Supporting Information for

Structures and Stabilities of $(CaO)_n$ Nanoclusters

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Ref. 32
Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision B.1, Gaussian, Inc., Wallingford CT, 2009.

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Werner, H.-J.; Knowles, P. J.; Knizia, G.; Manby, F. R.; Schütz, M.; Celani, P.; Korona, T.; Lindh, R.; Mitrushenkov, A.; Rauhut, G.; Shamasundar, K. R.; Adler, T. B.; Amos, R. D.; Bernhardsson, A.; Berning, A.; Cooper, D. L.; Deegan, M. J. O.; Dobbyn, A. J.; Eckert, F.; Goll, E.; Hampel, C.; Hesselmann, A.; Hetzer, G.; Hrenar, T.; Jansen, G.; Köppl, C.; Liu, Y.; Lloyd, A. W.; Mata, R. A.; May, A. J.; McNicholas, S. J.; Meyer, W.; Mura, M. E.; Nicklass, A.; O'Neill, D. P.; Palmieri, P.; Peng, D.; Pflüger, K.; Pitzer, R.; Reiher, M.; Shiozaki, T.; Stoll, H.; Stone, A. J.; Tarroni, R.; Thorsteinsson, T.; Wang, M. MOLPRO, version 2012.1, a pack-age of ab initio programs. See http://www.molpro.net.

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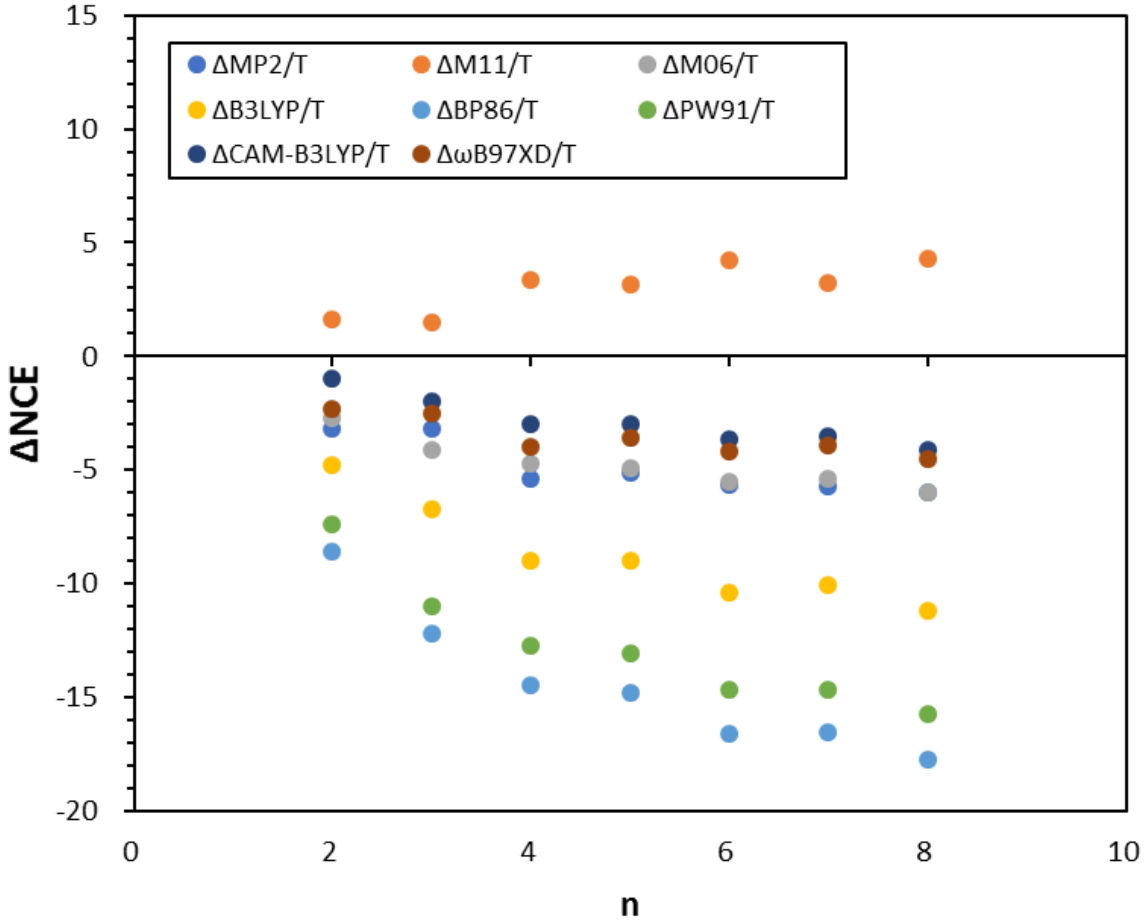


Figure S1. Deviation of NCEs calculated at different theoretical levels with cc-pVTZ basis sets from the CCSD(T)/T values for $(CaO)_n$, n = 2-8.

