.486983000	-4.633006000	-1.250552000
H	0.759964000	-2.349448000	-5.639981000
H	0.299815000	-2.174668000	-5.056459000
H	-0.861761000	2.251878000	5.620458000
H	-0.382821000	2.101328000	5.047799000
H	3.594173000	-2.143312000	4.455880000
H	3.127956000	-2.293457000	3.871686000
H	-2.746872000	4.106620000	-2.100380000
H	-3.111185000	4.731391000	-1.874206000
H	-2.166055000	4.761478000	3.190518000
H	-2.312365000	4.122987000	2.803136000
H	2.288094000	-4.155353000	-2.827338000
H	2.141111000	-4.798723000	-3.207845000
H	-1.684338000	-2.244783000	4.584474000
H	-1.420459000	-2.566231000	5.218105000
H	5.788914000	-1.249993000	1.584136000
H	5.250261000	-0.729635000	1.450448000
H	4.212135000	1.368992000	-3.049150000
H	4.969255000	1.357690000	-3.023192000
H	-4.596987000	-1.646923000	-2.308279000
H	-4.844364000	-2.085436000	-2.874231000
H	2.446443000	3.856773000	-4.085694000
H	2.468043000	3.170829000	-3.754932000
H	4.898828000	-2.159428000	-2.700892000

H	4.189472000	-2.289617000	-2.469725000
H	4.613274000	1.705321000	2.135317000
H	4.907392000	2.214293000	2.612195000
H	-3.224593000	2.239923000	-3.879309000
H	-3.712774000	2.085313000	-4.443413000
H	-4.359294000	-3.127461000	2.972904000
H	-3.734954000	-2.692986000	3.013224000
H	-4.724584000	1.979765000	3.023472000
H	-4.102959000	2.172690000	2.634570000
H	2.207037000	3.704089000	4.060441000
H	1.805435000	3.069301000	3.963798000
H	-5.292861000	0.705198000	-1.428714000
H	-5.833150000	1.229509000	-1.539927000
H	-1.900498000	-5.553983000	1.862273000
H	-1.799486000	-5.060562000	1.291877000
H	2.987011000	-4.824410000	1.870461000
H	2.658397000	-4.172560000	2.074632000
H	0.328513000	5.318258000	-0.580383000
H	-0.053419000	5.922708000	-0.830355000

$Ca_{12}O_{12}\cdot 24H_2$, ωB97XD/6-31++G(d,p)

Energy: -9063.361165 E_h

O	0.002414000	3.182308000	1.594094000
O	-0.002414000	3.182308000	-1.594094000
O	-3.179028000	1.593726000	-0.009096000
O	-3.179028000	-1.593726000	0.009096000
O	-1.592375000	-0.012865000	-3.178791000
O	1.592375000	0.012865000	-3.178791000
O	0.002414000	-3.182308000	-1.594094000
O	3.179028000	-1.593726000	-0.009096000
O	-0.002414000	-3.182308000	1.594094000

O	1.592375000	-0.012865000	3.178791000
O	3.179028000	1.593726000	0.009096000
O	-1.592375000	0.012865000	3.178791000
Ca	3.178744000	0.006112000	-1.620762000
Ca	0.008039000	-1.620901000	-3.174744000
Ca	-0.008039000	1.620901000	-3.174744000
Ca	1.621528000	-3.178793000	0.005100000
Ca	-1.621528000	-3.178793000	-0.005100000
Ca	-3.178744000	-0.006112000	-1.620762000
Ca	-3.178744000	0.006112000	1.620762000
Ca	-0.008039000	-1.620901000	3.174744000
Ca	-1.621528000	3.178793000	0.005100000
Ca	0.008039000	1.620901000	3.174744000
Ca	1.621528000	3.178793000	-0.005100000
Ca	3.178744000	-0.006112000	1.620762000
H	-1.695350000	-0.776818000	5.174768000
H	-1.577348000	-1.181316000	5.809643000
H	3.202214000	2.048826000	-4.657441000
H	2.819577000	1.476687000	-4.342024000
H	4.706335000	2.889290000	2.219183000
H	4.370184000	2.646709000	1.585010000
H	-5.848636000	-1.543730000	-1.113199000
H	-5.202360000	-1.669937000	-0.731023000
H	-2.215350000	-4.801571000	-2.748818000
H	-1.575747000	-4.439790000	-2.564479000
H	-1.575747000	4.439790000	2.564479000
H	-2.215350000	4.801571000	2.748818000
H	-5.848636000	1.543730000	1.113199000
H	-5.202360000	1.669937000	0.731023000
H	4.370184000	-2.646709000	-1.585010000
H	4.706335000	-2.889290000	-2.219183000

H	-2.819577000	-1.476687000	-4.342024000
H	-3.202214000	-2.048826000	-4.657441000
H	2.215350000	-4.801571000	2.748818000
H	1.575747000	-4.439790000	2.564479000
H	2.819577000	-1.476687000	4.342024000
H	3.202214000	-2.048826000	4.657441000
H	1.575747000	4.439790000	-2.564479000
H	2.215350000	4.801571000	-2.748818000
H	1.577348000	1.181316000	5.809643000
H	1.695350000	0.776818000	5.174768000
H	5.848636000	-1.543730000	1.113199000
H	5.202360000	-1.669937000	0.731023000
H	-0.789338000	-5.186154000	1.693942000
H	-1.187395000	-5.824003000	1.573220000
H	0.789338000	5.186154000	1.693942000
H	1.187395000	5.824003000	1.573220000
H	-1.577348000	1.181316000	-5.809643000
H	-1.695350000	0.776818000	-5.174768000
H	-4.706335000	2.889290000	-2.219183000
H	-4.370184000	2.646709000	-1.585010000
H	-4.706335000	-2.889290000	2.219183000
H	-4.370184000	-2.646709000	1.585010000
H	-0.789338000	5.186154000	-1.693942000
H	-1.187395000	5.824003000	-1.573220000
H	1.577348000	-1.181316000	-5.809643000
H	1.695350000	-0.776818000	-5.174768000
H	1.187395000	-5.824003000	-1.573220000
H	0.789338000	-5.186154000	-1.693942000
H	-2.819577000	1.476687000	4.342024000
H	-3.202214000	2.048826000	4.657441000
H	5.848636000	1.543730000	-1.113199000

H	5.202360000	1.669937000	-0.731023000

(H_2@$Ca_{12}O_{12}$)·24H_2, ωB97XD/6-31++G(d,p)

Energy: -9064.530438 E_h

O	0.075117000	-3.187194000	1.597234000
O	0.070724000	-3.194209000	-1.593419000
O	3.222616000	-1.520664000	-0.015688000
O	3.113158000	1.658692000	0.000063000
O	1.588454000	0.039358000	-3.181280000
O	-1.599052000	-0.049660000	-3.175938000
O	-0.076040000	3.189073000	-1.603661000
O	-3.222872000	1.520662000	-0.009752000
O	-0.070014000	3.192291000	1.586975000
O	-1.589893000	-0.015856000	3.176728000
O	-3.113156000	-1.658670000	0.015297000
O	1.600231000	0.026112000	3.171578000
Ca	-3.188951000	-0.080140000	-1.620137000
Ca	-0.044216000	1.612041000	-3.168969000
Ca	0.033691000	-1.622279000	-3.163756000
Ca	-1.692541000	3.133648000	-0.002577000
Ca	1.545417000	3.233633000	-0.013480000
Ca	3.183593000	0.074925000	-1.630975000
Ca	3.186475000	0.064244000	1.615801000
Ca	-0.021054000	1.623565000	3.159937000
Ca	1.692447000	-3.133663000	0.002111000
Ca	0.031400000	-1.613295000	3.165168000
Ca	-1.545518000	-3.233655000	0.002125000
Ca	-3.181278000	-0.058997000	1.626473000
H	1.635275000	0.784738000	5.184087000
H	1.492329000	1.175276000	5.822408000
H	-3.512185000	-1.911989000	-4.494422000

H	-2.993063000	-1.414876000	-4.254798000
H	-4.659533000	-2.950062000	2.221905000
H	-4.313769000	-2.717471000	1.589341000
H	5.824614000	1.619792000	-1.058366000
H	5.168376000	1.746608000	-0.695217000
H	2.083607000	4.854360000	-2.792974000
H	1.457034000	4.476895000	-2.594620000
H	1.664781000	-4.423841000	2.556930000
H	2.307604000	-4.780612000	2.740849000
H	5.891628000	-1.373986000	1.099391000
H	5.249981000	-1.525401000	0.718315000
H	-4.452148000	2.546974000	-1.569468000
H	-4.802038000	2.783468000	-2.198614000
H	2.980067000	1.401822000	-4.267532000
H	3.498979000	1.898140000	-4.509226000
H	-2.298898000	4.789097000	2.733085000
H	-1.656636000	4.431882000	2.548092000
H	-2.803291000	1.442849000	4.360919000
H	-3.167809000	2.020385000	4.687841000
H	-1.464884000	-4.484549000	-2.577072000
H	-2.091830000	-4.862386000	-2.773507000
H	-1.478927000	-1.162994000	5.827860000
H	-1.622585000	-0.772699000	5.189522000
H	-5.888544000	1.376058000	1.113491000
H	-5.248080000	1.526643000	0.730095000
H	0.684689000	5.211041000	1.668694000
H	1.076460000	5.851137000	1.538586000
H	-0.677500000	-5.206874000	1.685046000
H	-1.069043000	-5.847544000	1.557179000
H	1.504377000	-1.102074000	-5.837172000
H	1.636928000	-0.708490000	-5.198472000

H	4.794781000	-2.789938000	-2.205755000
H	4.446852000	-2.551727000	-1.576165000
H	4.665585000	2.956378000	2.199141000
H	4.318171000	2.722268000	1.568057000
H	0.862997000	-5.203754000	-1.617995000
H	1.260425000	-5.836393000	-1.472021000
H	-1.524172000	1.086119000	-5.834678000
H	-1.654625000	0.693747000	-5.194804000
H	-1.263022000	5.832847000	-1.483417000
H	-0.866727000	5.199558000	-1.629590000
H	2.823706000	-1.426034000	4.353702000
H	3.194009000	-2.000530000	4.679464000
H	-5.826984000	-1.624280000	-1.037258000
H	-5.169970000	-1.749700000	-0.675026000
H	-0.334467000	-0.166391000	-0.001073000
H	0.333998000	0.166485000	-0.004297000

$Ca_{12}O_{12}\cdot 25H_2$, ωB97XD/6-31++G(d,p)

Energy: -9064.527427 E_h

O	2.278113000	1.501104000	-2.319614000
O	3.024438000	1.764293000	0.771856000
O	2.991314000	-1.898230000	-0.541889000
O	0.359969000	-3.534919000	0.216418000
O	1.594469000	-1.101457000	3.004741000
O	-0.037817000	1.633267000	3.160047000
O	-2.210511000	-1.496004000	2.317164000
O	-2.929279000	1.899828000	0.560203000
O	-2.970095000	-1.770856000	-0.770306000
O	-1.546053000	1.088380000	-2.993874000
O	-0.305395000	3.532232000	-0.232348000
O	0.119968000	-1.622160000	-3.163233000

Ca	-1.229737000	2.851015000	1.732035000
Ca	-0.560688000	-0.559616000	3.472217000
Ca	2.115641000	1.091722000	2.685186000
Ca	-3.425248000	-0.247969000	0.850169000
Ca	-1.748360000	-3.015894000	0.693900000
Ca	2.048619000	-2.582314000	1.408987000
Ca	1.301059000	-2.848047000	-1.733607000
Ca	-2.043431000	-1.100683000	-2.684272000
Ca	3.486176000	0.245529000	-0.859108000
Ca	0.619125000	0.571663000	-3.469307000
Ca	1.808043000	3.014215000	-0.685323000
Ca	-2.003110000	2.579920000	-1.403959000
H	-0.947238000	-2.237022000	-4.928147000
H	-1.490416000	-2.380056000	-5.442708000
H	1.332777000	4.056186000	4.228658000
H	0.908540000	3.462890000	4.024893000
H	-0.569238000	5.345442000	-2.579743000
H	-0.439011000	4.976701000	-1.930613000
H	2.079197000	-5.682215000	1.130039000
H	1.543670000	-5.232392000	0.829421000
H	-2.203852000	-4.134432000	3.685371000
H	-2.257959000	-3.412261000	3.461796000
H	3.917747000	0.729100000	-3.633249000
H	4.510398000	0.358472000	-3.925539000
H	4.027586000	-4.333189000	-1.724577000
H	3.899635000	-3.677577000	-1.359382000
H	-4.030489000	2.528818000	2.401539000
H	-4.249386000	2.756789000	3.090297000
H	1.230883000	-2.759000000	4.462362000
H	0.983875000	-3.315052000	4.913072000
H	-5.265845000	-1.309455000	-2.560411000

H	-4.762566000	-1.483447000	-2.019442000
H	-3.610836000	1.680308000	-3.603413000
H	-4.315397000	1.955409000	-3.648751000
H	3.490040000	3.838871000	1.465154000
H	3.507931000	4.587646000	1.579668000
H	-1.203759000	1.347934000	-5.855901000
H	-1.439937000	1.324023000	-5.132097000
H	-4.419395000	4.240592000	-0.308887000
H	-4.129899000	3.625140000	0.031747000
H	-4.319761000	-3.384794000	-0.267575000
H	-4.644440000	-4.005234000	0.030448000
H	3.567965000	3.171673000	-2.790105000
H	3.935428000	3.838207000	-2.780678000
H	3.070099000	-0.204824000	5.326433000
H	2.680599000	-0.578570000	4.788995000
H	5.347665000	-2.418516000	1.203643000
H	4.832832000	-2.286452000	0.663467000
H	-0.419962000	-5.700561000	-1.674577000
H	-0.248800000	-5.230525000	-1.105348000
H	5.105971000	2.119389000	0.327013000
H	5.806311000	2.090038000	0.029676000
H	-0.384593000	1.202757000	5.996775000
H	-0.264268000	1.465408000	5.291742000
H	-4.991441000	-1.742278000	3.096513000
H	-4.235563000	-1.769350000	3.012085000
H	1.669861000	-1.922024000	-4.748339000
H	2.248163000	-1.909272000	-5.236934000
H	-1.456039000	5.870293000	1.031357000
H	-1.110575000	5.355752000	0.589098000
H	-6.399131000	-0.135424000	0.433997000
H	-6.202118000	-0.638535000	-0.080490000

$Ca_{12}O_{12}\cdot 26H_2$, ωB97XD/6-31++G(d,p)

Energy: -9065.693717 E_h

O	2.328837000	1.519315000	-2.210634000
O	2.871315000	1.909818000	0.909026000
O	3.061283000	-1.793908000	-0.289095000
O	0.450181000	-3.512184000	0.353686000
O	1.407733000	-0.947702000	3.132716000
O	-0.332727000	1.721962000	3.102325000
O	-2.326811000	-1.519733000	2.224627000
O	-3.057134000	1.794975000	0.320584000
O	-2.873644000	-1.911887000	-0.893761000
O	-1.423283000	0.934831000	-3.112985000
O	-0.455094000	3.510678000	-0.359800000
O	0.352126000	-1.710769000	-3.094857000
Ca	-1.476393000	2.852594000	1.564066000
Ca	-0.790724000	-0.480707000	3.446942000
Ca	1.863547000	1.254701000	2.779431000
Ca	-3.489137000	-0.362015000	0.644749000
Ca	-1.702512000	-3.065802000	0.681996000
Ca	2.020900000	-2.458591000	1.619427000
Ca	1.486666000	-2.842801000	-1.554053000
Ca	-1.855214000	-1.262430000	-2.767370000
Ca	3.492888000	0.360117000	-0.638275000
Ca	0.786094000	0.491867000	-3.434719000
Ca	1.701182000	3.063706000	-0.661985000
Ca	-2.036051000	2.453659000	-1.603654000
H	-0.576864000	-2.396927000	-4.912956000
H	-1.080095000	-2.568316000	-5.458435000
H	0.514989000	4.407441000	4.090942000
H	0.276899000	3.709899000	3.917517000
H	-0.647273000	5.224173000	-2.788316000

H	-0.540155000	4.886609000	-2.118360000
H	2.206883000	-5.565773000	1.408414000
H	1.670612000	-5.144834000	1.070071000
H	-2.284432000	-4.106656000	3.690081000
H	-2.357414000	-3.396943000	3.434425000
H	4.070905000	0.786177000	-3.408527000
H	4.691379000	0.433804000	-3.662843000
H	4.266809000	-4.186631000	-1.400014000
H	4.090156000	-3.536191000	-1.046089000
H	-4.311529000	2.411083000	2.065528000
H	-4.594194000	2.637521000	2.731142000
H	1.105588000	-2.633971000	4.571801000
H	0.917466000	-3.235323000	4.991605000
H	-5.071169000	-1.617867000	-2.837351000
H	-4.595568000	-1.749473000	-2.260574000
H	-3.468161000	1.422436000	-3.867185000
H	-4.179045000	1.665962000	-3.964530000
H	3.104470000	4.016634000	1.691740000
H	3.049836000	4.754509000	1.849938000
H	-0.904243000	1.144389000	-5.951286000
H	-1.186365000	1.126770000	-5.243881000
H	-4.596556000	4.028985000	-0.721231000
H	-4.299966000	3.440059000	-0.341886000
H	-4.164625000	-3.590846000	-0.454093000
H	-4.472107000	-4.225015000	-0.166751000
H	3.490013000	3.255081000	-2.738751000
H	3.800380000	3.950201000	-2.758497000
H	2.738777000	0.056372000	5.491583000
H	2.387194000	-0.344266000	4.947032000
H	5.246386000	-2.360164000	1.625137000
H	4.785758000	-2.202495000	1.043358000

H	-0.112264000	-5.760277000	-1.520544000
H	-0.000646000	-5.268830000	-0.954677000
H	4.853490000	2.651334000	0.425869000
H	5.541487000	2.790358000	0.134954000
H	-0.795496000	1.347210000	5.931017000
H	-0.652756000	1.597256000	5.225576000
H	-5.143514000	-1.915375000	2.784009000
H	-4.383014000	-1.899031000	2.760846000
H	2.007506000	-1.997211000	-4.570615000
H	2.614122000	-1.977579000	-5.023402000
H	-1.813680000	5.830015000	0.723560000
H	-1.410779000	5.318587000	0.329147000
H	-6.427213000	-0.338788000	0.017956000
H	-6.185121000	-0.857534000	-0.460494000
H	6.325064000	-0.400573000	-0.250124000
H	6.450909000	0.334889000	-0.257597000

$Ca_{12}O_{12}\cdot 27H_2$, ωB97XD/6-31++G(d,p)

Energy: -9066.859982 E_h

O	1.670453000	-1.604266000	-2.681925000
O	3.445634000	0.381014000	-0.924096000
O	2.081434000	-2.694306000	1.038145000
O	-0.470319000	-2.055596000	2.845711000
O	2.177389000	0.807321000	2.748072000
O	1.407497000	3.207866000	0.795573000
O	-1.615901000	1.662781000	2.696981000
O	-2.024246000	2.763808000	-1.002307000
O	-3.410383000	-0.320958000	0.956884000
O	-2.137387000	-0.742574000	-2.700858000
O	0.506962000	2.106660000	-2.830426000
O	-1.341041000	-3.156904000	-0.781081000