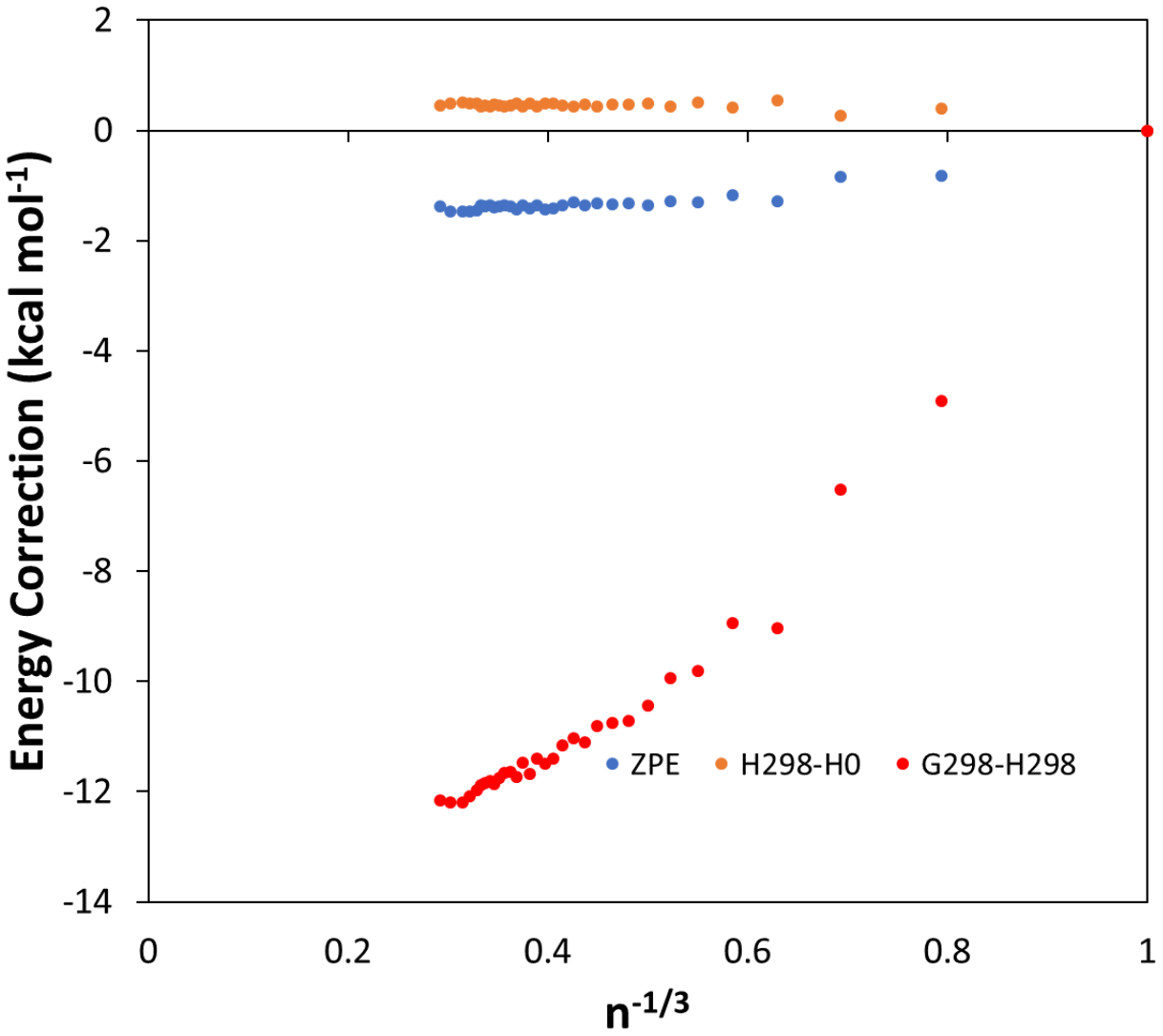
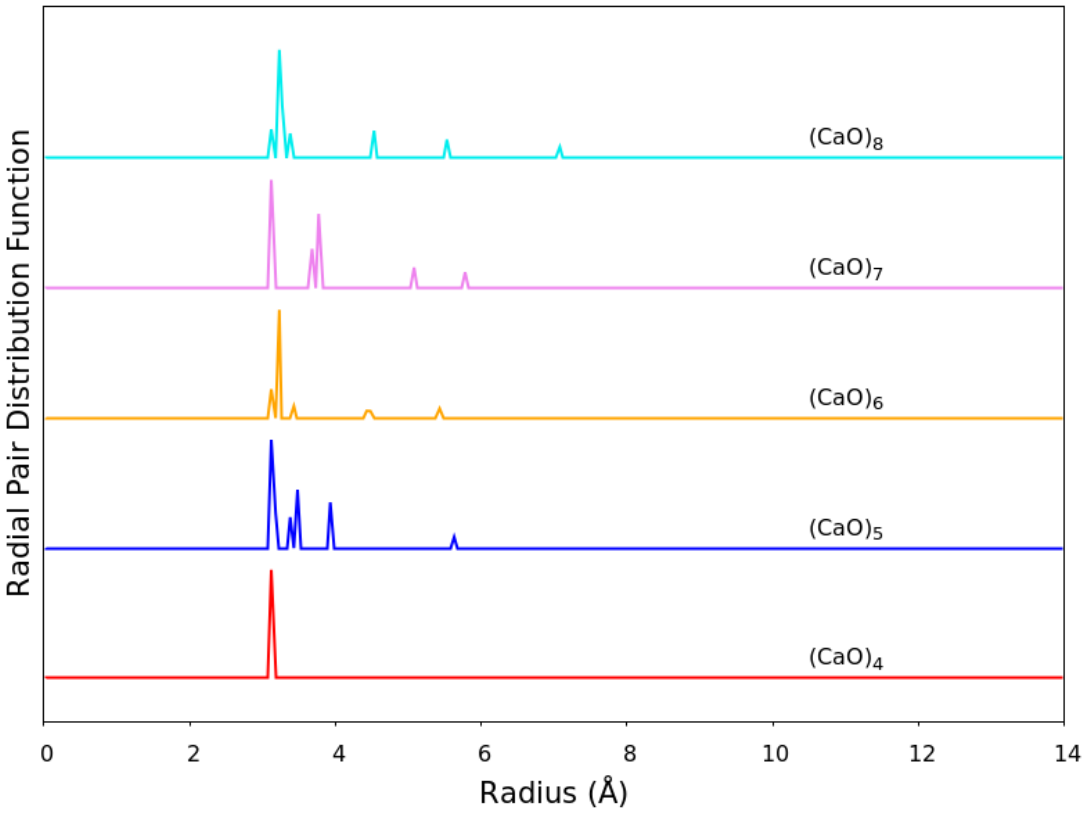