Ca	0.146292000	3.442954000	-1.024285000
Ca	0.499540000	2.338619000	2.691615000
Ca	3.077781000	1.676297000	0.845470000
Ca	-2.905187000	1.898016000	0.843158000
Ca	-2.107391000	-0.555298000	2.808799000
Ca	1.697231000	-1.361359000	2.836806000
Ca	-0.086791000	-3.389133000	1.044279000
Ca	-3.025567000	-1.631284000	-0.817136000
Ca	2.954309000	-1.839398000	-0.820779000
Ca	-0.448858000	-2.267937000	-2.669202000
Ca	2.155555000	0.617310000	-2.781118000
Ca	-1.661684000	1.430112000	-2.810605000
H	-2.711515000	-4.446415000	-1.849402000
H	-3.245921000	-4.797350000	-2.260013000
H	3.077236000	5.152896000	-0.730345000
H	2.701754000	4.698494000	-0.254970000
H	-0.093903000	1.654525000	-5.715629000
H	0.160471000	1.833765000	-5.024789000
H	0.871579000	-3.334816000	5.074924000
H	0.393106000	-3.075316000	4.542723000
H	-3.061922000	1.202964000	5.151679000
H	-2.682259000	1.476322000	4.550190000
H	2.493789000	-3.659765000	-3.003425000
H	2.819879000	-4.340588000	-2.940494000
H	2.025327000	-5.367673000	2.185629000
H	2.190926000	-4.680740000	1.904089000
H	-2.227335000	4.892642000	-0.333945000
H	-2.112411000	5.601498000	-0.092867000
H	1.858353000	1.095135000	4.937388000
H	1.606187000	1.262216000	5.632294000
H	-5.887092000	-0.109121000	-0.711249000

H	-5.338699000	-0.106490000	-0.190306000
H	-4.043765000	0.062844000	-3.539077000
H	-4.612966000	0.501781000	-3.778995000
H	4.561817000	2.053048000	-1.957018000
H	4.792866000	2.635549000	-2.380926000
H	-2.561671000	-2.544718000	-4.913399000
H	-2.580992000	-2.001995000	-4.378755000
H	-3.156276000	4.118061000	-3.317758000
H	-2.917249000	3.885108000	-2.634498000
H	-4.681741000	-1.966099000	1.767266000
H	-5.023463000	-2.583845000	2.039658000
H	2.976789000	-1.467331000	-4.385232000
H	3.439063000	-1.216426000	-4.936023000
H	4.534461000	2.297475000	3.499049000
H	3.903180000	1.873122000	3.453734000
H	4.591523000	-2.804228000	2.609620000
H	4.002622000	-2.873733000	2.136701000
H	-2.205375000	-4.433719000	3.294446000
H	-1.795069000	-3.797044000	3.310547000
H	5.207189000	-0.427531000	-1.906357000
H	5.732397000	-0.857934000	-2.247093000
H	2.014408000	5.034608000	2.957155000
H	1.930413000	4.657474000	2.300782000
H	-2.830486000	4.341299000	3.074551000
H	-2.484645000	3.667316000	3.100419000
H	-0.335542000	-5.149561000	-1.209662000
H	0.115930000	-5.755616000	-1.233916000
H	0.366904000	4.835953000	-3.812988000
H	0.431706000	4.086101000	-3.701722000
H	-5.488127000	1.018649000	2.637690000
H	-5.050255000	0.565650000	2.218933000

H	5.381885000	-3.353674000	-0.074817000
H	5.701277000	-3.003751000	-0.651278000
H	-5.690661000	-2.917970000	-1.049741000
H	-5.289010000	-3.447799000	-1.388228000

$Ca_{12}O_{12}\cdot 28H_2$, ωB97XD/6-31++G(d,p)

Energy: -9068.026359 E_h

O	1.564873000	-1.736700000	-2.652337000
O	3.276870000	0.555216000	-1.240413000
O	2.369446000	-2.431692000	1.100801000
O	-0.083774000	-1.858717000	3.059353000
O	2.259611000	1.204107000	2.483051000
O	1.125444000	3.342931000	0.410524000
O	-1.584124000	1.719972000	2.703924000
O	-2.370074000	2.431687000	-1.041167000
O	-3.297018000	-0.561780000	1.275775000
O	-2.301850000	-1.222059000	-2.439120000
O	0.053213000	1.829422000	-3.020654000
O	-1.123001000	-3.348168000	-0.373761000
Ca	-0.284485000	3.294422000	-1.311887000
Ca	0.450804000	2.572343000	2.442690000
Ca	2.928048000	1.968588000	0.444045000
Ca	-3.023664000	1.665273000	0.940662000
Ca	-1.851664000	-0.511202000	3.035670000
Ca	2.001554000	-0.981428000	2.812261000
Ca	0.280882000	-3.303140000	1.345292000
Ca	-2.947161000	-1.991993000	-0.396110000
Ca	3.004797000	-1.678152000	-0.893831000
Ca	-0.473531000	-2.580064000	-2.409587000
Ca	1.835575000	0.495873000	-2.996258000
Ca	-2.028121000	0.975816000	-2.754125000

H	-2.769519000	-4.710698000	-0.004383000
H	-3.458797000	-5.009160000	0.116584000
H	2.310046000	5.323317000	-1.468086000
H	2.086163000	4.873543000	-0.901055000
H	0.222909000	1.025252000	-5.887234000
H	0.112053000	1.318576000	-5.197994000
H	1.546245000	-2.934699000	5.207086000
H	1.006469000	-2.731822000	4.710513000
H	-1.430180000	1.375448000	5.653769000
H	-1.476346000	1.598570000	4.930994000
H	2.573730000	-3.727800000	-2.844472000
H	2.978995000	-4.359224000	-2.740182000
H	2.631056000	-5.057716000	2.296030000
H	2.717862000	-4.365961000	1.989586000
H	-2.756118000	4.557521000	-0.457484000
H	-2.722636000	5.283513000	-0.243272000
H	2.241490000	1.351687000	4.717103000
H	2.140064000	1.327482000	5.467044000
H	-5.966621000	-0.908895000	0.072513000
H	-5.342243000	-0.759446000	0.477550000
H	-4.330629000	-0.586524000	-3.156529000
H	-4.938900000	-0.191383000	-3.373262000
H	4.218399000	2.230346000	-2.393056000
H	4.422580000	2.827616000	-2.811286000
H	-2.049931000	-1.527791000	-5.403192000
H	-2.201415000	-1.457336000	-4.665322000
H	-3.804925000	3.488298000	-3.333852000
H	-3.487958000	3.330668000	-2.660406000
H	-4.612459000	-0.637859000	2.991996000
H	-4.900277000	-0.648414000	3.696421000
H	2.763353000	-1.664157000	-4.448169000

H	3.172154000	-1.434193000	-5.047350000
H	4.426249000	3.055438000	2.994379000
H	3.858753000	2.548092000	3.006181000
H	4.976727000	-2.235215000	2.476329000
H	4.362179000	-2.382573000	2.056307000
H	-1.710323000	-4.218094000	3.888377000
H	-1.302009000	-3.587418000	3.791075000
H	5.026145000	-0.196795000	-2.285119000
H	5.562483000	-0.614456000	-2.624537000
H	1.637883000	5.423990000	2.339942000
H	1.561253000	4.975813000	1.728035000
H	-4.008617000	3.056013000	3.560005000
H	-3.322159000	2.738540000	3.474987000
H	-0.586211000	-5.213822000	-1.390529000
H	-0.346152000	-5.737778000	-1.885275000
H	-0.487252000	4.413285000	-4.238924000
H	-0.327368000	3.690681000	-4.063160000
H	-5.945219000	2.413529000	0.832659000
H	-5.981431000	1.673158000	0.917055000
H	5.610635000	-2.901257000	-0.208852000
H	5.849705000	-2.599451000	-0.847923000
H	-3.876386000	-3.677654000	-3.137385000
H	-3.512433000	-3.016695000	-3.088178000
H	5.325790000	3.750021000	0.410335000
H	5.335510000	3.523433000	-0.300607000

$Ca_{12}O_{12}\cdot 29H_2$, ωB97XD/6-31++G(d,p)

Energy: -9069.190928 E_h

O	1.670257000	-0.995670000	-2.966107000
O	3.482087000	0.410540000	-0.746939000
O	1.885610000	-2.952517000	0.387434000

O	-0.689176000	-2.644963000	2.247044000
O	2.082283000	0.019379000	2.888125000
O	1.502638000	2.855172000	1.556120000
O	-1.661251000	1.069561000	2.948000000
O	-1.872255000	3.038970000	-0.389057000
O	-3.473286000	-0.342722000	0.738871000
O	-2.084149000	0.048048000	-2.877810000
O	0.695778000	2.702215000	-2.250932000
O	-1.481265000	-2.794170000	-1.568364000
Ca	0.324950000	3.587767000	-0.186797000
Ca	0.482310000	1.608794000	3.163458000
Ca	3.098524000	1.271438000	1.283174000
Ca	-2.863851000	1.810115000	1.172104000
Ca	-2.262827000	-1.079001000	2.518155000
Ca	1.508957000	-2.080369000	2.449055000
Ca	-0.308599000	-3.516390000	0.179497000
Ca	-3.089237000	-1.211612000	-1.287323000
Ca	2.874921000	-1.740549000	-1.190004000
Ca	-0.474759000	-1.532886000	-3.167433000
Ca	2.265627000	1.153873000	-2.520258000
Ca	-1.501700000	2.155030000	-2.451983000
H	-2.847219000	-3.706691000	-2.983308000
H	-3.365203000	-3.914133000	-3.498657000
H	3.117811000	5.135082000	0.527246000
H	2.786911000	4.563469000	0.898291000
H	0.174734000	2.985720000	-5.175151000
H	0.414503000	2.980803000	-4.456549000
H	-1.292930000	-2.539546000	5.191523000
H	-1.071122000	-2.694309000	4.485730000
H	-3.479300000	0.258168000	5.061746000
H	-3.001298000	0.606054000	4.583336000

H	2.491972000	-2.909887000	-3.754296000
H	2.824602000	-3.585590000	-3.840241000
H	1.743274000	-5.849713000	0.331312000
H	1.933539000	-5.113742000	0.364147000
H	-1.996584000	4.959727000	0.759524000
H	-1.853160000	5.583732000	1.164253000
H	1.693417000	-0.199871000	5.082902000
H	1.419781000	-0.187288000	5.789079000
H	-5.847229000	0.412258000	-0.943874000
H	-5.333240000	0.262583000	-0.410199000
H	-3.913814000	1.141770000	-3.556965000
H	-4.447671000	1.659560000	-3.701252000
H	4.854812000	2.176879000	-0.899057000
H	5.227411000	2.833763000	-0.853555000
H	-2.502144000	-1.140660000	-5.474857000
H	-2.517737000	-0.742761000	-4.825208000
H	-2.916130000	4.935315000	-2.333214000
H	-2.697358000	4.540583000	-1.721135000
H	-4.901026000	-2.024695000	1.053841000
H	-5.304833000	-2.659704000	1.132866000
H	2.865195000	-0.465017000	-4.669777000
H	3.299981000	-0.093552000	-5.172880000
H	4.448981000	1.198347000	4.091015000
H	3.811912000	0.821756000	3.914699000
H	4.291459000	-3.695417000	1.934495000
H	3.721004000	-3.586800000	1.446290000
H	-2.938781000	-4.581194000	2.526537000
H	-2.327669000	-4.135018000	2.512897000
H	5.145285000	-0.107682000	-2.142337000
H	5.603851000	-0.399136000	-2.669337000
H	2.171401000	4.048800000	4.111580000

H	2.078800000	3.850970000	3.382228000
H	-2.645681000	3.711315000	3.913775000
H	-2.373514000	3.016058000	3.786342000
H	-0.512234000	-4.619317000	-2.539545000
H	-0.072573000	-5.186935000	-2.774757000
H	0.634140000	5.595118000	-2.566830000
H	0.682676000	4.839199000	-2.633475000
H	-5.578133000	0.754669000	2.559736000
H	-5.140368000	0.360335000	2.085265000
H	5.361790000	-3.262611000	-0.712801000
H	5.676127000	-2.732633000	-1.133109000
H	-5.776334000	-2.304881000	-1.896990000
H	-5.380691000	-2.738498000	-2.357398000
H	5.875489000	-0.254530000	0.930276000
H	5.355573000	-0.133622000	0.394762000
H	0.162642000	-4.484190000	3.218507000
H	0.620430000	-5.017362000	3.498590000

$Ca_{12}O_{12}\cdot 30H_2$, ωB97XD/6-31++G(d,p)

Energy: -9070.358890 E_h

O	2.158023000	0.805504000	-2.697817000
O	2.301816000	2.732391000	-0.159329000
O	3.386431000	-0.942041000	0.550347000
O	1.156665000	-2.720183000	1.983868000
O	1.252599000	0.989209000	3.179725000
O	-1.010229000	2.827924000	1.897271000
O	-2.163422000	-0.805043000	2.692279000
O	-3.399312000	0.945290000	-0.548396000
O	-2.296900000	-2.741869000	0.163724000
O	-1.264704000	-1.005525000	-3.166879000
O	-1.155726000	2.702385000	-1.982826000

O	1.020452000	-2.829809000	-1.903298000
Ca	-2.213333000	2.802673000	0.023645000
Ca	-1.017644000	1.009388000	3.262828000
Ca	1.252714000	2.811303000	1.815970000
Ca	-3.385266000	-0.837162000	0.778854000
Ca	-1.066340000	-2.697857000	2.078149000
Ca	2.329120000	-0.853555000	2.560494000
Ca	2.210470000	-2.801485000	-0.026877000
Ca	-1.251371000	-2.822495000	-1.814662000
Ca	3.389794000	0.831167000	-0.789337000
Ca	1.009597000	-1.009201000	-3.262189000
Ca	1.064011000	2.695912000	-2.067648000
Ca	-2.339535000	0.848830000	-2.560386000
H	0.458286000	-4.449469000	-3.232218000
H	0.064799000	-4.949605000	-3.649067000
H	-1.219775000	5.750132000	1.323319000
H	-1.140746000	5.042272000	1.579217000
H	-1.771399000	3.031292000	-4.848140000
H	-1.565497000	3.081902000	-4.119426000
H	3.205575000	-3.595512000	3.824431000
H	2.621651000	-3.498874000	3.345095000
H	-2.627810000	-2.763349000	4.764171000
H	-2.599871000	-2.156869000	4.304056000
H	4.146014000	0.137643000	-3.440702000
H	4.864544000	-0.094431000	-3.507193000
H	5.368672000	-2.730957000	-0.659905000
H	4.966844000	-2.183100000	-0.321071000
H	-4.913240000	2.061311000	0.651174000
H	-5.287124000	2.542731000	1.101605000
H	0.940268000	0.236099000	5.265373000
H	0.679275000	-0.047545000	5.917600000

H	-4.415067000	-3.621237000	-1.747108000
H	-3.961419000	-3.439634000	-1.169469000
H	-3.276652000	-1.398768000	-4.054277000
H	-4.007818000	-1.388697000	-4.252810000
H	2.117665000	4.959701000	-0.057316000
H	1.942774000	5.688490000	0.046336000
H	-0.520100000	-2.049692000	-5.764487000
H	-0.859952000	-1.795662000	-5.132166000
H	-5.212210000	2.087178000	-2.512982000
H	-4.851430000	1.805283000	-1.905409000
H	-3.795515000	-3.849187000	1.372697000
H	-4.275533000	-4.135869000	1.883458000
H	2.758567000	2.241519000	-4.179549000
H	2.843014000	2.876828000	-4.591392000
H	1.939327000	3.282026000	4.830188000
H	1.783033000	2.602118000	4.527123000
H	5.518293000	-0.689213000	2.485733000
H	5.054412000	-0.772218000	1.887431000
H	0.888310000	-5.683672000	1.828747000
H	1.002976000	-4.941266000	1.925840000
H	4.038751000	3.608389000	-1.259435000
H	4.648870000	3.731572000	-1.690429000
H	-1.680487000	3.743424000	4.560843000
H	-1.520775000	3.653501000	3.821622000
H	-4.815941000	0.131613000	3.612358000
H	-4.109978000	-0.120689000	3.499757000
H	2.788207000	-3.284375000	-3.208813000
H	3.366571000	-3.267010000	-3.697085000
H	-1.542737000	5.591054000	-2.124680000
H	-1.439566000	4.839045000	-2.159209000
H	-6.235083000	-1.665067000	0.583239000

H	-5.924343000	-2.331807000	0.708243000
H	6.079171000	1.045843000	0.340368000
H	6.132500000	1.712432000	0.009190000
H	-2.022378000	-4.964250000	-0.110835000
H	-1.811948000	-5.656251000	-0.332332000
H	4.323611000	3.618499000	1.869123000
H	3.917794000	3.433046000	1.258240000
H	3.633253000	-4.978553000	1.310772000
H	4.144754000	-4.929655000	0.770032000
H	-3.919696000	5.002982000	-0.973304000
H	-4.443585000	4.678315000	-0.552738000

$Ca_{12}O_{12}\cdot 31H_2$, ωB97XD/6-31++G(d,p)

Energy: -9071.524552 E_h

O	0.553377000	-2.054863000	2.823204000
O	-0.488076000	-3.554718000	0.212071000
O	3.039283000	-1.904120000	-0.171781000
O	3.002087000	0.891573000	-1.710731000
O	0.473719000	-1.727357000	-3.099876000
O	-2.541497000	-1.253451000	-2.174162000
O	-0.534845000	2.023227000	-2.869800000
O	-3.003575000	1.861071000	0.114494000
O	0.516060000	3.523822000	-0.258679000
O	-0.448640000	1.705277000	3.052306000
O	-2.989908000	-0.919479000	1.679231000
O	2.560356000	1.204551000	2.137172000
Ca	-3.532773000	-0.280177000	-0.436483000
Ca	-1.046520000	-0.067803000	-3.413813000
Ca	-1.021718000	-2.911825000	-1.860269000
Ca	-1.541267000	3.014699000	-1.092233000
Ca	1.520408000	2.518775000	-2.037522000

Ca	2.481602000	-1.250601000	-2.276789000
Ca	3.554528000	0.242913000	0.391668000
Ca	1.047413000	2.873439000	1.817355000
Ca	1.562057000	-3.048771000	1.058458000
Ca	1.066228000	0.037441000	3.378120000
Ca	-1.503632000	-2.550107000	1.988092000
Ca	-2.462542000	1.220221000	2.229882000
H	3.195994000	2.700865000	3.574107000
H	3.253964000	3.321521000	4.010086000
H	-4.207007000	-3.699514000	-2.247650000
H	-3.879541000	-3.016038000	-2.268656000
H	-3.528107000	-1.880394000	4.433162000
H	-3.502533000	-1.571890000	3.740917000
H	4.946070000	0.045237000	-3.670090000
H	4.512564000	0.398708000	-3.153131000
H	0.890360000	3.425036000	-4.963881000
H	0.397600000	3.059241000	-4.513188000
H	2.222716000	-2.419166000	4.269646000
H	2.814104000	-2.359505000	4.739131000
H	5.882744000	-1.814282000	-1.056058000
H	5.179799000	-1.952738000	-0.813037000
H	-4.710320000	2.165051000	-1.302497000
H	-5.261657000	2.085921000	-1.816097000
H	1.065480000	-1.063490000	-5.159622000
H	1.182226000	-0.704999000	-5.816449000
H	-0.446699000	5.772774000	1.445886000
H	-0.215609000	5.284166000	0.916167000
H	-1.626270000	3.447113000	3.795841000
H	-2.158879000	3.967812000	3.936143000
H	-2.269119000	-4.886954000	0.399292000
H	-2.933012000	-5.216794000	0.553048000

H	0.527564000	1.943318000	5.769637000
H	0.185122000	2.003022000	5.092073000
H	-5.149080000	2.851225000	1.806747000
H	-4.662534000	2.656390000	1.256275000
H	0.526889000	5.316054000	-1.566790000
H	0.511770000	5.834473000	-2.118868000
H	-0.131720000	-3.629845000	4.141417000
H	-0.538601000	-4.174367000	4.482600000
H	-0.579807000	-3.824285000	-4.831715000
H	-0.218642000	-3.243368000	-4.500279000
H	3.514339000	-4.711182000	-1.084571000
H	3.507296000	-3.979502000	-0.892037000
H	4.849118000	3.216932000	-1.628508000
H	4.456120000	2.570705000	-1.676154000
H	0.064938000	-5.390087000	1.415720000
H	0.417949000	-5.879793000	1.871350000
H	-3.357373000	-1.386025000	-4.954558000
H	-3.271698000	-1.439037000	-4.199911000
H	-2.851975000	3.362964000	-4.109365000
H	-2.216210000	3.000090000	-3.910646000
H	4.407637000	0.377326000	3.084735000
H	5.053690000	0.008604000	3.229701000
H	-5.871581000	-0.502802000	1.942626000
H	-5.131480000	-0.670244000	1.974270000
H	-2.784820000	5.720970000	-1.210624000
H	-2.063018000	5.909951000	-1.208088000
H	4.571072000	-3.237903000	2.034606000
H	4.328261000	-2.870561000	1.419601000
H	2.315221000	4.817642000	0.196663000
H	2.938165000	5.128886000	0.490907000
H	0.187216000	-5.781296000	-1.679118000

H	0.054858000	-5.328998000	-1.087265000
H	6.166969000	1.601632000	0.144900000
H	6.272893000	1.380975000	0.849761000
H	-6.240473000	-1.535570000	-0.546361000
H	-5.955329000	-1.813048000	-1.177352000
H	-3.999559000	1.480223000	4.780833000
H	-4.220443000	0.800514000	4.567817000

$Ca_{12}O_{12}\cdot 32H_2$, ωB97XD/6-31++G(d,p)

Energy: -9072.692705 E_h

O	-0.993321000	0.523727000	3.420320000
O	-2.143473000	2.562777000	1.261097000
O	-3.323437000	-1.124271000	0.754525000
O	-1.751189000	-2.692494000	-1.537746000
O	-2.439353000	1.080122000	-2.342318000
O	0.088929000	2.974561000	-1.893826000
O	0.952848000	-0.540651000	-3.328750000
O	3.288372000	1.116157000	-0.687026000
O	2.140465000	-2.584065000	-1.188968000
O	2.406528000	-1.093648000	2.405487000
O	1.736060000	2.661212000	1.629323000
O	-0.124768000	-2.982001000	1.980747000
Ca	1.921106000	2.924240000	-0.625344000
Ca	-0.377626000	1.241074000	-3.291173000
Ca	-1.958882000	2.813887000	-0.942516000
Ca	2.830690000	-0.589464000	-2.042273000
Ca	0.269694000	-2.523727000	-2.483844000
Ca	-3.116399000	-0.876421000	-1.496563000
Ca	-1.950197000	-2.939755000	0.717689000
Ca	1.935261000	-2.826863000	1.026911000
Ca	-2.855452000	0.580976000	2.121640000

Ca	0.349047000	-1.244901000	3.367787000
Ca	-0.282824000	2.504308000	2.554764000
Ca	3.101965000	0.850804000	1.566541000
H	0.968191000	-4.646577000	2.854430000
H	1.507880000	-5.147940000	3.042912000
H	0.633649000	5.829786000	-1.292984000
H	0.398804000	5.150717000	-1.534672000
H	2.328882000	3.351635000	4.442415000
H	2.277142000	3.220890000	3.696789000
H	-2.241721000	-3.460540000	-4.363353000
H	-2.240436000	-3.315648000	-3.620117000
H	-0.610135000	-0.752511000	-5.866894000
H	-0.131992000	-0.795595000	-5.281495000
H	-2.502559000	-0.393414000	4.804346000
H	-3.115388000	-0.706771000	5.119377000
H	-4.518729000	-2.795541000	2.900056000
H	-4.315887000	-2.312044000	2.354024000
H	4.439823000	1.714468000	-2.473042000
H	4.749866000	1.791206000	-3.161580000
H	-3.452138000	0.107604000	-4.100507000
H	-3.790727000	-0.381062000	-4.568604000
H	4.898552000	-3.413229000	-0.459998000
H	4.220317000	-3.235789000	-0.746289000
H	4.616540000	-1.395342000	2.446269000
H	5.367512000	-1.339393000	2.360270000
H	-2.168126000	4.791505000	1.170444000
H	-2.115049000	5.525215000	0.988290000
H	2.763765000	-2.342061000	4.995993000
H	2.821130000	-2.028939000	4.304215000
H	5.759602000	2.185545000	0.427493000
H	5.173994000	1.936140000	0.012277000

H	2.891829000	-3.664551000	-2.990435000
H	3.001956000	-3.962002000	-3.677786000
H	-1.365838000	1.937186000	5.015756000
H	-1.420973000	2.570760000	5.433633000
H	-3.203433000	3.257223000	-4.212890000
H	-3.091623000	2.651827000	-3.772094000
H	-5.679313000	-2.413483000	-0.569252000
H	-5.154403000	-2.144419000	-0.096061000
H	-0.627921000	-5.498719000	-1.912683000
H	-1.043414000	-4.880379000	-1.794386000
H	-3.632475000	3.198734000	2.711361000
H	-4.161053000	3.225574000	3.257001000
H	0.125518000	4.016365000	-4.580006000
H	0.140390000	3.885865000	-3.829215000
H	3.120062000	-1.020605000	-5.199830000
H	2.469729000	-0.902254000	-4.824556000
H	-1.217136000	-3.632012000	3.830650000
H	-1.558736000	-3.684495000	4.504087000
H	3.621654000	4.844649000	1.229865000
H	3.146845000	4.304034000	1.475066000
H	5.637670000	-1.175203000	-2.875098000
H	5.445338000	-1.850845000	-2.624385000
H	-5.305597000	-0.006174000	1.071940000
H	-5.816963000	0.506766000	1.286779000
H	2.146333000	-4.837947000	-0.876832000
H	2.100506000	-5.529691000	-0.576028000
H	-4.018167000	4.619758000	-2.029713000
H	-3.985280000	4.930386000	-1.352057000
H	-3.367022000	-4.226598000	-1.366647000
H	-3.878666000	-4.721612000	-1.109307000
H	3.384131000	4.818768000	-2.415799000

H	3.902259000	4.284628000	-2.364260000
H	5.044580000	1.440887000	3.763635000
H	4.641557000	2.068078000	3.788596000
H	-5.387507000	1.478753000	-1.916257000
H	-4.656530000	1.473855000	-2.108179000

(H_2@$Ca_{12}O_{12}$)·32H_2 , ωB97XD/6-31++G(d,p)

Energy: -9073.861560 E_h

O	0.407667000	-0.594205000	3.464458000
O	0.342123000	-3.190191000	1.626369000
O	3.358458000	-0.795388000	0.939766000
O	2.964593000	1.111921000	-1.590749000
O	1.531869000	-2.498791000	-2.047777000
O	-1.632150000	-2.688465000	-1.695526000
O	-0.391934000	0.547783000	-3.446513000
O	-3.352063000	0.726134000	-0.932081000
O	-0.358109000	3.145370000	-1.604222000
O	-1.521976000	2.460807000	2.052877000
O	-2.969277000	-1.131975000	1.632193000
O	1.643885000	2.635747000	1.735674000
Ca	-3.177123000	-1.509832000	-0.603058000
Ca	-0.249948000	-1.651325000	-3.173543000
Ca	0.142774000	-3.526709000	-0.563234000
Ca	-1.985225000	1.754967000	-2.356903000
Ca	1.233121000	1.951449000	-2.709548000
Ca	3.120715000	-1.136383000	-1.297954000
Ca	3.180825000	1.452203000	0.641058000
Ca	-0.129000000	3.481263000	0.586724000
Ca	1.982604000	-1.808168000	2.382542000
Ca	0.249434000	1.610557000	3.199540000
Ca	-1.235661000	-1.986913000	2.732057000

Ca	-3.123666000	1.105626000	1.300756000
H	1.612957000	4.568593000	2.705294000
H	1.472993000	5.260712000	2.986742000
H	-3.626207000	-4.721166000	-0.854210000
H	-3.064159000	-4.304300000	-1.145636000
H	-3.905127000	-1.101798000	4.432754000
H	-3.780770000	-1.091121000	3.683979000
H	5.704980000	1.101690000	-2.458443000
H	4.973333000	1.152256000	-2.252759000
H	1.608047000	0.664263000	-5.666759000
H	1.019517000	0.573231000	-5.199026000
H	1.776425000	0.154110000	5.084567000
H	2.212822000	0.576546000	5.536842000
H	6.220574000	-0.558321000	0.146165000
H	5.532120000	-0.652374000	0.444728000
H	-4.557629000	0.641420000	-2.768252000
H	-4.829748000	0.665707000	-3.476998000
H	2.316854000	-2.602081000	-4.121361000
H	2.457317000	-2.544183000	-4.864071000
H	-2.116657000	5.495313000	-1.342510000
H	-1.661133000	4.909200000	-1.501159000
H	-3.205665000	3.902960000	1.847586000
H	-3.859993000	4.252790000	1.691684000
H	-1.022424000	-4.853689000	2.151956000
H	-1.587617000	-5.318336000	2.351568000
H	-1.361148000	3.873802000	4.562751000
H	-1.522830000	3.594018000	3.872357000
H	-6.050689000	1.246504000	0.023367000
H	-5.404423000	1.103052000	-0.350464000
H	0.053190000	4.358179000	-3.357303000
H	0.321868000	4.626999000	-4.016317000

H	0.011157000	-1.822686000	5.210139000
H	-0.256733000	-2.343776000	5.695083000
H	1.482684000	-5.326924000	-2.716864000
H	1.595936000	-4.576931000	-2.656735000
H	4.561562000	-3.533220000	1.263024000
H	4.374852000	-2.810439000	1.143710000
H	3.687683000	4.001795000	-2.150400000
H	3.640812000	3.265638000	-1.986854000
H	1.293535000	-4.343695000	3.197638000
H	1.741406000	-4.572989000	3.768292000
H	-1.761413000	-4.163141000	-4.172462000
H	-1.827158000	-3.878529000	-3.468217000
H	-1.774222000	2.092992000	-5.490479000
H	-1.338155000	1.633923000	-5.069859000
H	3.424431000	2.749378000	3.102859000
H	4.099350000	2.645386000	3.430621000
H	-5.706324000	-2.042983000	1.261364000
H	-5.024107000	-1.802580000	1.495326000
H	-4.052934000	3.650580000	-3.387248000
H	-3.535492000	4.145424000	-3.177888000
H	4.532799000	-0.726532000	2.843486000
H	4.755906000	-0.764140000	3.566112000
H	0.000595000	6.414242000	0.220947000
H	0.381605000	6.388602000	0.862162000
H	-0.321137000	-6.480198000	-0.657441000
H	-0.451715000	-6.350244000	0.065555000
H	5.787753000	2.891853000	0.468004000
H	5.726012000	2.605688000	-0.218473000
H	-5.512435000	-2.445420000	-2.223605000
H	-5.599529000	-1.707297000	-2.287333000
H	-5.131237000	1.892361000	3.373597000

H	-5.150393000	1.152036000	3.462863000
H	5.305009000	-1.362860000	-3.297056000
H	4.923571000	-1.972456000	-3.496687000
H	0.011570000	-0.031945000	0.390770000
H	0.016298000	-0.009558000	-0.355533000

$Ca_{12}O_{12}\cdot 33H_2$, ωB97XD/6-31++G(d,p)

Energy: -9073.855484 E_h

O	1.955964000	-0.332277000	2.986091000
O	2.393293000	-2.576138000	0.764246000
O	3.392283000	1.034246000	-0.366817000
O	1.217545000	2.468036000	-2.209800000
O	1.596381000	-1.363821000	-2.859021000
O	-0.709471000	-3.129533000	-1.537826000
O	-1.936378000	0.304936000	-2.939653000
O	-3.347156000	-1.049087000	0.425585000
O	-2.366098000	2.551670000	-0.706228000
O	-1.563320000	1.339928000	2.924931000
O	-1.201990000	-2.493941000	2.288320000
O	0.742357000	3.093090000	1.604116000
Ca	-2.067232000	-2.905468000	0.225155000
Ca	-0.655016000	-1.511790000	-3.136518000
Ca	1.540214000	-2.981625000	-1.259667000
Ca	-3.317791000	0.531195000	-1.141024000
Ca	-0.982787000	2.324152000	-2.500044000
Ca	2.527194000	0.620638000	-2.424880000
Ca	2.086478000	2.889878000	-0.157222000
Ca	-1.509582000	2.942738000	1.325877000
Ca	3.339873000	-0.552394000	1.208636000
Ca	0.692210000	1.488004000	3.201537000
Ca	1.003346000	-2.351178000	2.555137000

Ca	-2.493209000	-0.637661000	2.494382000
H	-0.000412000	4.821237000	2.687466000
H	-0.443666000	5.348174000	3.010531000
H	-0.705805000	-5.962848000	-0.620731000
H	-0.692659000	-5.278491000	-0.943705000
H	-0.900141000	-3.027842000	5.180260000
H	-1.086660000	-2.933573000	4.450930000
H	3.104398000	3.033210000	-4.335448000
H	2.560377000	3.025415000	-3.803543000
H	-1.283547000	1.209337000	-5.697044000
H	-1.525573000	0.914141000	-5.043122000
H	3.291446000	0.991274000	4.207498000
H	3.605358000	1.573578000	4.576447000
H	5.128762000	3.101222000	-1.623707000
H	4.795910000	2.513840000	-1.282026000
H	-5.020292000	-1.688429000	-0.910360000
H	-5.517574000	-1.755388000	-1.478401000
H	1.754282000	-0.798513000	-5.014886000
H	1.755616000	-0.511395000	-5.714863000
H	-4.687051000	3.711247000	0.709268000
H	-4.151270000	3.435102000	0.249518000
H	-3.656434000	1.709486000	3.589407000
H	-4.399662000	1.667600000	3.733486000
H	2.278845000	-4.761048000	1.208958000
H	2.122883000	-5.481419000	1.380584000
H	-1.098036000	2.764380000	5.402301000
H	-1.368417000	2.409948000	4.784830000
H	-5.370713000	-1.980722000	2.313753000
H	-4.941128000	-1.775402000	1.721730000
H	-3.459130000	3.700074000	-2.275409000
H	-3.678808000	4.035433000	-2.917509000

H	2.735214000	-1.575228000	4.572938000
H	2.894024000	-2.155741000	5.038395000
H	2.274587000	-3.927631000	-4.215099000
H	2.116901000	-3.216090000	-4.012364000
H	5.923004000	-0.502804000	-0.719511000
H	5.342392000	-0.017434000	-0.720610000
H	0.524731000	5.298233000	-2.776946000
H	0.808366000	4.605467000	-2.657875000
H	4.143868000	-3.131509000	2.072952000
H	4.744478000	-3.113378000	2.532253000
H	-0.620718000	-4.548731000	-4.150617000
H	-0.645469000	-4.329124000	-3.426955000
H	-4.525993000	1.402853000	-3.965992000
H	-3.828609000	1.133981000	-3.854516000
H	2.554772000	4.172700000	2.324645000
H	3.248285000	4.467640000	2.405446000
H	-3.106274000	-4.672672000	2.572151000
H	-2.584025000	-4.124905000	2.648439000
H	-6.225681000	1.155493000	-0.902964000
H	-5.954129000	1.846579000	-0.831441000
H	4.897021000	1.789232000	1.171079000
H	5.305962000	1.898374000	1.796624000
H	-2.054531000	4.846153000	-0.612242000
H	-1.843848000	5.539816000	-0.403756000
H	4.539601000	-3.773727000	-0.966487000
H	4.112087000	-3.492069000	-0.410080000
H	2.593413000	5.681860000	-1.000852000
H	2.813854000	5.778668000	-0.294728000
H	-2.744979000	-4.012583000	-2.191836000
H	-3.474085000	-4.206271000	-2.204905000
H	-3.644047000	-1.024141000	5.228085000

H	-3.264905000	-1.663490000	5.165039000
H	4.572214000	-1.441047000	-3.469159000
H	3.834120000	-1.580436000	-3.394912000
H	-3.377202000	-1.827878000	-4.530256000
H	-3.156545000	-1.196438000	-4.179068000

(H_2@$Ca_{12}O_{12}$)·$33H_2$, ωB97XD/6-31++G(d,p)

Energy: -9075.024741 E_h

O	1.987983000	-0.512871000	2.947175000
O	2.368972000	-2.644492000	0.609335000
O	3.381664000	0.998300000	-0.346116000
O	1.230096000	2.564912000	-2.092821000
O	1.545548000	-1.230584000	-2.941406000
O	-0.766629000	-3.037807000	-1.684350000
O	-1.971179000	0.485306000	-2.902674000
O	-3.323139000	-1.014474000	0.400355000
O	-2.346880000	2.617075000	-0.550722000
O	-1.511645000	1.203546000	3.010671000
O	-1.215563000	-2.599136000	2.175209000
O	0.801543000	2.993882000	1.749951000
Ca	-2.102846000	-2.896297000	0.102205000
Ca	-0.710854000	-1.334346000	-3.190020000
Ca	1.485551000	-2.923243000	-1.422791000
Ca	-3.336793000	0.641043000	-1.086302000
Ca	-0.975222000	2.456221000	-2.359588000
Ca	2.510602000	0.715474000	-2.423608000
Ca	2.126322000	2.872089000	-0.031932000
Ca	-1.453428000	2.876432000	1.485955000
Ca	3.353114000	-0.664001000	1.149863000
Ca	0.748485000	1.309068000	3.261562000
Ca	0.994596000	-2.487153000	2.416625000