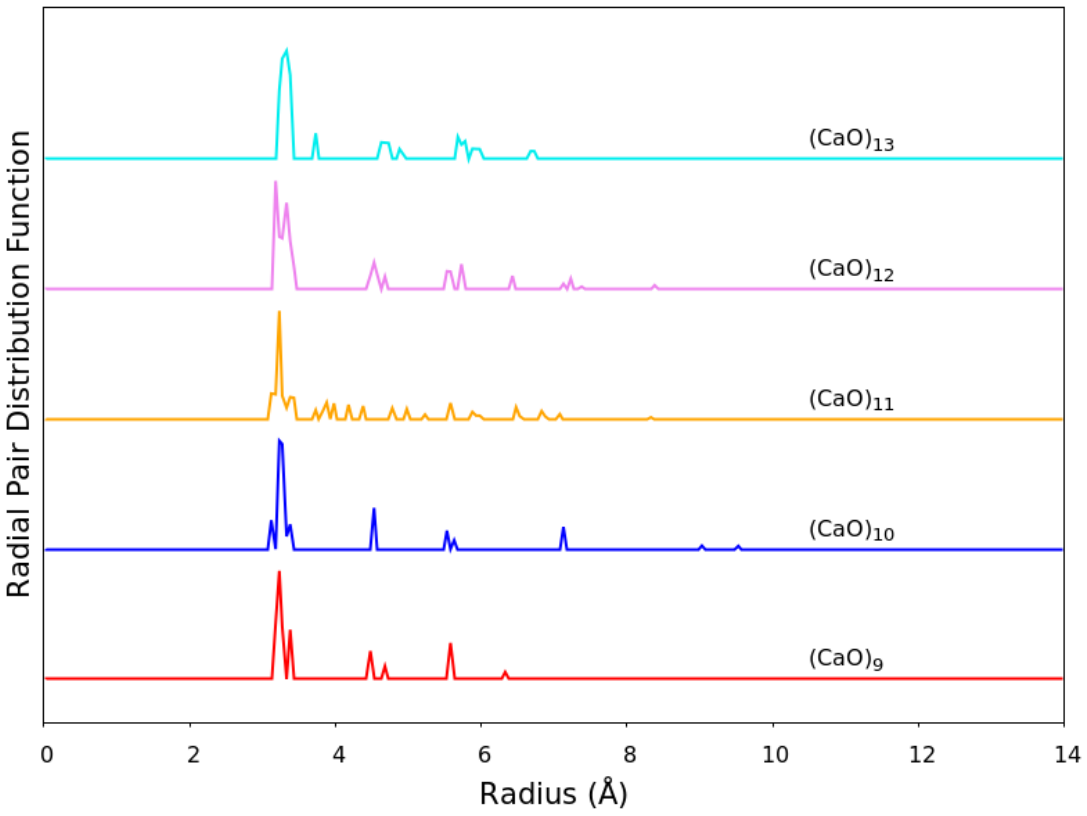
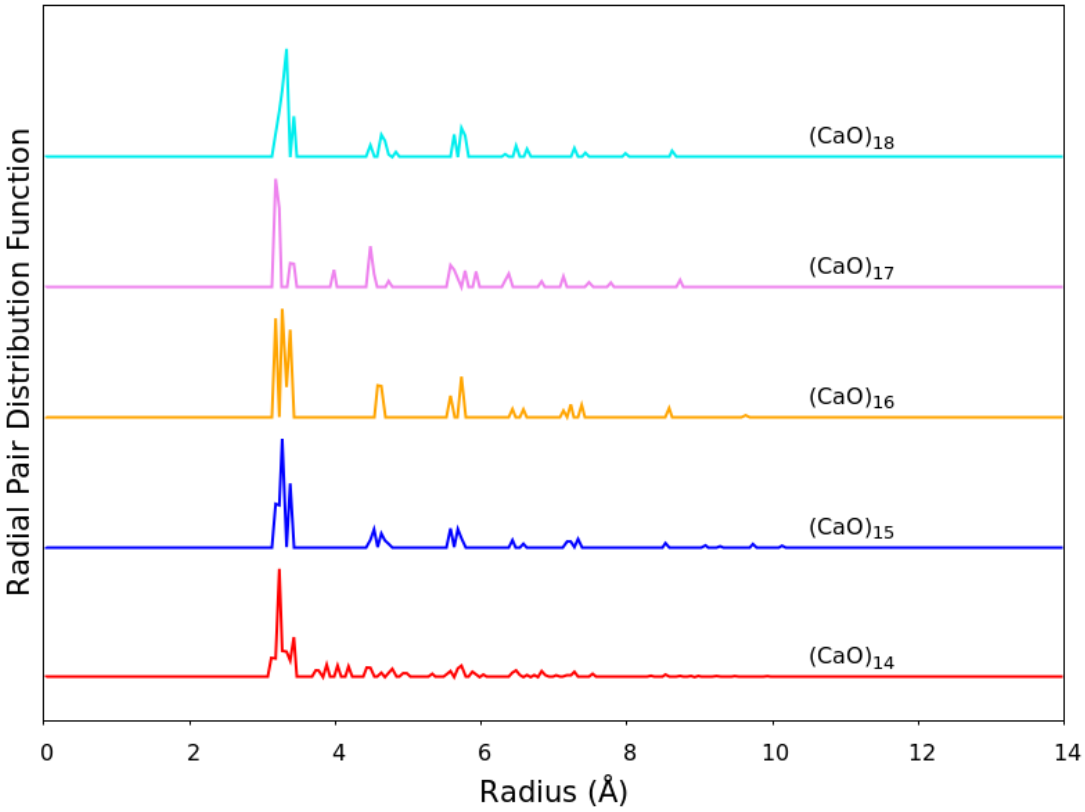