Ca	-2.472780000	-0.735802000	2.491909000
H	0.096094000	4.682719000	2.912906000
H	-0.333284000	5.204530000	3.262044000
H	-0.876960000	-5.898534000	-0.860981000
H	-0.821282000	-5.211079000	-1.172712000
H	-0.926616000	-3.244306000	5.048402000
H	-1.103539000	-3.123063000	4.320822000
H	3.125326000	3.204927000	-4.193713000
H	2.579519000	3.181869000	-3.664132000
H	-1.318572000	1.410849000	-5.654314000
H	-1.562696000	1.131154000	-4.994452000
H	3.360273000	0.727145000	4.208092000
H	3.693933000	1.284655000	4.597688000
H	5.163475000	3.090895000	-1.515209000
H	4.818402000	2.494880000	-1.202488000
H	-5.038505000	-1.571634000	-0.941986000
H	-5.545677000	-1.601017000	-1.503867000
H	1.713411000	-0.560904000	-5.063295000
H	1.730577000	-0.232643000	-5.744879000
H	-4.645401000	3.739116000	0.916645000
H	-4.108169000	3.478461000	0.449055000
H	-3.586432000	1.564436000	3.725338000
H	-4.328083000	1.524067000	3.878577000
H	2.242162000	-4.857375000	0.858912000
H	2.086835000	-5.594401000	0.933152000
H	-0.998471000	2.520564000	5.539744000
H	-1.280181000	2.194949000	4.911697000
H	-5.383004000	-1.970635000	2.243257000
H	-4.945726000	-1.751437000	1.662023000
H	-3.426335000	3.857345000	-2.059506000
H	-3.642346000	4.224776000	-2.685078000

H	2.734482000	-1.838484000	4.476187000
H	2.880010000	-2.442055000	4.916288000
H	2.172503000	-3.732609000	-4.431675000
H	2.026895000	-3.030052000	-4.191889000
H	5.885598000	-0.558118000	-0.825647000
H	5.313382000	-0.064399000	-0.791685000
H	0.600878000	5.432819000	-2.513110000
H	0.862979000	4.726172000	-2.431873000
H	4.106431000	-3.311429000	1.874422000
H	4.707380000	-3.336771000	2.333300000
H	-0.719333000	-4.349771000	-4.348146000
H	-0.733359000	-4.152711000	-3.617589000
H	-4.544781000	1.663600000	-3.862911000
H	-3.850156000	1.381240000	-3.766783000
H	2.636803000	4.007672000	2.501920000
H	3.336424000	4.287316000	2.586160000
H	-3.177421000	-4.736521000	2.378877000
H	-2.638857000	-4.207776000	2.474428000
H	-6.232929000	1.322239000	-0.824728000
H	-5.938061000	1.992928000	-0.684127000
H	4.936671000	1.655353000	1.196512000
H	5.361477000	1.725813000	1.816808000
H	-1.988176000	4.894575000	-0.353255000
H	-1.759202000	5.574334000	-0.119795000
H	4.512407000	-3.707353000	-1.208660000
H	4.081196000	-3.469861000	-0.634898000
H	2.685306000	5.681519000	-0.761202000
H	2.936338000	5.741819000	-0.061222000
H	-2.824944000	-3.848878000	-2.365355000
H	-3.557528000	-4.029136000	-2.380551000
H	-3.616894000	-1.187786000	5.214395000

H	-3.260775000	-1.837535000	5.127850000
H	4.512225000	-1.319548000	-3.584428000
H	3.772959000	-1.452102000	-3.509404000
H	-3.466935000	-1.566862000	-4.547366000
H	-3.230008000	-0.952347000	-4.177364000
H	0.331163000	0.099486000	-0.032599000
H	-0.374043000	-0.134050000	0.042965000

$Ca_{12}O_{12}\cdot 34H_2$, ωB97XD/6-31++G(d,p)

Energy: -9075.023868 E_h

O	0.851877000	-0.717827000	3.410581000
O	0.639660000	-3.214857000	1.439604000
O	3.473783000	-0.706005000	0.506601000
O	2.725091000	1.263169000	-1.892774000
O	1.356850000	-2.362993000	-2.311516000
O	-1.732596000	-2.671414000	-1.586007000
O	-0.834106000	0.676571000	-3.393301000
O	-3.449647000	0.645261000	-0.497777000
O	-0.630608000	3.174850000	-1.417604000
O	-1.324401000	2.331208000	2.310121000
O	-2.711121000	-1.287451000	1.927682000
O	1.772704000	2.622813000	1.622905000
Ca	-3.182117000	-1.595524000	-0.279544000
Ca	-0.572847000	-1.531399000	-3.174792000
Ca	0.190082000	-3.499973000	-0.718518000
Ca	-2.302156000	1.772787000	-2.037833000
Ca	0.843928000	2.080216000	-2.760404000
Ca	2.991073000	-0.986297000	-1.702034000
Ca	3.208338000	1.543987000	0.306828000
Ca	-0.149839000	3.461269000	0.737500000
Ca	2.318354000	-1.816839000	2.067544000

Ca	0.595021000	1.495108000	3.197908000
Ca	-0.830202000	-2.118061000	2.777941000
Ca	-2.970619000	0.955194000	1.708072000
H	1.810411000	4.557618000	2.582951000
H	1.678904000	5.252958000	2.860833000
H	-3.509623000	-4.820519000	-0.557510000
H	-3.011102000	-4.368310000	-0.905899000
H	-3.300609000	-1.548706000	4.806831000
H	-3.276234000	-1.458961000	4.053594000
H	5.351091000	1.391236000	-3.062571000
H	4.645213000	1.403981000	-2.777286000
H	0.822211000	0.806689000	-5.861265000
H	0.314465000	0.732042000	-5.304562000
H	2.394225000	0.006187000	4.854450000
H	2.888490000	0.410374000	5.261234000
H	5.203742000	-0.696724000	2.930728000
H	4.883891000	-0.651073000	2.246182000
H	-4.881614000	0.602413000	-2.167535000
H	-5.242751000	0.651181000	-2.833778000
H	1.907796000	-2.380379000	-4.465600000
H	1.970881000	-2.298250000	-5.216167000
H	-2.495418000	5.416765000	-0.933667000
H	-2.016332000	4.864861000	-1.137209000
H	-3.064885000	3.721754000	2.377790000
H	-3.744398000	4.052582000	2.319761000
H	-0.580325000	-4.936271000	2.105573000
H	-1.098516000	-5.418862000	2.377480000
H	-0.825321000	3.802948000	4.761789000
H	-1.078750000	3.504392000	4.109373000
H	-6.012389000	1.083538000	0.812678000
H	-5.419391000	0.963397000	0.352326000

H	-0.287145000	4.581341000	-3.023373000
H	-0.042566000	4.927906000	-3.654931000
H	1.034547000	-2.288826000	4.986945000
H	0.985790000	-2.915803000	5.408401000
H	1.365506000	-5.173496000	-3.048422000
H	1.448595000	-4.420023000	-2.983303000
H	6.208872000	-0.352006000	-0.636563000
H	5.570245000	-0.477640000	-0.251922000
H	3.306948000	4.198886000	-2.413393000
H	3.295965000	3.455516000	-2.280820000
H	1.917383000	-4.490499000	2.634033000
H	2.477750000	-4.764506000	3.069272000
H	-1.967971000	-4.243757000	-4.015269000
H	-1.993365000	-3.932123000	-3.321572000
H	-2.084412000	2.824964000	-5.074804000
H	-1.711672000	2.236336000	-4.782003000
H	3.706263000	2.771260000	2.764898000
H	4.422168000	2.688134000	2.997523000
H	-5.466226000	-2.223725000	1.827407000
H	-4.764701000	-1.983258000	1.994750000
H	-4.607924000	3.533815000	-2.737151000
H	-4.096128000	4.064866000	-2.625451000
H	4.572784000	-2.694528000	0.494612000
H	4.795876000	-3.414327000	0.550358000
H	-0.335665000	6.401655000	0.451094000
H	0.120363000	6.405108000	1.041829000
H	-0.272903000	-6.456090000	-0.832193000
H	-0.295843000	-6.346059000	-0.094630000
H	5.608548000	2.802366000	-0.795689000
H	5.739609000	3.062337000	-0.108551000
H	-5.488149000	-2.606384000	-1.887015000

H	-5.692105000	-1.890468000	-1.838357000
H	-4.621899000	1.522736000	4.139348000
H	-4.618882000	0.777155000	4.164281000
H	4.911977000	-1.046703000	-3.968937000
H	4.520430000	-1.654450000	-4.154136000
H	-2.704289000	-0.673989000	-5.295730000
H	-2.279649000	-0.197696000	-4.888473000
H	-0.240609000	-0.127643000	5.331143000
H	-0.631388000	0.236777000	5.864785000

(H_2@$Ca_{12}O_{12}$)·34H_2 , ωB97XD/6-31++G(d,p)

Energy: -9076.189738 E_h

O	-1.618598000	-1.923817000	-2.578789000
O	-1.903269000	-3.041468000	0.392229000
O	-3.487942000	0.471712000	-0.168246000
O	-1.756708000	2.925683000	0.898013000
O	-1.599154000	-0.268638000	3.135200000
O	1.040948000	-2.020870000	2.742516000
O	1.632852000	1.840386000	2.517639000
O	3.470302000	-0.550323000	0.099935000
O	1.915860000	2.953131000	-0.460876000
O	1.597150000	0.186218000	-3.215811000
O	1.763182000	-3.009108000	-0.973566000
O	-1.042163000	1.920960000	-2.801887000
Ca	2.493787000	-2.343997000	1.074771000
Ca	0.618463000	0.092283000	3.471543000
Ca	-1.174161000	-2.377793000	2.394688000
Ca	3.125501000	1.522483000	0.827887000
Ca	0.428729000	3.269235000	1.230342000
Ca	-2.780268000	1.150784000	1.878883000
Ca	-2.492358000	2.263530000	-1.152159000

Ca	1.177677000	2.279272000	-2.463661000
Ca	-3.103018000	-1.604988000	-0.902500000
Ca	-0.625224000	-0.179775000	-3.541339000
Ca	-0.410588000	-3.362275000	-1.297558000
Ca	2.768446000	-1.226951000	-1.955748000
H	-0.486889000	3.125309000	-4.522211000
H	-0.107523000	3.533610000	-5.039477000
H	1.386313000	-4.957406000	3.139175000
H	1.301567000	-4.205551000	3.129909000
H	1.797655000	-4.746269000	-3.367224000
H	1.900971000	-4.327134000	-2.743414000
H	-4.269565000	4.435593000	1.293205000
H	-3.595458000	4.101913000	1.207019000
H	0.730392000	2.839800000	5.170886000
H	1.036414000	2.708221000	4.491148000
H	-3.040468000	-1.482989000	-4.251014000
H	-3.415053000	-1.171820000	-4.831358000
H	-5.857910000	2.217549000	0.283590000
H	-5.306159000	1.721087000	0.139348000
H	5.130759000	-0.282975000	1.589668000
H	5.589646000	-0.019994000	2.131834000
H	-2.257746000	1.179922000	4.706587000
H	-2.518891000	1.773513000	5.096797000
H	4.215900000	3.704849000	-2.170066000
H	3.666427000	3.583891000	-1.662488000
H	3.655607000	0.582548000	-3.958073000
H	4.406004000	0.610419000	-4.063937000
H	-1.425593000	-5.164069000	0.886070000
H	-1.145348000	-5.857377000	1.002791000
H	1.116663000	0.349503000	-6.067862000
H	1.388326000	0.335046000	-5.356626000

H	5.784830000	-1.798108000	-1.181810000
H	5.276573000	-1.446596000	-0.740092000
H	2.727382000	4.813452000	0.456732000
H	2.867364000	5.419526000	0.887872000
H	-2.074535000	-3.835206000	-3.471836000
H	-2.109561000	-4.576299000	-3.640649000
H	-1.993020000	-2.010454000	5.510008000
H	-1.927919000	-1.459039000	4.995940000
H	-5.726685000	-1.320398000	0.786832000
H	-5.264791000	-0.751431000	0.604242000
H	-1.219816000	5.759210000	0.020159000
H	-1.493617000	5.089648000	0.237527000
H	-3.445053000	-4.385128000	-0.568264000
H	-4.005027000	-4.659241000	-0.996386000
H	0.946792000	-2.195359000	5.707551000
H	0.995261000	-2.298163000	4.959384000
H	3.794939000	3.773928000	3.147199000
H	3.188541000	3.324026000	3.099081000
H	-2.930249000	2.263376000	-3.941385000
H	-3.652239000	2.371418000	-4.145285000
H	4.007215000	-4.715709000	-0.271228000
H	3.412191000	-4.356496000	-0.580844000
H	5.907535000	2.553900000	0.521056000
H	5.544362000	3.063697000	0.115151000
H	-4.996604000	0.220249000	-1.878280000
H	-5.372048000	-0.029404000	-2.483777000
H	1.352365000	4.890961000	-1.585923000
H	1.087382000	5.377652000	-2.098043000
H	-3.971340000	-3.751811000	2.446299000
H	-3.545110000	-3.661943000	1.828053000
H	-3.961494000	4.803342000	-1.364694000

H	-3.935279000	4.674887000	-2.099301000
H	3.113867000	-2.283540000	3.723955000
H	3.858775000	-2.364076000	3.817052000
H	4.162990000	-2.488290000	-4.276982000
H	3.904347000	-3.105515000	-3.947397000
H	-4.577538000	-0.695453000	3.613819000
H	-3.823454000	-0.695136000	3.632633000
H	3.485470000	0.644681000	4.624528000
H	3.133903000	1.068958000	4.109781000
H	-0.349215000	-0.014070000	-0.054431000
H	0.392456000	-0.048995000	0.024794000
H	-1.672284000	4.185405000	2.807058000
H	-1.433102000	4.553257000	3.421779000

$Ca_{12}O_{12}\cdot 35H_2$, ωB97XD/6-31++G(d,p)

Energy: -9076.189934 E_h

O	-0.812606000	-3.140753000	-1.518985000
O	-0.645616000	-3.088211000	1.662650000
O	-3.467539000	-0.849419000	0.202161000
O	-2.768151000	2.263492000	0.121158000
O	-1.418653000	0.396633000	3.267850000
O	1.678729000	-0.341357000	3.106979000
O	0.771074000	3.124456000	1.540252000
O	3.419394000	0.836037000	-0.159665000
O	0.596905000	3.091466000	-1.650460000
O	1.376915000	-0.390134000	-3.237322000
O	2.735796000	-2.283380000	-0.114427000
O	-1.729954000	0.297756000	-3.084856000
Ca	3.151231000	-0.707938000	1.478318000
Ca	0.501946000	1.603921000	3.153918000
Ca	-0.235546000	-1.548539000	3.218680000

Ca	2.258230000	2.734886000	-0.138296000
Ca	-0.896810000	3.467512000	0.028159000
Ca	-3.037846000	0.727097000	1.779237000
Ca	-3.199777000	0.686376000	-1.456302000
Ca	0.175255000	1.531479000	-3.199647000
Ca	-2.305869000	-2.741754000	0.144039000
Ca	-0.532502000	-1.625126000	-3.127347000
Ca	0.845583000	-3.477723000	0.004258000
Ca	3.005524000	-0.731370000	-1.757121000
H	-1.718619000	0.934263000	-5.150917000
H	-1.538254000	1.241844000	-5.823010000
H	3.548715000	-2.398325000	4.173318000
H	3.020378000	-1.870982000	4.043515000
H	3.313480000	-4.563712000	-1.936822000
H	3.280190000	-3.967952000	-1.470528000
H	-5.567885000	2.715224000	0.817697000
H	-4.845458000	2.691446000	0.584035000
H	-0.870879000	5.235387000	2.812328000
H	-0.363651000	4.723390000	2.578352000
H	-2.329268000	-3.998828000	-2.851255000
H	-2.862532000	-4.194890000	-3.354817000
H	-6.143330000	-0.285579000	-0.773274000
H	-5.509072000	-0.527113000	-0.430363000
H	4.794201000	2.164268000	0.969993000
H	5.127085000	2.727165000	1.353936000
H	-2.007562000	2.247860000	4.425262000
H	-2.068062000	2.933046000	4.739680000
H	2.327179000	3.930411000	-3.895020000
H	1.905033000	3.825823000	-3.274080000
H	3.136690000	0.502076000	-4.309403000
H	3.813159000	0.780120000	-4.505518000

H	0.392516000	-4.389166000	3.144425000
H	0.788837000	-4.694546000	3.713190000
H	0.975087000	-1.082503000	-6.031974000
H	1.181848000	-0.857650000	-5.335722000
H	6.011418000	0.401188000	-1.388243000
H	5.393698000	0.598813000	-0.991718000
H	0.616291000	5.315328000	-1.527784000
H	0.497903000	6.040657000	-1.346246000
H	-0.575117000	-5.299169000	-1.477757000
H	-0.345637000	-6.007127000	-1.320343000
H	-1.366939000	-0.269088000	6.094603000
H	-1.450208000	-0.016176000	5.382398000
H	-5.149206000	-1.720686000	2.500918000
H	-4.793468000	-1.575146000	1.847725000
H	-3.477632000	4.668540000	-1.467786000
H	-3.429066000	4.029926000	-1.062278000
H	-1.845879000	-4.867733000	1.877383000
H	-2.380282000	-5.405996000	1.815837000
H	1.959258000	0.692660000	5.809205000
H	1.974583000	0.314710000	5.149342000
H	2.256575000	5.673901000	1.002770000
H	1.803635000	5.120317000	1.246626000
H	-3.581633000	-0.567297000	-3.984922000
H	-4.278250000	-0.833981000	-4.118473000
H	5.703535000	-2.498133000	-0.017370000
H	4.950715000	-2.548301000	-0.071275000
H	4.508775000	4.286962000	-1.338433000
H	3.960575000	4.519247000	-1.787808000
H	-4.078170000	-4.765555000	-1.097944000
H	-4.477122000	-4.726170000	-0.468822000
H	-0.732831000	4.147827000	-3.222798000

H	-1.191090000	4.291959000	-3.804452000
H	-1.189802000	-2.826969000	5.728700000
H	-1.013658000	-3.449500000	5.356787000
H	-5.141671000	2.665145000	-2.458236000
H	-5.247074000	2.193651000	-3.026560000
H	5.895845000	-0.427558000	2.629936000
H	5.913413000	0.040397000	2.048983000
H	4.945742000	-2.072171000	-3.584928000
H	4.935909000	-2.572256000	-3.031542000
H	-5.120927000	2.113211000	3.403291000
H	-4.634763000	1.953824000	3.946601000
H	2.654353000	3.709630000	3.825593000
H	2.238723000	3.714045000	3.194379000
H	-1.012503000	-3.648750000	-5.234155000
H	-0.598852000	-3.191148000	-5.654242000
H	3.319750000	-4.053131000	1.173566000
H	3.312509000	-4.680090000	1.595845000