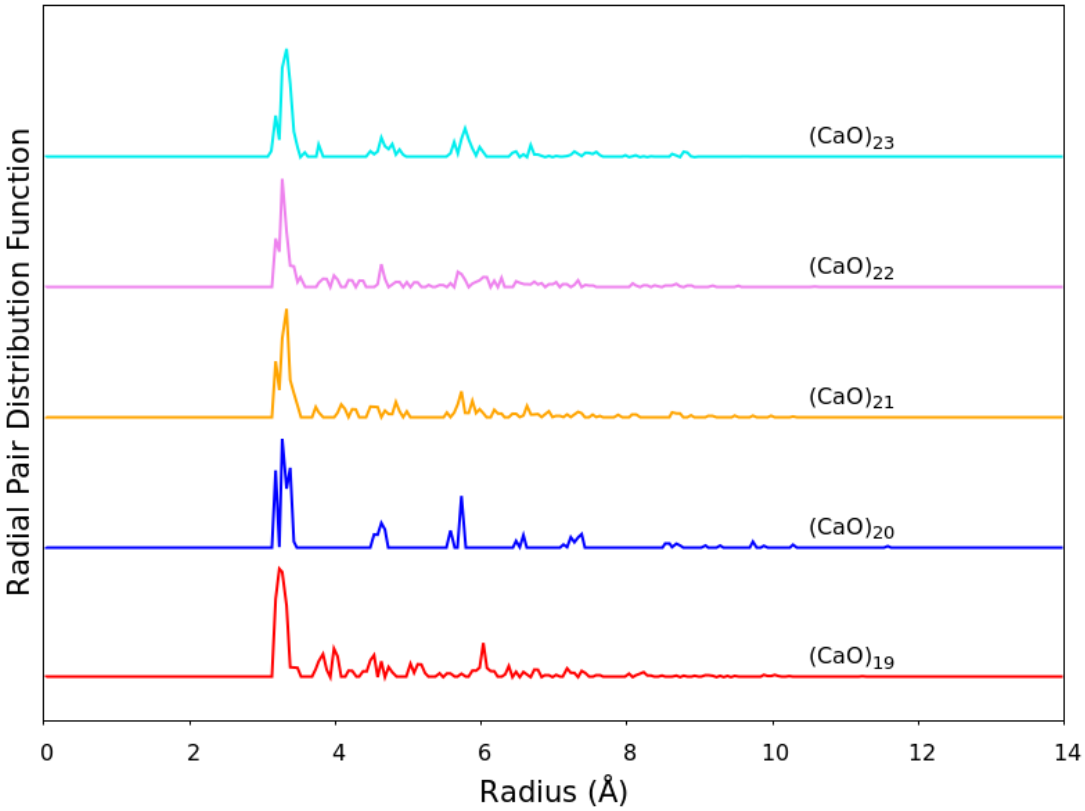
Figure S2. Energy corrections to NCE(n) as functions of $n^{-1/3}$. "ZPE" denotes zero-point energy correction, "H298 – H0" denotes $\Delta H_{298K} - \Delta H_{0K}$, and "G298 – H298" denotes $\Delta G_{298K} - \Delta H_{298K}$.