$Ca_{12}O_{12}\cdot 36H_2$, ωB97XD/6-31++G(d,p)

Energy: -9077.35249326 E_h

O	-0.022815000	-3.357224000	-1.272909000
O	-0.093395000	-3.023774000	1.899397000
O	-3.200561000	-1.553044000	0.098333000
O	-3.176252000	1.623869000	-0.214460000
O	-1.662098000	0.344125000	3.131754000
O	1.521725000	0.279489000	3.187614000
O	0.024014000	3.325772000	1.270008000
O	3.211926000	1.531237000	-0.096981000
O	0.061854000	3.000215000	-1.898730000
O	1.654915000	-0.342202000	-3.128625000
O	3.148412000	-1.648799000	0.216693000

O	-1.529471000	-0.312989000	-3.186122000
Ca	3.141642000	0.100769000	1.672548000
Ca	-0.040371000	1.924902000	3.011670000
Ca	-0.098689000	-1.297440000	3.322155000
Ca	1.663117000	3.134484000	-0.293972000
Ca	-1.578623000	3.184619000	-0.332336000
Ca	-3.222114000	0.190154000	1.555571000
Ca	-3.153478000	-0.125469000	-1.673338000
Ca	0.084206000	1.282482000	-3.328355000
Ca	-1.679622000	-3.159075000	0.272762000
Ca	0.035890000	-1.937352000	-3.003115000
Ca	1.557234000	-3.214034000	0.353017000
Ca	3.216589000	-0.217940000	-1.551599000
H	-1.472824000	0.139391000	-5.314428000
H	-1.301687000	0.424104000	-5.998321000
H	3.697761000	-1.245808000	4.531635000
H	3.083083000	-0.852694000	4.327737000
H	4.156391000	-3.954447000	-1.437650000
H	4.038956000	-3.332883000	-1.024323000
H	-6.117205000	1.236251000	-0.001541000
H	-5.392504000	1.433397000	-0.095368000
H	-1.696151000	4.952316000	3.079872000
H	-1.235003000	4.626268000	2.576791000
H	-1.370715000	-4.365972000	-2.797756000
H	-1.808874000	-4.526013000	-3.392329000
H	-5.776491000	-1.862295000	-1.207114000
H	-5.153310000	-1.880148000	-0.772332000
H	4.074536000	3.204779000	1.192616000
H	4.183657000	3.824066000	1.610669000
H	-2.839036000	1.867440000	4.240391000
H	-3.194706000	2.455316000	4.558861000

H	1.784659000	4.152660000	-4.031870000
H	1.328296000	3.961742000	-3.459289000
H	2.995055000	0.917626000	-4.414316000
H	3.443725000	1.412479000	-4.769599000
H	1.089613000	-3.816643000	3.647147000
H	1.479417000	-3.886872000	4.291661000
H	1.529966000	-1.643036000	-5.733552000
H	1.675385000	-1.222568000	-5.117184000
H	6.159102000	1.400694000	-0.028213000
H	5.407287000	1.491752000	-0.045893000
H	-0.429679000	5.192100000	-1.936018000
H	-0.732059000	5.872082000	-1.799939000
H	0.069312000	-5.540013000	-1.055560000
H	0.139555000	-6.279512000	-0.907699000
H	-1.600691000	-0.567209000	5.903909000
H	-1.736321000	-0.232852000	5.234792000
H	-4.894299000	-2.498144000	2.354981000
H	-4.512799000	-2.364546000	1.714143000
H	-4.271014000	3.643214000	-2.096991000
H	-4.111883000	3.079939000	-1.616477000
H	-0.297405000	-5.236519000	2.019636000
H	-0.416844000	-5.979849000	1.948565000
H	1.293238000	1.455170000	5.846204000
H	1.459927000	1.068297000	5.213516000
H	0.962246000	6.079477000	0.647269000
H	0.621023000	5.453096000	0.900144000
H	-3.130398000	-1.542866000	-4.131331000
H	-3.761985000	-1.932352000	-4.285462000
H	6.119118000	-1.473559000	0.241953000
H	5.373024000	-1.595585000	0.248015000
H	4.142456000	3.027317000	-1.547024000

H	4.254065000	3.603247000	-2.022999000
H	-2.509642000	-5.830277000	-0.632991000
H	-3.185351000	-5.651181000	-0.371984000
H	-1.338888000	3.642805000	-3.625085000
H	-1.774816000	3.647171000	-4.240655000
H	-2.147817000	-3.714762000	4.014952000
H	-1.633905000	-3.683732000	3.463087000
H	-5.365770000	1.264812000	-3.053132000
H	-5.274826000	0.743852000	-3.579158000
H	5.799747000	0.982105000	2.572401000
H	5.576194000	0.730368000	3.238325000
H	5.903545000	0.546178000	-2.537052000
H	5.610654000	0.383061000	-3.203593000
H	-5.757813000	1.199884000	2.726451000
H	-5.329078000	1.248047000	3.335039000
H	1.784153000	4.362800000	3.535558000
H	1.384147000	4.262695000	2.903911000
H	1.342617000	-4.367372000	-2.822781000
H	1.766163000	-4.504068000	-3.432663000
H	3.998911000	-3.167478000	1.678830000
H	4.082466000	-3.749691000	2.153659000
H	-4.187830000	3.941080000	1.423644000
H	-4.071514000	3.316508000	1.015367000

$Ca_{12}O_{12}\cdot 37H_2$, ωB97XD/6-31++G(d,p)

Energy: -9078.51702376 E_h

O	-3.456134000	-0.572880000	0.721950000
O	-2.375352000	2.408382000	1.116605000
O	-2.208506000	1.137510000	-2.549089000
O	0.688134000	0.225085000	-3.512509000
O	0.685185000	3.327495000	-1.136867000

O	1.444482000	2.636017000	1.883336000
O	3.418396000	0.572526000	-0.747918000
O	2.201645000	-1.150197000	2.531073000
O	2.359741000	-2.405854000	-1.164943000
O	-0.694479000	-3.322930000	1.086122000
O	-0.705834000	-0.222719000	3.443860000
O	-1.458246000	-2.634814000	-1.929689000
Ca	1.296810000	0.827209000	3.190634000
Ca	2.544901000	2.512501000	-0.104128000
Ca	-0.410522000	3.444308000	0.852809000
Ca	3.279210000	-1.264993000	0.575762000
Ca	2.514865000	-0.569335000	-2.495751000
Ca	-0.227457000	2.193130000	-2.829128000
Ca	-1.305281000	-0.831600000	-3.242224000
Ca	0.398958000	-3.447363000	-0.904876000
Ca	-3.301957000	1.261948000	-0.616375000
Ca	-2.551114000	-2.510781000	0.062434000
Ca	-2.526385000	0.574020000	2.452666000
Ca	0.199765000	-2.197575000	2.797892000
H	-1.020672000	-3.618970000	-3.896119000
H	-0.824112000	-3.784694000	-4.607651000
H	3.380475000	2.705914000	3.117892000
H	3.959191000	2.533846000	3.570364000
H	5.472547000	0.393493000	-2.809856000
H	5.045126000	0.514421000	-2.193476000
H	-5.108755000	-1.514483000	-0.537200000
H	-5.510453000	-1.946282000	-1.009024000
H	4.200650000	-0.568305000	3.360735000
H	4.894644000	-0.321950000	3.530363000
H	2.217168000	4.227586000	-2.494830000
H	2.822022000	4.419601000	-2.907090000

H	3.024301000	-5.127140000	-0.100144000
H	2.999407000	-4.433472000	-0.399587000
H	-2.363784000	3.820788000	2.887123000
H	-2.176598000	4.301323000	3.439812000
H	-2.241575000	-4.530162000	3.328037000
H	-1.870021000	-4.313406000	2.705870000
H	2.338015000	-3.856711000	-2.911984000
H	2.133101000	-4.351444000	-3.445109000
H	-5.459678000	0.061638000	1.356754000
H	-6.123597000	0.350792000	1.579290000
H	-3.996588000	3.504894000	-2.831032000
H	-3.516973000	2.923189000	-2.903294000
H	1.875318000	-1.658001000	-5.483940000
H	1.492959000	-1.133903000	-5.093817000
H	2.581838000	5.369596000	2.060862000
H	2.286937000	4.673272000	2.088219000
H	-3.396568000	-2.626870000	-3.206472000
H	-3.946173000	-2.422035000	-3.680554000
H	0.290398000	0.435987000	6.103919000
H	-0.090609000	0.201785000	5.489522000
H	3.480651000	-3.032611000	2.702827000
H	3.935174000	-3.615847000	2.548882000
H	-6.223694000	1.189461000	-0.980264000
H	-6.077957000	1.553423000	-1.615159000
H	-5.173849000	3.066174000	1.888361000
H	-4.444078000	2.976557000	1.712142000
H	0.041473000	1.075395000	-5.476491000
H	-0.271684000	1.485736000	-6.030128000
H	0.713770000	3.631292000	4.625868000
H	0.923823000	3.526237000	3.907678000
H	2.339557000	-1.887511000	4.649275000

H	2.190929000	-2.175798000	5.332930000
H	-0.969396000	5.146985000	-2.902667000
H	-0.512782000	4.850751000	-2.378433000
H	5.920169000	1.256514000	0.697951000
H	5.314526000	1.084533000	0.276396000
H	-4.481134000	-2.125932000	2.045709000
H	-4.671831000	-2.762522000	2.404383000
H	-2.007235000	-1.403478000	4.830721000
H	-2.469845000	-1.857065000	5.221637000
H	3.009842000	1.730324000	-4.753961000
H	2.367533000	1.384092000	-4.563390000
H	0.995358000	5.475593000	-0.569980000
H	0.988701000	6.150976000	-0.229930000
H	-2.954792000	4.452057000	0.295831000
H	-2.942639000	5.141306000	-0.013648000
H	5.118794000	3.870398000	0.441005000
H	4.678462000	4.382578000	0.757609000
H	-3.025843000	-5.149906000	-1.753554000
H	-2.583417000	-4.560728000	-1.926784000
H	-0.986793000	-5.468286000	0.503553000
H	-0.974483000	-6.134406000	0.145029000
H	0.693426000	-4.830689000	2.178018000
H	1.209292000	-5.128258000	2.640747000
H	6.141342000	-2.090457000	0.893806000
H	6.232893000	-1.367285000	0.736629000
H	4.446076000	-2.835022000	-1.852718000
H	5.167559000	-2.837666000	-2.078857000
H	-3.086218000	0.885242000	-4.516813000
H	-3.286617000	0.626476000	-5.202887000
H	-4.547326000	0.104678000	4.574652000
H	-5.013789000	0.176038000	3.996705000

$Ca_{12}O_{12}\cdot 38H_2$, ωB97XD/6-31++G(d,p)

Energy: -9079.68395489 E_h

O	3.407211000	0.771903000	-0.636190000
O	1.936123000	2.391851000	1.677702000
O	2.228899000	-1.439791000	2.364113000
O	-0.463073000	-3.067628000	1.807597000
O	-1.006583000	0.474969000	3.350007000
O	-1.915527000	2.703755000	1.255612000
O	-3.438156000	-0.838257000	0.603187000
O	-2.271750000	1.380358000	-2.390768000
O	-1.995167000	-2.448404000	-1.741523000
O	0.979703000	-0.544319000	-3.403292000
O	0.428419000	2.989634000	-1.862924000
O	1.870771000	-2.748668000	-1.284131000
Ca	-1.646179000	3.020004000	-0.941157000
Ca	-2.834334000	0.773443000	2.030194000
Ca	-0.093376000	2.404900000	2.586012000
Ca	-3.186367000	-0.511844000	-1.631783000
Ca	-2.247108000	-2.773068000	0.491186000
Ca	0.139801000	-1.430390000	3.264805000
Ca	1.628198000	-3.075385000	0.903209000
Ca	0.057576000	-2.469588000	-2.627047000
Ca	3.129787000	0.459253000	1.599407000
Ca	2.798376000	-0.836133000	-2.065652000
Ca	2.216834000	2.709208000	-0.546239000
Ca	-0.195622000	1.355319000	-3.315793000
H	2.141891000	-4.281659000	-2.796484000
H	2.058472000	-4.742172000	-3.395666000
H	-3.918968000	3.579855000	0.670278000
H	-4.528791000	3.829336000	0.300238000
H	-4.690195000	-1.381743000	3.326426000

H	-4.477847000	-1.372945000	2.602678000
H	5.258555000	-0.550516000	-0.690600000
H	5.746936000	-1.118665000	-0.786840000
H	-2.964190000	3.217537000	-3.465848000
H	-3.119375000	3.928371000	-3.673458000
H	-2.310257000	1.155206000	4.921444000
H	-2.852095000	1.422819000	5.381355000
H	-4.777120000	-3.148211000	-2.515645000
H	-4.041475000	-3.118381000	-2.340260000
H	1.653102000	4.578272000	2.158078000
H	1.368544000	5.251719000	2.353420000
H	2.353536000	1.453363000	-5.217457000
H	2.104209000	0.851548000	-4.836675000
H	-1.829431000	-4.611249000	-2.263673000
H	-1.602733000	-5.307266000	-2.456859000
H	5.205132000	1.968380000	-0.167278000
H	5.751374000	2.433142000	0.076500000
H	3.597602000	-0.038182000	4.674093000
H	3.242687000	-0.509091000	4.202776000
H	-1.216415000	-5.749891000	0.610634000
H	-0.935273000	-5.171470000	1.005704000
H	-3.058370000	4.025232000	3.662376000
H	-2.814909000	3.755434000	2.998914000
H	-5.381072000	-3.099357000	0.403672000
H	-5.023299000	-2.434855000	0.455093000
H	3.792755000	-3.801065000	-0.828520000
H	4.388658000	-4.131762000	-0.498473000
H	1.077308000	5.793665000	-1.105544000
H	0.847336000	5.131400000	-1.390901000
H	-3.272384000	0.695138000	-4.272169000
H	-3.613195000	0.316137000	-4.831180000

H	6.024340000	0.740679000	2.168878000
H	5.920828000	0.123624000	2.574774000
H	4.471880000	3.273530000	2.797382000
H	3.772325000	3.148940000	2.529203000
H	1.970345000	-5.944803000	1.507251000
H	2.405316000	-5.939130000	0.900920000
H	-1.525418000	5.653636000	0.824578000
H	-1.665516000	4.955720000	1.078321000
H	-0.281659000	4.402364000	-4.378778000
H	-0.073199000	4.177373000	-3.686821000
H	2.517882000	-2.861053000	4.074231000
H	2.425874000	-3.326953000	4.662701000
H	-6.076663000	0.532561000	0.603223000
H	-5.443464000	0.118376000	0.595082000
H	4.575817000	1.263422000	-2.519438000
H	4.840855000	1.276197000	-3.227114000
H	2.262821000	3.683006000	-3.120466000
H	2.968841000	3.817144000	-3.345786000
H	0.537732000	-5.219521000	3.574246000
H	0.220967000	-4.685754000	3.141048000
H	0.126775000	0.491886000	5.305506000
H	0.600688000	0.350635000	5.878249000
H	-0.108796000	3.707081000	5.277562000
H	-0.546663000	3.112892000	5.387414000
H	-5.063058000	2.235119000	3.359663000
H	-5.480452000	1.722463000	3.014605000
H	2.886430000	-2.071669000	-5.100996000
H	2.329956000	-1.663574000	-4.789960000
H	-2.195720000	-2.676822000	-4.781804000
H	-2.312700000	-2.661302000	-4.037331000
H	-0.033003000	-0.570571000	-5.401876000

H	-0.476680000	-0.434890000	-5.999703000
H	-4.541010000	1.818495000	-2.201289000
H	-5.273379000	1.757409000	-2.032076000
H	-2.817432000	-3.994152000	3.420066000
H	-2.146291000	-3.831621000	3.113321000
H	4.313482000	-2.251329000	2.365766000
H	5.026194000	-2.482768000	2.264976000
H	3.895752000	5.179411000	-0.649088000
H	4.366625000	4.738258000	-0.274540000

$Ca_{12}O_{12}\cdot 39H_2$, ωB97XD/6-31++G(d,p)

Energy: -9080.85280673 E_h

O	3.432078000	0.838653000	0.652410000
O	2.462609000	-2.077229000	1.488286000
O	2.265903000	-1.387790000	-2.349330000
O	-0.683338000	-0.742656000	-3.378435000
O	-0.525616000	-3.445437000	-0.570357000
O	-1.324336000	-2.362489000	2.323256000
O	-3.401960000	-0.802282000	-0.592447000
O	-2.249901000	1.438362000	2.391974000
O	-2.470687000	2.130539000	-1.442538000
O	0.552054000	3.485543000	0.626786000
O	0.694332000	0.797627000	3.428566000
O	1.342556000	2.392641000	-2.255131000
Ca	-1.253592000	-0.370476000	3.338760000
Ca	-2.422305000	-2.581586000	0.343025000
Ca	0.569207000	-3.232808000	1.402920000
Ca	-3.338254000	1.218020000	0.450672000
Ca	-2.531695000	0.112045000	-2.486354000
Ca	0.312355000	-2.551520000	-2.426189000
Ca	1.263216000	0.424875000	-3.292944000

Ca	-0.546319000	3.271173000	-1.340647000
Ca	3.342027000	-1.176744000	-0.398295000
Ca	2.443421000	2.614772000	-0.285627000
Ca	2.539627000	-0.065553000	2.542472000
Ca	-0.297388000	2.609130000	2.487244000
H	1.397835000	4.451137000	-2.927248000
H	1.257646000	5.189427000	-3.046373000
H	-3.124415000	-2.436632000	3.655880000
H	-3.690078000	-2.269327000	4.130173000
H	-4.436247000	-3.288345000	-1.996134000
H	-4.299250000	-2.598503000	-1.722545000
H	5.094796000	1.639515000	-0.630823000
H	5.517168000	2.004671000	-1.141082000
H	2.531065000	-2.207514000	-5.192992000
H	2.568001000	-2.039869000	-4.455224000
H	-4.312035000	0.992145000	3.141773000
H	-5.038613000	0.795599000	3.219565000
H	-1.818914000	-5.188720000	-0.552993000
H	-2.395051000	-5.676640000	-0.470682000
H	-5.162918000	2.646844000	-2.525734000
H	-4.462844000	2.568919000	-2.246668000
H	3.275831000	-2.619234000	3.442073000
H	3.520265000	-2.616332000	4.161567000
H	2.375401000	5.446275000	1.789560000
H	1.840154000	4.987672000	1.506667000
H	-2.397855000	3.287057000	-3.428862000
H	-2.176942000	3.702783000	-4.019046000
H	5.344296000	0.241350000	1.562019000
H	5.924823000	-0.064918000	1.941980000
H	4.034496000	-3.792785000	-2.239980000
H	3.572437000	-3.215299000	-2.397632000