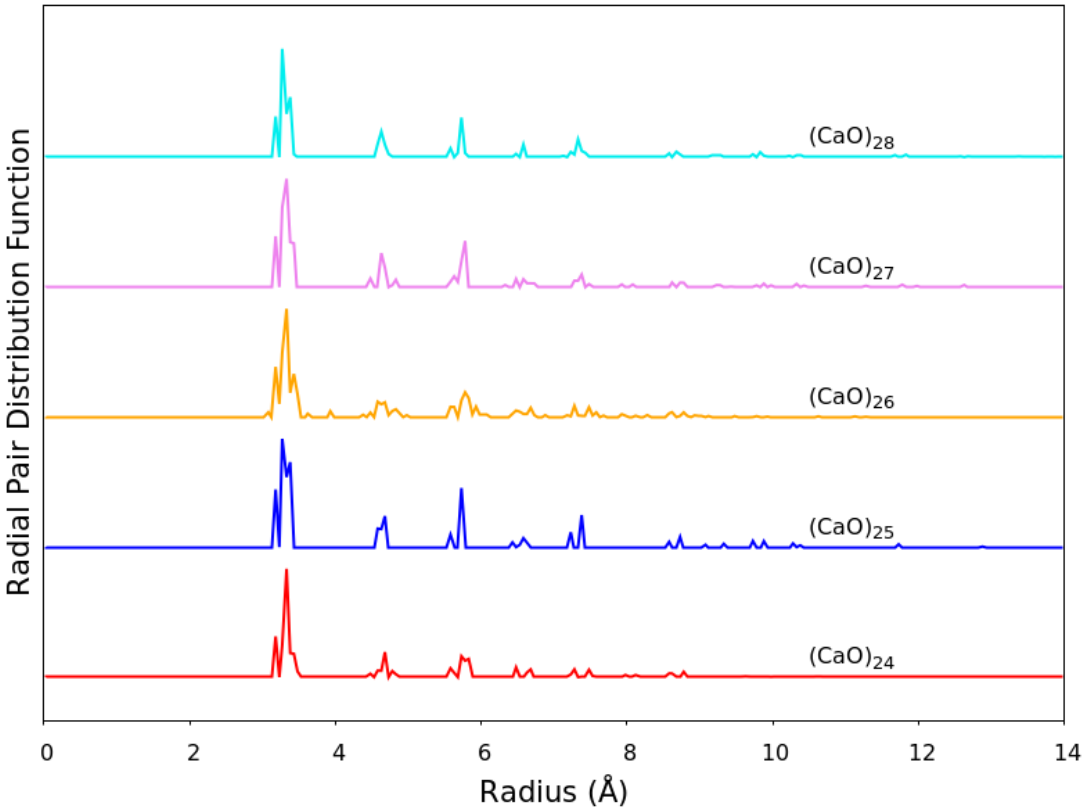
(a)