H	-1.227523000	0.048652000	-6.100598000
H	-1.092230000	-0.194957000	-5.391671000
H	-1.969058000	-5.237492000	2.747588000
H	-1.852091000	-4.490182000	2.734553000
H	-5.808842000	-0.111898000	-2.213438000
H	-5.285535000	-0.342888000	-1.719312000
H	3.111384000	2.594676000	-3.584035000
H	3.686160000	2.491804000	-4.067368000
H	-0.207835000	0.436991000	6.162310000
H	0.145447000	0.607337000	5.510466000
H	-3.486853000	3.362742000	2.289813000
H	-3.910656000	3.946009000	2.067126000
H	6.260875000	-1.572798000	-0.202180000
H	6.180241000	-1.980102000	-0.821747000
H	4.205090000	-4.384914000	0.919772000
H	3.761697000	-3.810187000	1.139014000
H	1.133219000	1.104712000	-6.171594000
H	1.710329000	1.549450000	-6.010120000
H	-0.250038000	-3.086879000	5.043114000
H	-0.566282000	-3.012459000	4.360958000
H	-2.464447000	2.409267000	4.398824000
H	-2.355721000	2.768703000	5.055884000
H	1.388831000	-4.522675000	-4.349373000
H	1.056241000	-5.014613000	-3.897928000
H	-5.767950000	-1.506445000	1.081825000
H	-5.212701000	-1.330540000	0.599186000
H	4.385656000	2.572977000	1.782319000
H	4.554595000	3.247037000	2.077158000
H	1.742986000	2.411428000	4.539931000
H	2.039091000	3.056550000	4.805538000
H	-2.050492000	-3.122274000	-4.559887000

H	-1.768927000	-2.447353000	-4.364496000
H	0.701702000	-5.247627000	-1.006454000
H	1.194649000	-5.804036000	-1.153164000
H	1.186940000	-6.061980000	2.188894000
H	1.100597000	-6.142680000	1.452459000
H	-4.345875000	-4.466435000	1.600306000
H	-4.853982000	-4.014547000	1.294378000
H	3.902228000	5.065231000	-1.164375000
H	3.655606000	5.309032000	-0.504195000
H	-3.123130000	5.005919000	-0.816282000
H	-3.119336000	4.271882000	-0.994466000
H	-0.704415000	5.207254000	1.340716000
H	-1.197714000	5.661147000	1.692018000
H	-6.156803000	2.156958000	0.644818000
H	-6.059530000	2.209707000	-0.092848000
H	-4.109649000	1.203228000	-4.745146000
H	-3.613587000	0.815910000	-5.146020000
H	4.292844000	-0.714674000	-3.102591000
H	4.985345000	-0.430070000	-3.201542000
H	4.152273000	1.141167000	4.707278000
H	4.732545000	0.905246000	4.302251000

$Ca_{12}O_{12}\cdot 40H_2$, ωB97XD/6-31++G(d,p)

Energy: -9082.01800634 E_h

O	3.203964000	1.252505000	0.987837000
O	1.798352000	-0.832175000	2.946057000
O	2.640729000	-2.296483000	-0.566226000
O	0.116144000	-2.482573000	-2.510607000
O	-0.695526000	-3.268502000	1.223353000
O	-2.080209000	-0.854833000	2.789720000
O	-3.225617000	-1.214327000	-0.922856000

O	-2.663027000	2.340249000	0.602661000
O	-1.837092000	0.856831000	-2.911669000
O	0.671262000	3.292037000	-1.173664000
O	-0.138135000	2.523359000	2.541181000
O	2.068220000	0.888938000	-2.729433000
Ca	-2.097960000	1.374131000	2.581420000
Ca	-2.672712000	-2.161131000	1.027045000
Ca	-0.107392000	-1.967365000	2.992331000
Ca	-3.236646000	1.051399000	-1.132123000
Ca	-1.832875000	-1.405289000	-2.709247000
Ca	0.680895000	-3.445936000	-0.531409000
Ca	2.078482000	-1.325987000	-2.546059000
Ca	0.089123000	1.992405000	-2.942362000
Ca	3.206669000	-1.013098000	1.178391000
Ca	2.650263000	2.195858000	-0.965514000
Ca	1.785290000	1.435213000	2.759615000
Ca	-0.694756000	3.491310000	0.564257000
H	2.410749000	2.248324000	-4.406065000
H	2.342597000	2.781995000	-4.942381000
H	-4.163482000	-0.295613000	3.458258000
H	-4.804045000	0.077927000	3.606788000
H	-4.146397000	-4.098791000	-0.998352000
H	-4.009052000	-3.365290000	-1.111293000
H	5.231313000	1.359894000	0.029348000
H	5.823869000	1.421517000	-0.436097000
H	3.904049000	-4.443396000	-2.147311000
H	3.622870000	-3.901834000	-1.698495000
H	-4.856335000	2.188501000	1.032506000
H	-5.589638000	2.012192000	1.087795000
H	-1.356287000	-5.186305000	0.199601000
H	-1.443138000	-5.753024000	-0.292900000

H	-4.050322000	0.143423000	-4.758091000
H	-3.494955000	0.429512000	-4.331480000
H	1.987108000	-0.201619000	5.035398000
H	2.022285000	0.195266000	5.682013000
H	2.428737000	5.603454000	-0.704387000
H	1.902854000	5.075021000	-0.843873000
H	-3.298919000	4.896052000	1.989801000
H	-3.274845000	4.227186000	1.636401000
H	-1.182053000	0.860468000	-5.118460000
H	-0.785319000	0.948964000	-5.754497000
H	4.739165000	1.349154000	2.575342000
H	5.151771000	1.329012000	3.210770000
H	4.160438000	-4.024727000	1.373025000
H	3.795067000	-3.715289000	0.788658000
H	1.687021000	-4.539955000	-3.972536000
H	1.216261000	-4.053564000	-3.635442000
H	-3.010065000	-2.900716000	4.721145000
H	-2.845161000	-2.330410000	4.251981000
H	-5.513399000	-1.386161000	-2.788914000
H	-4.958286000	-1.374114000	-2.274242000
H	4.209678000	0.868307000	-3.304861000
H	4.958375000	0.849583000	-3.418832000
H	-1.755283000	3.670577000	4.661280000
H	-1.228722000	3.475816000	4.148080000
H	-3.742960000	3.781298000	-0.791398000
H	-4.084102000	4.102371000	-1.383972000
H	5.835693000	-1.122369000	2.518763000
H	5.885088000	-1.803939000	2.220014000
H	3.095684000	-3.122107000	4.287599000
H	2.784910000	-2.497053000	3.991766000
H	4.371336000	-2.500672000	-4.003601000

H	4.448097000	-1.800240000	-4.248735000
H	-1.761524000	0.249886000	5.605447000
H	-1.882819000	-0.143459000	4.973099000
H	-1.804415000	6.126602000	-0.306022000
H	-1.256546000	6.019296000	-0.801193000
H	1.959907000	-5.991371000	-1.303610000
H	1.412122000	-6.308110000	-0.908725000
H	-5.732917000	-1.335011000	0.760772000
H	-5.206239000	-1.273031000	0.223386000
H	3.999116000	3.368142000	1.262936000
H	4.153295000	4.104908000	1.207520000
H	0.736052000	4.547315000	2.842449000
H	1.008759000	5.251967000	2.784538000
H	-1.925360000	-4.483232000	-3.396347000
H	-1.304977000	-4.095385000	-3.203582000
H	0.778159000	-4.892534000	1.927521000
H	1.374918000	-5.345040000	2.016207000
H	-1.942479000	-5.097800000	3.194921000
H	-1.608738000	-4.686163000	2.654621000
H	-4.372282000	-4.051575000	2.523691000
H	-4.878521000	-3.910970000	1.994410000
H	4.458998000	3.632691000	-2.801645000
H	4.234808000	4.237760000	-2.427987000
H	-2.656512000	3.480608000	-4.114138000
H	-2.557716000	2.776744000	-3.857968000
H	0.116537000	4.815009000	-2.619925000
H	-0.131868000	5.214348000	-3.216402000
H	-5.942594000	1.851789000	-2.075234000
H	-5.911301000	1.167200000	-2.369863000
H	-0.279521000	-2.047688000	-5.476863000
H	-0.087486000	-2.257552000	-4.777582000

H	4.877324000	-1.892274000	-0.935558000
H	5.577576000	-1.612886000	-0.925719000
H	2.826020000	3.705435000	4.337576000
H	3.467846000	3.325330000	4.331418000

$Ca_{12}O_{12}\cdot 41H_2$, ωB97XD/6-31++G(d,p)

Energy: -9083.18296194 E_h

O	-3.161188000	1.420324000	0.930299000
O	-3.039996000	-0.105424000	-1.869264000
O	-2.342386000	-2.383535000	1.231390000
O	0.751889000	-2.998536000	1.705008000
O	-0.284711000	-2.862140000	-2.052043000
O	0.504502000	-0.136287000	-3.505362000
O	3.136930000	-1.362843000	-0.904261000
O	2.330207000	2.443355000	-1.197536000
O	3.020348000	0.165865000	1.895524000
O	0.259265000	2.932052000	2.085786000
O	-0.763269000	3.053784000	-1.662204000
O	-0.526518000	0.199631000	3.516844000
Ca	0.843216000	1.976262000	-2.855223000
Ca	1.678525000	-1.823351000	-2.535905000
Ca	-1.457554000	-1.178377000	-3.028943000
Ca	3.486932000	0.783617000	-0.241715000
Ca	2.674169000	-1.983617000	1.233766000
Ca	-0.729294000	-3.474347000	0.053393000
Ca	-0.850914000	-1.908285000	2.887046000
Ca	1.437685000	1.245207000	3.050888000
Ca	-3.501058000	-0.727762000	0.269998000
Ca	-1.702605000	1.879448000	2.562642000
Ca	-2.691521000	2.043726000	-1.204437000
Ca	0.716618000	3.533248000	-0.017816000

H	0.130124000	0.878020000	5.464387000
H	0.521036000	1.184586000	6.040215000
H	2.232146000	0.543879000	-4.824657000
H	2.808251000	0.927814000	-5.126919000
H	3.642807000	-4.248498000	-1.709905000
H	3.656472000	-3.540297000	-1.451072000
H	-4.416028000	1.281752000	2.821355000
H	-4.641032000	1.245790000	3.542008000
H	-2.601599000	-4.874513000	2.819874000
H	-2.644666000	-4.254307000	2.386985000
H	4.159826000	2.275105000	-2.528859000
H	4.795539000	2.048158000	-2.868568000
H	0.557261000	-4.957700000	-1.999556000
H	0.810839000	-5.638717000	-1.792419000
H	5.816658000	-0.709244000	2.313934000
H	5.116085000	-0.428483000	2.256114000
H	-3.476801000	0.555499000	-4.006631000
H	-3.446319000	0.709703000	-4.745368000
H	-0.947425000	5.655984000	1.631080000
H	-0.678190000	5.001764000	1.895532000
H	2.691577000	4.992889000	-2.675471000
H	2.695035000	4.346753000	-2.281425000
H	3.377146000	-0.547122000	4.057284000
H	3.302832000	-0.719429000	4.788034000
H	-5.283494000	1.902918000	0.516774000
H	-5.990427000	2.038953000	0.283942000
H	-4.690628000	-3.717919000	-0.034869000
H	-4.075703000	-3.504044000	0.350468000
H	1.733735000	-4.211574000	4.167654000
H	1.475357000	-3.939133000	3.506837000
H	-5.175289000	0.369360000	-2.177425000

H	-5.903295000	0.574399000	-2.209897000
H	0.426584000	-1.630878000	-6.066868000
H	0.485253000	-1.199336000	-5.448270000
H	5.951420000	-2.019411000	-0.240929000
H	5.249836000	-1.871436000	-0.482463000
H	-2.118071000	-0.403970000	4.966460000
H	-2.669542000	-0.755805000	5.348241000
H	-0.287845000	4.721522000	-3.988323000
H	-0.506612000	4.386999000	-3.341511000
H	4.001029000	3.590016000	-0.189486000
H	4.578958000	3.816233000	0.241645000
H	-6.453625000	-0.627927000	0.345647000
H	-6.401072000	-1.313469000	0.634718000
H	-4.339003000	-2.443024000	-3.252485000
H	-4.164691000	-1.813602000	-2.872618000
H	-0.498666000	-3.523581000	5.345208000
H	-0.990239000	-3.043447000	5.635767000
H	-0.640107000	1.695220000	-5.626878000
H	-0.380467000	1.123149000	-5.208414000
H	1.756554000	6.240661000	-0.561722000
H	1.417517000	6.415335000	0.079376000
H	-1.557988000	-6.217478000	0.780407000
H	-1.214363000	-6.410163000	0.147146000
H	4.626633000	-1.262860000	-3.511171000
H	4.398732000	-1.278774000	-2.790653000
H	-3.712671000	3.551988000	1.568106000
H	-3.708281000	4.240685000	1.877205000
H	-2.107440000	4.823180000	-1.302650000
H	-2.681219000	5.280553000	-1.116632000
H	2.120445000	-5.549025000	0.936099000
H	1.772698000	-4.933908000	1.205358000

H	-2.046571000	-4.340157000	-2.269746000
H	-2.633024000	-4.793501000	-2.133023000
H	-0.443995000	-4.049102000	-4.762926000
H	-0.380950000	-3.825632000	-4.042555000
H	2.195209000	-3.629973000	-4.807599000
H	2.912743000	-3.566902000	-4.613977000
H	-0.550054000	3.987951000	4.753008000
H	-0.244239000	3.825220000	4.080413000
H	4.370164000	2.429312000	3.319876000
H	4.173836000	1.812344000	2.929398000
H	1.854744000	4.424433000	2.587730000
H	2.441829000	4.899156000	2.627878000
H	6.401290000	1.372355000	-0.378333000
H	6.425960000	0.715974000	-0.025009000
H	4.743944000	-3.232974000	2.943589000
H	4.177741000	-3.692399000	3.102084000
H	-4.096428000	-2.178468000	2.663861000
H	-4.696978000	-1.948017000	3.059268000
H	-4.639911000	3.672702000	-2.738777000
H	-5.035446000	3.042551000	-2.682234000

$Ca_{12}O_{12}\cdot 42H_2$, ωB97XD/6-31++G(d,p)

Energy: -9084.35047169 E_h

O	2.405554000	-2.527056000	-0.757414000
O	3.347496000	0.490232000	-1.176752000
O	2.463863000	-0.422193000	2.525102000
O	-0.408871000	0.601354000	3.467311000
O	1.458214000	3.048816000	1.073467000
O	0.421580000	2.972846000	-1.939357000
O	-2.396190000	2.528813000	0.728981000
O	-2.463340000	0.413680000	-2.555444000

O	-3.339840000	-0.492214000	1.141972000
O	-1.440015000	-3.060716000	-1.111411000
O	0.409306000	-0.605394000	-3.492263000
O	-0.418440000	-2.974099000	1.902843000
Ca	-0.554259000	1.438723000	-3.241599000
Ca	-0.517474000	3.534073000	0.054845000
Ca	2.395878000	2.498634000	-0.912723000
Ca	-3.390990000	0.971355000	-0.597559000
Ca	-2.341114000	1.061496000	2.467697000
Ca	1.503076000	1.624621000	2.783180000
Ca	0.544165000	-1.443729000	3.203654000
Ca	-2.390477000	-2.503097000	0.872793000
Ca	3.396665000	-0.970084000	0.567107000
Ca	0.524349000	-3.533330000	-0.084747000
Ca	2.346381000	-1.067679000	-2.499125000
Ca	-1.494384000	-1.632268000	-2.818028000
H	-1.176046000	-4.928316000	2.287549000
H	-1.494148000	-5.617233000	2.349557000
H	-1.068491000	4.197031000	-3.152438000
H	-1.635202000	4.418221000	-3.600208000
H	-1.950986000	4.961572000	2.491995000
H	-2.206235000	4.358221000	2.117457000
H	3.228854000	-4.259351000	0.459134000
H	3.326525000	-4.842330000	0.929153000
H	2.867426000	-0.427329000	5.468235000
H	2.884229000	-0.425155000	4.710856000
H	-3.870402000	2.043271000	-3.182166000
H	-4.360315000	2.619413000	-3.203836000
H	1.394522000	5.203198000	1.288451000
H	1.217318000	5.941638000	1.271370000
H	-5.483684000	-2.320815000	0.064063000

H	-5.064105000	-1.769118000	0.363181000
H	4.151654000	1.712686000	-2.929063000
H	4.270220000	2.248380000	-3.448435000
H	-0.882976000	-4.864838000	-3.421291000
H	-1.052726000	-4.508448000	-2.775554000
H	-3.120544000	-0.125024000	-5.403116000
H	-3.043526000	0.086044000	-4.680124000
H	-5.281110000	0.178918000	1.901289000
H	-5.919798000	0.476902000	2.180021000
H	4.397945000	-3.151352000	-1.521467000
H	5.084764000	-3.258968000	-1.818756000
H	5.199927000	0.753787000	2.861540000
H	4.508137000	0.451233000	2.888437000
H	-1.530982000	-0.061890000	6.042014000
H	-1.219144000	0.142103000	5.377636000
H	5.305513000	-0.201771000	-1.870615000
H	5.954632000	-0.507897000	-2.113947000
H	1.298610000	5.808132000	-2.000662000
H	1.062248000	5.093616000	-2.074000000
H	-4.872206000	3.113408000	2.292754000
H	-4.284308000	3.073981000	1.819449000
H	1.042779000	-4.188045000	3.171041000
H	1.591226000	-4.396817000	3.647381000
H	-0.014669000	0.412150000	-6.176259000
H	0.150734000	0.026495000	-5.541904000
H	-4.558315000	-0.491325000	-2.728496000
H	-5.249407000	-0.763184000	-2.595137000
H	6.299741000	-1.440038000	0.326461000
H	6.277087000	-1.533422000	1.066152000
H	-4.070971000	-1.706830000	2.958728000
H	-4.163316000	-2.234794000	3.489941000

H	5.475134000	2.267678000	0.028076000
H	5.057511000	1.736302000	-0.307445000
H	-0.132306000	-2.240870000	5.971149000
H	0.119179000	-2.910081000	5.757350000
H	1.589326000	3.357009000	-4.674637000
H	1.358476000	3.387557000	-3.955133000
H	-3.587619000	-2.722917000	-4.621965000
H	-3.537238000	-3.300426000	-4.152399000
H	3.058787000	2.248665000	5.225645000
H	3.150032000	2.913962000	4.901324000
H	-3.898342000	4.610603000	-0.782231000
H	-3.545867000	4.107322000	-0.341529000
H	2.294860000	-4.403464000	-2.057923000
H	2.059810000	-5.032866000	-2.402907000
H	1.128545000	-2.304291000	-4.764861000
H	1.498810000	-2.896922000	-5.056789000
H	-0.317431000	3.177124000	4.983229000
H	-0.440107000	2.489871000	4.691233000
H	3.335415000	3.739071000	2.036765000
H	3.969095000	3.851715000	2.436646000
H	4.034191000	5.032307000	-0.816778000
H	3.701591000	4.995478000	-0.150245000
H	-1.061704000	6.320832000	-0.820490000
H	-1.746420000	6.167772000	-0.567888000
H	0.805176000	-6.499947000	0.099439000
H	0.271108000	-6.387671000	0.608100000
H	-4.356147000	-4.740588000	1.067301000
H	-3.883629000	-4.971713000	1.595791000
H	-3.283611000	-4.100913000	-1.600918000
H	-3.970788000	-4.402480000	-1.714664000
H	-6.237961000	1.795913000	-0.882925000

H	-6.241059000	1.577850000	-0.169606000
H	-4.437924000	0.801841000	4.550048000
H	-3.845397000	0.789226000	5.003359000
H	3.844501000	-2.124642000	3.085639000
H	4.320455000	-2.711740000	3.072746000
H	4.122093000	-1.213075000	-4.871833000
H	4.638143000	-1.066442000	-4.353223000

$Ca_{12}O_{12}\cdot 43H_2$, ωB97XD/6-31++G(d,p)

Energy: -9085.51378215 E_h

O	-2.107096000	-2.810119000	0.737334000
O	-3.524665000	0.042642000	0.538409000
O	-1.849397000	-1.132179000	-2.785713000
O	0.971256000	0.239909000	-3.358159000
O	-1.636568000	2.618108000	-1.711010000
O	-1.197192000	3.058267000	1.414867000
O	2.111961000	2.781461000	-0.638037000
O	1.856713000	1.105715000	2.881910000
O	3.528984000	-0.071514000	-0.439264000
O	1.642634000	-2.648325000	1.817075000
O	-0.963160000	-0.262851000	3.452062000
O	1.195821000	-3.077972000	-1.309797000
Ca	-0.275593000	1.871643000	3.072220000
Ca	0.014921000	3.536354000	-0.448214000
Ca	-2.848055000	2.138552000	0.151033000
Ca	3.047267000	1.577993000	1.049232000
Ca	2.599076000	1.133855000	-2.129943000
Ca	-1.155239000	0.999818000	-3.176826000
Ca	0.288225000	-1.892137000	-2.973282000
Ca	2.851440000	-2.166885000	-0.046993000
Ca	-3.040178000	-1.604974000	-0.951673000

Ca	-0.009711000	-3.564224000	0.554145000
Ca	-2.587917000	-1.160460000	2.228268000
Ca	1.162358000	-1.025043000	3.278255000
H	2.645337000	-3.646042000	-2.939524000
H	3.085859000	-3.708917000	-3.549927000
H	-0.163070000	4.639758000	2.714920000
H	0.265030000	4.985853000	3.231310000
H	1.701613000	4.945775000	-2.712749000
H	1.960151000	4.421626000	-2.235081000
H	-2.332223000	-4.832770000	-0.306497000
H	-2.193182000	-5.481399000	-0.667492000
H	-1.914339000	-1.296297000	-5.747236000
H	-1.985107000	-1.305549000	-4.993328000
H	2.739419000	3.043117000	3.579028000
H	3.060759000	3.721995000	3.665795000
H	-1.134947000	3.792615000	-3.581111000
H	-0.898949000	4.009020000	-4.265609000
H	5.684052000	-1.313303000	1.249582000
H	5.241929000	-0.897203000	0.800349000
H	-4.745904000	1.126145000	2.148966000
H	-5.020219000	1.575378000	2.689274000
H	0.827680000	-3.936138000	4.429235000
H	1.077276000	-3.768423000	3.736853000
H	2.064487000	0.772493000	5.836247000
H	2.086233000	0.980698000	5.109025000
H	5.436384000	0.895064000	-1.007927000
H	6.026569000	1.299810000	-1.253976000
H	-4.061754000	-3.744781000	1.141266000
H	-4.764847000	-3.991536000	1.273638000
H	-3.013476000	5.256090000	-1.659776000
H	-2.669493000	4.589213000	-1.751641000

H	-4.719563000	-0.628777000	-3.517641000
H	-3.974396000	-0.747253000	-3.477773000
H	2.353334000	-0.736901000	-5.693052000
H	1.989311000	-0.428583000	-5.099719000
H	-5.437095000	-0.987499000	1.020438000
H	-6.027377000	-1.421629000	1.206904000
H	-2.510200000	5.690637000	1.156673000
H	-2.169006000	5.025664000	1.279269000
H	4.762174000	3.884909000	-1.357355000
H	4.064871000	3.670273000	-1.155321000
H	0.146740000	-4.638883000	-2.638951000
H	-0.281083000	-4.967551000	-3.166543000
H	-1.173461000	1.190130000	5.971229000
H	-1.171121000	0.690006000	5.399057000
H	4.022840000	0.735611000	3.517134000
H	4.771334000	0.636567000	3.516882000
H	-5.638359000	-3.005058000	-1.097841000
H	-5.553247000	-2.934881000	-1.835441000
H	4.830340000	-1.353468000	-1.824283000
H	5.121463000	-1.926569000	-2.219900000
H	-5.716681000	1.414253000	-0.974678000
H	-5.269577000	0.953598000	-0.575215000
H	0.824319000	-2.850438000	-5.727610000
H	0.546984000	-3.497961000	-5.483075000
H	-2.893117000	3.468791000	3.880974000
H	-2.554236000	3.483010000	3.206365000
H	3.971068000	-2.419461000	3.728548000
H	3.460064000	-2.613111000	3.207552000
H	-2.000850000	1.299403000	-6.003321000
H	-2.005404000	2.027364000	-5.840997000
H	2.368885000	5.388143000	0.851173000

H	2.440392000	4.750566000	0.453144000
H	-1.975524000	-4.416973000	2.360434000
H	-1.729598000	-4.928721000	2.858191000
H	-1.490457000	-1.836064000	4.948315000
H	-1.705433000	-2.432134000	5.362180000
H	1.865325000	2.663951000	-4.917127000
H	1.579956000	2.017976000	-4.648901000
H	-3.508289000	2.590327000	-3.029100000
H	-4.055386000	2.407662000	-3.515397000
H	-5.244614000	3.831968000	0.656307000
H	-4.718420000	4.356907000	0.718534000
H	-0.604643000	6.425876000	-0.539027000
H	0.096958000	6.495433000	-0.782185000
H	2.086016000	-5.858428000	-0.759782000
H	1.918708000	-5.161130000	-1.000144000
H	4.674648000	-4.475200000	0.220464000
H	5.143091000	-4.058545000	-0.183583000
H	2.600307000	-4.630034000	1.967267000
H	2.905634000	-5.322308000	1.945922000
H	5.482578000	3.095959000	1.836876000
H	5.468802000	3.259718000	1.109275000
H	4.909488000	0.672872000	-3.944332000
H	4.354190000	0.548707000	-4.427024000
H	-2.771933000	-3.115874000	-3.352577000
H	-3.118783000	-3.787188000	-3.360006000
H	-4.290429000	-2.493745000	4.260832000
H	-4.623006000	-2.769187000	3.652491000

$Ca_{12}O_{12}\cdot 44H_2$, ωB97XD/6-31++G(d,p)

Energy: -9086.68206203 E_h

O	0.796343000	3.474860000	0.212410000
O	3.061949000	1.435384000	1.152176000
O	2.115443000	1.139767000	-2.627337000
O	0.178253000	-1.307744000	-3.282223000
O	2.835628000	-2.083952000	-0.538315000
O	1.682813000	-1.986803000	2.431297000
O	-0.805937000	-3.462383000	-0.188308000
O	-2.126251000	-1.130501000	2.644480000
O	-3.071207000	-1.422083000	-1.133457000
O	-2.856284000	2.100022000	0.558088000
O	-0.195917000	1.319377000	3.292380000
O	-1.677623000	1.996494000	-2.397640000
Ca	-0.007620000	-0.939933000	3.453704000
Ca	1.277320000	-3.279976000	0.606957000
Ca	3.240358000	-0.790441000	1.286961000
Ca	-2.529913000	-2.400306000	0.847291000
Ca	-1.345718000	-2.485138000	-2.169473000
Ca	2.293212000	-1.123719000	-2.485134000
Ca	-0.008811000	0.952248000	-3.429327000
Ca	-3.249947000	0.803228000	-1.270660000
Ca	2.513209000	2.410524000	-0.828601000
Ca	-1.286819000	3.290044000	-0.582968000
Ca	1.337026000	2.497035000	2.192273000
Ca	-2.308629000	1.132372000	2.499963000
H	-3.469058000	2.704619000	-3.383744000
H	-4.179433000	2.842137000	-3.615082000
H	0.925599000	-3.533005000	3.932184000
H	0.515148000	-3.907084000	4.443905000
H	0.774361000	-5.601040000	-1.649582000

H	0.269360000	-5.150096000	-1.317239000
H	0.684982000	5.196209000	-1.245822000
H	0.482157000	5.680382000	-1.789878000
H	2.679224000	0.875638000	-5.523927000
H	2.636129000	0.999331000	-4.777719000
H	-2.416738000	-3.209921000	3.543774000
H	-2.494214000	-3.953489000	3.648509000
H	3.288374000	-3.711324000	-2.068625000
H	3.336157000	-4.119090000	-2.702419000
H	-5.916243000	-1.252740000	-0.208742000
H	-5.222942000	-1.358714000	-0.489915000
H	-4.909043000	1.647547000	1.423256000
H	-5.495423000	1.380693000	1.816878000
H	4.214258000	1.138006000	3.099467000
H	4.537991000	0.856935000	3.721059000
H	-3.373517000	4.118486000	2.710056000
H	-3.318480000	3.708029000	2.077347000
H	-2.801288000	-0.882869000	5.524022000
H	-2.715293000	-1.001123000	4.781085000
H	-4.205917000	-3.198488000	-1.850690000
H	-4.461493000	-3.854220000	-2.127889000
H	2.137498000	5.132819000	0.828989000
H	2.645090000	5.624381000	1.099201000
H	4.923507000	-3.925447000	0.460235000
H	4.411779000	-3.464136000	0.145554000
H	5.046180000	1.685092000	-2.786536000
H	4.316225000	1.506539000	-2.871497000
H	-1.042566000	-1.261868000	-5.923484000
H	-0.698949000	-1.345671000	-5.250596000
H	4.355594000	3.149088000	1.662894000
H	4.731501000	3.784037000	1.829696000

H	3.846826000	-3.889939000	3.143794000
H	3.275606000	-3.407167000	3.031683000
H	-2.657588000	-5.673311000	-0.856684000
H	-2.144616000	-5.149895000	-0.667964000
H	-1.097330000	3.626861000	-3.826550000
H	-0.765867000	4.094927000	-4.320320000
H	-0.122087000	0.752276000	6.139134000
H	-0.156276000	1.037409000	5.435223000
H	-4.337840000	-1.510657000	2.866465000
H	-5.062975000	-1.698693000	2.765351000
H	4.539140000	4.552006000	-0.774219000
H	4.614839000	4.404307000	-1.501366000
H	-4.215368000	-1.070385000	-3.097173000
H	-4.532724000	-0.758213000	-3.706709000
H	5.888058000	0.805413000	0.317541000
H	5.228570000	1.098159000	0.539741000
H	-0.555907000	1.337681000	-6.327080000
H	-0.702862000	2.035495000	-6.108196000
H	2.666890000	-1.181295000	5.167010000
H	2.549100000	-1.467713000	4.478125000
H	-3.963995000	1.390682000	4.932839000
H	-4.222431000	2.010585000	4.608274000
H	3.882717000	-1.401136000	-4.959333000
H	4.127712000	-2.034849000	-4.651715000
H	-0.381970000	-5.639375000	1.853736000
H	-0.625706000	-5.175290000	1.309817000
H	-0.321370000	5.180604000	1.279384000
H	-0.850619000	5.634128000	1.567678000
H	-0.433212000	3.338489000	4.238249000
H	-0.391898000	4.074015000	4.413583000
H	0.918046000	-3.903685000	-4.549227000

H	0.728337000	-3.216115000	-4.296634000
H	4.879644000	-1.618546000	-1.475072000
H	5.437387000	-1.348665000	-1.905354000
H	5.977195000	-1.339538000	2.330183000
H	5.768528000	-2.041478000	2.189197000
H	3.005115000	-5.660014000	0.909369000
H	2.366132000	-6.041932000	0.863952000
H	-2.252522000	6.036385000	-1.222385000
H	-2.914112000	5.695234000	-1.175246000
H	-6.056620000	1.758437000	-1.553008000
H	-6.209848000	1.028722000	-1.547564000
H	-4.349896000	3.509498000	-0.248748000
H	-4.805384000	3.977648000	-0.632567000
H	-4.719259000	-4.330942000	1.423344000
H	-4.450642000	-4.639109000	0.799540000
H	-2.945661000	-3.608262000	-4.410033000
H	-2.379420000	-3.321181000	-4.802099000
H	2.382538000	3.211233000	-3.538687000
H	2.446637000	3.954615000	-3.655057000
H	2.672450000	3.721298000	4.542627000
H	3.262965000	3.663330000	4.090307000

$Ca_{12}O_{12}\cdot 45H_2$, ωB97XD/6-31++G(d,p)

Energy: -9087.84793426 E_h

O	1.511413000	3.220081000	-0.421264000
O	3.304318000	0.990990000	0.991346000
O	2.310272000	0.150248000	-2.695431000
O	-0.092650000	-1.936908000	-2.968568000
O	2.341003000	-2.665329000	-0.002076000
O	1.241606000	-1.758011000	2.849883000
O	-1.500734000	-3.170237000	0.460981000

O	-2.304636000	-0.112345000	2.740822000
O	-3.300066000	-0.948171000	-0.947925000
O	-2.346724000	2.714212000	0.031176000
O	0.094278000	1.970264000	2.972744000
O	-1.219912000	1.783976000	-2.797247000
Ca	-0.190277000	-0.201724000	3.579282000
Ca	0.571963000	-3.270768000	1.292093000
Ca	3.011569000	-1.153284000	1.557579000
Ca	-2.965622000	-1.598818000	1.206555000
Ca	-1.833921000	-2.520594000	-1.690092000
Ca	2.016028000	-2.029021000	-2.121311000
Ca	0.201330000	0.246364000	-3.544433000
Ca	-3.010619000	1.194433000	-1.526358000
Ca	2.967671000	1.640678000	-1.161501000
Ca	-0.563121000	3.302506000	-1.253668000
Ca	1.839744000	2.570265000	1.732017000
Ca	-2.011633000	2.065421000	2.146537000
H	-2.771196000	2.748606000	-3.959782000
H	-3.413263000	3.030588000	-4.251006000
H	0.151625000	-2.781795000	4.584220000
H	-0.335144000	-2.948498000	5.136778000
H	0.954156000	-2.608849000	-5.650707000
H	0.650032000	-2.490212000	-4.967571000
H	-0.449098000	-5.898535000	-0.268673000
H	-0.844613000	-5.272216000	-0.122282000
H	1.757792000	4.587698000	-2.204273000
H	1.659605000	4.977850000	-2.844318000
H	3.093744000	-0.681628000	-5.433582000
H	2.966809000	-0.440507000	-4.727860000
H	-3.103519000	-1.830286000	3.991736000
H	-3.370493000	-2.497619000	4.224942000

H	2.364774000	-4.641655000	-1.145888000
H	2.296324000	-5.177863000	-1.672991000
H	-5.973757000	0.205800000	-0.126699000
H	-5.362358000	-0.171077000	-0.356920000
H	-4.440531000	2.931800000	0.878745000
H	-5.072490000	2.898814000	1.290377000
H	4.293392000	0.924695000	3.055337000
H	4.518285000	0.756867000	3.755710000
H	-2.380588000	5.185465000	1.738570000
H	-2.425663000	4.659545000	1.197628000
H	-2.807546000	0.822960000	5.519830000
H	-2.789634000	0.553459000	4.812840000
H	-4.902221000	-2.457165000	-1.173492000
H	-5.391142000	-3.032303000	-1.225852000
H	3.172348000	4.654119000	-0.104559000
H	3.774596000	5.074938000	0.075653000
H	3.972802000	-4.674107000	1.446066000
H	3.580466000	-4.190125000	1.016634000
H	5.312106000	0.075758000	-2.667761000
H	4.571039000	0.014173000	-2.802277000
H	-2.434889000	-2.202340000	-4.869781000
H	-1.772838000	-2.148649000	-4.511678000
H	4.924709000	2.470524000	1.218510000
H	5.424300000	3.036349000	1.276757000
H	2.920399000	-3.889117000	4.031515000
H	2.474370000	-3.326828000	3.791120000
H	-3.857853000	-4.968863000	0.242483000
H	-3.219643000	-4.570301000	0.315691000
H	-0.267538000	2.839441000	-4.551983000
H	0.176000000	3.035476000	-5.132914000
H	0.176372000	1.978279000	5.871947000

H	0.169668000	2.116742000	5.124354000
H	-4.524046000	0.184390000	2.973902000
H	-5.275552000	0.237191000	2.918802000
H	5.332179000	3.380821000	-1.465077000
H	5.413771000	3.039698000	-2.123247000
H	-4.449815000	-0.737439000	-2.909457000
H	-4.734073000	-0.477905000	-3.559466000
H	5.931339000	-0.411121000	0.561893000
H	5.356208000	0.071353000	0.647755000
H	-0.319396000	-0.365921000	-6.383438000
H	-0.512875000	0.353628000	-6.421979000
H	2.358713000	-0.664536000	5.432429000
H	2.188595000	-1.046555000	4.803780000
H	-3.599163000	3.083956000	4.418622000
H	-3.733138000	3.668468000	3.975053000
H	3.313534000	-3.293047000	-4.453615000
H	3.668230000	-3.709049000	-3.946322000
H	-1.613135000	-4.856100000	2.970522000
H	-1.730713000	-4.492549000	2.319684000
H	0.780419000	5.297356000	0.233859000
H	0.360709000	5.900851000	0.403150000
H	0.260443000	4.145084000	3.493725000
H	0.442276000	4.879497000	3.524528000
H	-0.452677000	-4.897052000	-3.327326000
H	-0.269940000	-4.164395000	-3.355099000
H	4.416116000	-2.868883000	-0.944993000
H	5.009057000	-2.828087000	-1.410518000
H	5.486192000	-1.980881000	2.985621000
H	5.056282000	-2.564911000	3.159704000
H	1.681630000	-5.773743000	2.417412000
H	1.007377000	-6.053871000	2.265584000

H	-0.891988000	5.996531000	-2.489382000
H	-1.613498000	5.823995000	-2.412369000
H	-5.479484000	2.738778000	-2.140943000
H	-5.811334000	2.073645000	-2.085419000
H	-3.482288000	4.246044000	-1.082195000
H	-3.814065000	4.731309000	-1.560238000
H	-5.604956000	-2.616403000	2.123126000
H	-5.632676000	-2.849413000	1.415201000
H	-3.775393000	-4.527069000	-2.671013000
H	-3.248873000	-4.675883000	-3.177793000
H	3.024718000	1.931489000	-3.950185000
H	3.251804000	2.613873000	-4.178965000
H	3.357432000	4.104903000	3.765292000
H	3.934743000	3.853211000	3.365263000

$Ca_{12}O_{12}\cdot 46H_2$, ωB97XD/6-31++G(d,p)

Energy: -9089.01333546 E_h

O	-2.891677000	-1.445299000	-1.508582000
O	-3.379100000	0.371212000	1.064465000
O	-1.877718000	2.299283000	-1.974093000
O	1.259362000	2.840810000	-1.759988000
O	-0.644083000	3.113685000	1.640446000
O	-0.324870000	0.534866000	3.484229000
O	2.895655000	1.449768000	1.501133000
O	1.883758000	-2.293028000	1.977810000
O	3.387230000	-0.368110000	-1.070597000
O	0.650157000	-3.104651000	-1.637916000
O	-1.254060000	-2.830952000	1.758900000
O	0.332041000	-0.529285000	-3.487073000
Ca	0.064963000	-1.633794000	3.175480000
Ca	1.106502000	2.092548000	2.679083000

Ca	-2.079596000	1.544071000	2.455262000
Ca	3.300943000	-0.762686000	1.168292000
Ca	2.979673000	1.843474000	-0.735072000
Ca	-0.559234000	3.498260000	-0.563021000
Ca	-0.060556000	1.637469000	-3.171634000
Ca	2.087620000	-1.543431000	-2.461230000
Ca	-3.296978000	0.767303000	-1.172297000
Ca	-1.098626000	-2.088896000	-2.681037000
Ca	-2.974096000	-1.839962000	0.728660000
Ca	0.565053000	-3.489425000	0.564610000
H	1.100923000	-1.523329000	-5.248107000
H	1.460423000	-1.930847000	-5.778283000
H	0.965309000	0.123957000	5.285865000
H	1.441282000	-0.153957000	5.803680000
H	-2.987817000	-5.105704000	0.856940000
H	-2.491371000	-4.625913000	1.163951000
H	0.869082000	5.141071000	-3.584913000
H	1.026733000	4.574370000	-3.109173000
H	3.349312000	4.358129000	2.204040000
H	3.383228000	3.632927000	1.998849000
H	-3.638959000	-1.451175000	-3.664797000
H	-3.682600000	-1.471799000	-4.418512000
H	-1.933738000	4.584086000	-3.868074000
H	-1.997892000	4.013810000	-3.375572000
H	3.306087000	-1.897228000	3.742163000
H	3.823066000	-1.603006000	4.206008000
H	0.350518000	5.150675000	1.529874000
H	0.695646000	5.782273000	1.299919000
H	5.008550000	-2.879170000	-1.490432000
H	4.708768000	-2.198584000	-1.362848000
H	2.295094000	-4.652415000	-1.364852000

H	2.822218000	-5.117365000	-1.089061000
H	-4.394983000	0.112968000	3.094855000
H	-4.550314000	0.119643000	3.833784000
H	-0.658856000	-5.786310000	-1.258432000
H	-0.325130000	-5.154525000	-1.504051000
H	1.971065000	-4.561908000	3.881337000
H	2.022512000	-3.994465000	3.383139000
H	5.551675000	0.089552000	-0.900777000
H	6.266064000	0.305131000	-0.777113000
H	-5.066644000	-1.791653000	-1.647218000
H	-5.820724000	-1.854641000	-1.629497000
H	-1.006134000	4.482541000	4.226158000
H	-0.931069000	4.212655000	3.521123000
H	-4.389775000	3.825510000	-1.358052000
H	-3.721688000	3.556547000	-1.585944000
H	3.494586000	2.838230000	-3.806087000
H	2.886324000	2.941108000	-3.371713000
H	-5.543157000	-0.084684000	0.888030000
H	-6.255302000	-0.304797000	0.759313000
H	-2.069573000	0.496991000	5.817201000
H	-1.555446000	0.493929000	5.258241000
H	5.826647000	1.903756000	1.564502000
H	5.075488000	1.823178000	1.604354000
H	-0.928427000	0.018295000	-5.288378000
H	-1.372732000	0.377780000	-5.783854000
H	-0.861450000	-4.972876000	3.767054000
H	-1.024212000	-4.472751000	3.223070000
H	3.750688000	-3.524767000	1.615718000
H	4.428721000	-3.776657000	1.397543000
H	-6.199447000	0.880552000	-1.724189000
H	-6.029719000	1.499282000	-2.104359000

H	4.388478000	-0.099418000	-3.100291000
H	4.545721000	-0.100208000	-3.839225000
H	-4.956345000	2.899408000	1.551047000
H	-4.678600000	2.215570000	1.394703000
H	0.797839000	3.260503000	-5.479054000
H	0.610579000	2.656159000	-5.874474000
H	-1.180667000	-2.792984000	5.609571000
H	-1.171812000	-2.076251000	5.816617000
H	1.162427000	-6.075988000	1.850720000
H	1.101130000	-6.358325000	1.163085000
H	-1.100339000	6.127464000	-1.785792000
H	-1.144003000	6.368855000	-1.081465000
H	3.732102000	1.503689000	4.392698000
H	3.673480000	1.477713000	3.640113000
H	-3.376988000	-3.621562000	-2.019177000
H	-3.341084000	-4.345424000	-2.229724000
H	-2.983685000	-2.966826000	3.273480000
H	-3.640381000	-2.875340000	3.633401000
H	3.108629000	5.030693000	-0.855538000
H	2.576174000	4.590860000	-1.161894000
H	-2.268478000	4.674848000	1.392314000
H	-2.793391000	5.150648000	1.130365000
H	-3.934042000	2.918425000	4.347330000
H	-3.341450000	3.363417000	4.430004000
H	1.421712000	3.938904000	4.977805000
H	2.120204000	3.677765000	4.990979000
H	-2.038469000	-3.651512000	-5.039240000
H	-1.329202000	-3.881938000	-5.029271000
H	3.443997000	-3.417028000	-4.331477000
H	4.066273000	-3.146537000	-4.022368000
H	0.951167000	-4.260866000	-3.495763000

H	1.035591000	-4.560898000	-4.185973000
H	6.031898000	-1.413133000	2.163284000
H	6.182508000	-0.765605000	1.825357000
H	5.724909000	2.852814000	-1.198668000
H	5.375919000	3.444057000	-1.489876000
H	-3.323350000	1.935205000	-3.719609000
H	-3.853017000	1.651218000	-4.175929000
H	-5.364400000	-3.544292000	1.247007000
H	-5.680836000	-3.037497000	0.800738000

$Ca_{12}O_{12}\cdot 47H_2$, ωB97XD/6-31++G(d,p)

Energy: -9090.17819506 E_h

O	-0.008959000	2.260028000	-2.786164000
O	0.005964000	3.559553000	0.126566000
O	3.185600000	1.450109000	-0.691060000
O	3.189701000	-1.460181000	0.610213000
O	1.608092000	1.297486000	2.877437000
O	-1.580599000	1.301635000	2.889311000
O	0.008225000	-2.262813000	2.727017000
O	-3.186780000	-1.452418000	0.636002000
O	-0.005830000	-3.561311000	-0.185494000
O	-1.608303000	-1.295550000	-2.933325000
O	-3.188781000	1.457845000	-0.664999000
O	1.580274000	-1.299845000	-2.944673000
Ca	-3.183268000	0.664778000	1.465736000
Ca	0.014041000	-0.180909000	3.543856000
Ca	0.013090000	2.781340000	2.223934000
Ca	-1.620028000	-2.912728000	1.278824000
Ca	1.622492000	-2.915191000	1.264757000
Ca	3.196747000	0.657392000	1.439556000
Ca	3.183723000	-0.666873000	-1.520260000

Ca	-0.013172000	-2.780239000	-2.281658000
Ca	1.619677000	2.909691000	-1.337352000
Ca	-0.014434000	0.179264000	-3.602488000
Ca	-1.622650000	2.912563000	-1.322430000
Ca	-3.197428000	-0.659196000	-1.494245000
H	1.525251000	-2.095894000	-5.011781000
H	1.412785000	-2.333303000	-5.721200000
H	-3.774797000	3.365538000	3.093774000
H	-3.174756000	2.913980000	3.169919000
H	-4.193631000	2.755728000	-3.199183000
H	-4.088626000	2.379343000	-2.553299000
H	6.148653000	-1.336960000	0.551629000
H	5.398525000	-1.428806000	0.592084000
H	1.802433000	-2.295976000	5.152836000
H	1.361205000	-2.439940000	4.557463000
H	1.324469000	2.394783000	-4.637219000
H	1.751271000	2.225796000	-5.236891000
H	6.149118000	1.289114000	-0.649362000
H	5.401106000	1.395214000	-0.686485000
H	-4.081438000	-2.372002000	2.525860000
H	-4.186704000	-2.747466000	3.172253000
H	3.212069000	0.420496000	4.248390000
H	3.813524000	0.058491000	4.525799000
H	-1.812422000	-5.365153000	-1.800855000
H	-1.371546000	-5.027671000	-1.289469000
H	-3.198458000	-2.893122000	-3.237148000
H	-3.797316000	-3.348357000	-3.171129000
H	-1.336867000	5.046219000	1.221465000
H	-1.774812000	5.396094000	1.727113000
H	-3.843832000	-0.034747000	-4.541107000
H	-3.234817000	-0.397595000	-4.282766000

H	-6.148968000	-1.299811000	0.601373000
H	-5.400121000	-1.402039000	0.635574000
H	-0.007766000	-5.563976000	0.749939000
H	-0.008737000	-6.206609000	1.149302000
H	-0.005193000	4.293583000	-3.656452000
H	-0.002028000	5.019620000	-3.869188000
H	1.466041000	2.500045000	5.582768000
H	1.569670000	2.195671000	4.897862000
H	4.209272000	4.189539000	0.055775000
H	4.096127000	3.460727000	-0.104965000
H	4.188956000	-4.206231000	-0.158730000
H	4.083376000	-3.477358000	0.006391000
H	0.013278000	5.558428000	-0.824566000
H	0.017739000	6.196528000	-1.230978000
H	-1.418424000	2.512110000	5.593432000
H	-1.527244000	2.205326000	4.910543000
H	-0.001693000	-5.034275000	3.785525000
H	0.002599000	-4.305956000	3.581406000
H	3.814068000	-0.045894000	-4.559907000
H	3.203573000	-0.406235000	-4.301481000
H	-6.149304000	1.322747000	-0.608033000
H	-5.399987000	1.419672000	-0.647925000
H	-4.096267000	-3.460560000	0.035751000
H	-4.209485000	-4.187384000	-0.133487000
H	2.341300000	5.529271000	-2.514145000
H	3.043007000	5.293678000	-2.423490000
H	1.333618000	-5.040256000	-1.299440000
H	1.765262000	-5.383842000	-1.814763000
H	1.822501000	5.373108000	1.717087000
H	1.376358000	5.030019000	1.214085000
H	6.050034000	-1.088833000	-2.126873000

H	5.801769000	-1.329772000	-2.787526000
H	-6.052380000	1.014703000	2.100598000
H	-5.801726000	1.291860000	2.745965000
H	-6.073011000	-1.016331000	-2.097741000
H	-5.828254000	-1.281412000	-2.750387000
H	6.073941000	0.922690000	2.081845000
H	5.830021000	1.224709000	2.718571000
H	-1.787246000	-2.286160000	5.152334000
H	-1.344958000	-2.432052000	4.558251000
H	-1.348670000	2.403386000	-4.632700000
H	-1.776731000	2.237678000	-5.232364000
H	-4.086161000	3.476513000	-0.075247000
H	-4.192824000	4.206900000	0.082474000
H	4.195655000	-2.754160000	3.145311000
H	4.089628000	-2.379590000	2.498553000
H	3.218893000	2.894914000	3.147384000
H	3.823828000	3.338914000	3.065143000
H	0.036380000	5.143219000	4.041677000
H	0.034202000	4.602976000	4.555743000
H	0.014850000	0.340850000	6.456872000
H	0.019319000	-0.402525000	6.515976000
H	-0.041047000	-4.472683000	-4.701652000
H	-0.033794000	-5.042683000	-4.220736000
H	-1.567670000	-2.096403000	-4.996851000
H	-1.459575000	-2.336982000	-5.705838000
H	-3.044821000	-5.312083000	2.329657000
H	-2.343224000	-5.551573000	2.410393000
H	2.323913000	-5.553709000	2.404989000
H	3.028088000	-5.323433000	2.319898000
H	4.082310000	2.366458000	-2.581127000
H	4.188477000	2.740626000	-3.228150000

H	-3.787074000	0.075587000	4.545379000
H	-3.182956000	0.433022000	4.267653000
H	-3.022613000	5.318657000	-2.389702000
H	-2.317946000	5.544091000	-2.483299000
H	3.159417000	-2.907512000	-3.266830000
H	3.755384000	-3.367462000	-3.208867000

$Ca_{12}O_{12}\cdot 48H_2$, ωB97XD/6-31++G(d,p)

Energy: -9091.34437648 E_h

O	-0.073160000	-3.525079000	0.521324000
O	1.559184000	-1.801607000	2.649852000
O	-2.264869000	-1.016015000	2.557598000
O	-3.008589000	1.648047000	0.971452000
O	0.313472000	1.880835000	3.010102000
O	2.950550000	1.564553000	1.246441000
O	0.073076000	3.525287000	-0.521465000
O	2.265162000	1.016120000	-2.557727000
O	-1.558861000	1.801578000	-2.650191000
O	-0.313340000	-1.880863000	-3.010332000
O	3.008872000	-1.648102000	-0.971884000
O	-2.950510000	-1.564487000	-1.246738000
Ca	3.468661000	0.559671000	-0.683381000
Ca	1.255839000	3.078693000	1.323117000
Ca	2.010795000	0.369403000	2.936976000
Ca	0.597591000	2.504841000	-2.484430000
Ca	-2.084035000	2.825991000	-0.689641000
Ca	-1.807866000	1.192474000	2.848073000
Ca	-3.468263000	-0.559910000	0.683159000
Ca	-2.010518000	-0.369372000	-2.937321000
Ca	-0.597323000	-2.504655000	2.484302000
Ca	-1.255725000	-3.078821000	-1.323454000

Ca	2.083993000	-2.826021000	0.689224000
Ca	1.807996000	-1.192307000	-2.848333000
H	-4.047227000	-2.766152000	-2.745909000
H	-4.344558000	-3.181722000	-3.303543000
H	5.709630000	0.388775000	1.598741000
H	5.052995000	0.758924000	1.638671000
H	3.432000000	-4.562337000	-1.639038000
H	3.429737000	-3.809621000	-1.582252000
H	-5.420913000	1.818281000	2.686759000
H	-4.825969000	1.831461000	2.219201000
H	-0.515217000	5.740117000	1.444207000
H	-0.434873000	5.280223000	0.850968000
H	-1.807382000	-5.006342000	0.661689000
H	-2.457004000	-5.378025000	0.563779000
H	-4.745983000	-0.585928000	4.124139000
H	-4.103028000	-0.752263000	3.761768000
H	3.332649000	2.995829000	-2.951743000
H	3.509265000	3.726727000	-3.018352000
H	-0.862144000	3.661864000	3.825869000
H	-1.406229000	4.150454000	4.013147000
H	-1.440335000	1.280961000	-5.621125000
H	-1.471097000	1.558299000	-4.919679000
H	0.233260000	-1.395961000	-5.175430000
H	0.572162000	-1.145947000	-5.801888000
H	3.711814000	-1.825416000	3.415940000
H	4.410976000	-1.635120000	3.627487000
H	1.405139000	-4.152428000	-4.010655000
H	0.861505000	-3.663029000	-3.824170000
H	4.747856000	0.589530000	-4.122861000
H	4.104411000	0.754503000	-3.760754000
H	-2.052148000	3.676127000	-3.719952000

H	-2.172397000	4.359732000	-4.020919000
H	0.464820000	-5.349979000	1.652288000
H	0.693509000	-5.918579000	2.095979000
H	1.960208000	3.463137000	4.901899000
H	1.486803000	3.069975000	4.461828000
H	-1.664751000	-1.786218000	5.413916000
H	-1.941901000	-1.532361000	4.759301000
H	-5.277759000	2.626218000	-0.763618000
H	-4.821948000	2.348086000	-0.230014000
H	2.052946000	-3.674853000	3.721201000
H	2.173505000	-4.357960000	4.023217000
H	4.341607000	3.188756000	3.301815000
H	4.045911000	2.770478000	2.745071000
H	-0.692669000	5.919449000	-2.095284000
H	-0.464573000	5.350399000	-1.651925000
H	-4.873837000	-3.393020000	0.193510000
H	-4.422476000	-3.025530000	-0.287119000
H	5.419754000	-1.821457000	-2.690392000
H	4.825859000	-1.833868000	-2.221818000
H	1.943185000	1.532196000	-4.759547000
H	1.666642000	1.785935000	-5.414421000
H	-0.518324000	-4.836214000	4.306226000
H	-1.155965000	-4.556621000	4.573367000
H	-3.711112000	1.825460000	-3.417562000
H	-4.410242000	1.635032000	-3.629130000
H	1.440044000	-1.279927000	5.620659000
H	1.470868000	-1.557568000	4.919340000
H	-6.207050000	-0.658715000	1.803002000
H	-6.360732000	-1.066451000	1.197954000
H	6.212071000	0.639819000	-1.791481000
H	6.365892000	1.050232000	-1.188320000

H	3.818505000	-1.872945000	-4.911266000
H	3.250533000	-2.221260000	-5.246241000
H	-3.819436000	1.872400000	4.908407000
H	-3.252722000	2.223553000	5.242147000
H	2.454974000	5.379885000	-0.558739000
H	1.805708000	5.007958000	-0.658352000
H	0.429754000	-5.281603000	-0.849828000
H	0.507905000	-5.742432000	-1.442739000
H	4.822989000	-2.346097000	0.229167000
H	5.279649000	-2.622939000	0.762692000
H	-3.433589000	4.561651000	1.640180000
H	-3.430753000	3.809003000	1.582730000
H	-0.233130000	1.394148000	5.174512000
H	-0.572559000	1.143844000	5.800664000
H	3.698631000	0.603157000	5.380548000
H	3.663628000	1.324608000	5.195035000
H	2.567349000	5.227426000	2.880325000
H	2.266438000	5.680874000	2.370421000
H	-2.284688000	-5.677910000	-2.361078000
H	-2.591137000	-5.223567000	-2.867030000
H	-3.661253000	-1.324089000	-5.198526000
H	-3.692007000	-0.602823000	-5.385483000
H	-1.486923000	-3.070347000	-4.461162000
H	-1.960533000	-3.463324000	-4.901195000
H	1.155697000	4.557166000	-4.573566000
H	0.515497000	4.834018000	-4.309643000
H	-3.330824000	5.308611000	-1.714079000
H	-3.860279000	5.165788000	-1.208736000
H	-3.333550000	-2.994803000	2.952209000
H	-3.511214000	-3.725499000	3.018454000
H	4.877252000	3.387386000	-0.196827000

H	4.425028000	3.022296000	0.285005000
H	3.863417000	-5.159420000	1.211655000
H	3.337425000	-5.298678000	1.721448000
H	-5.053583000	-0.757658000	-1.635361000
H	-5.710181000	-0.387626000	-1.593024000