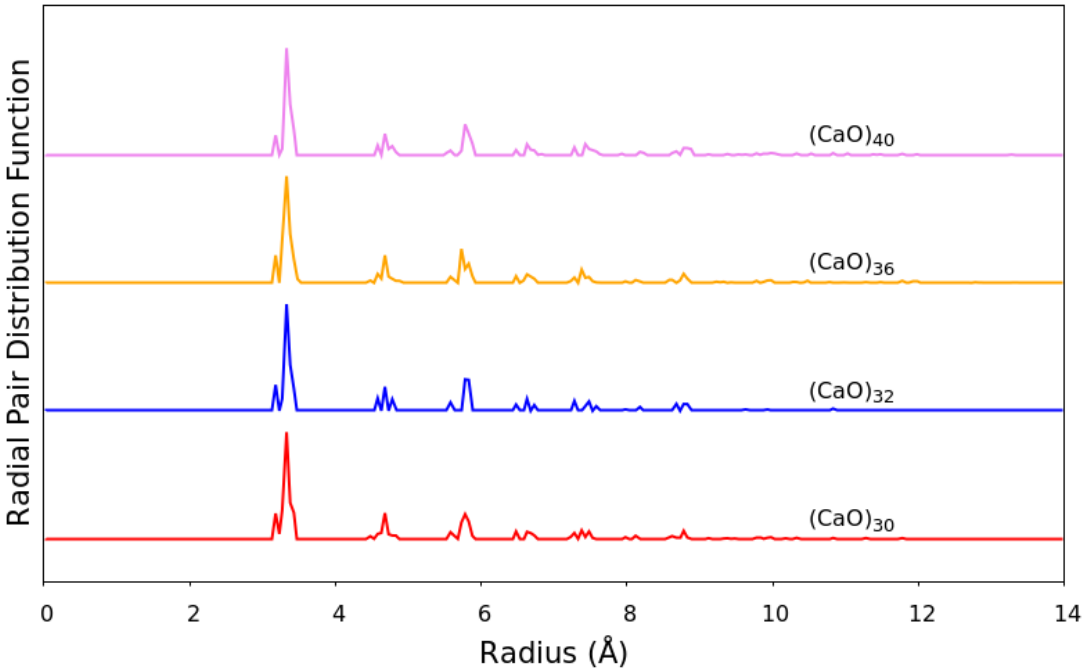

Radial Pair Distribution Function
(CaO)8
(CaO)7
(CaO)6
(CaO)5
(CaO)4
0
2
4
6
8
10
12
14
Radius (Å)


Radial Pair Distribution Function
(CaO)13
(CaO)12
(CaO)11
(CaO)10
(CaO)9
0
2
4
6
8
10
12
14
Radius (Å)

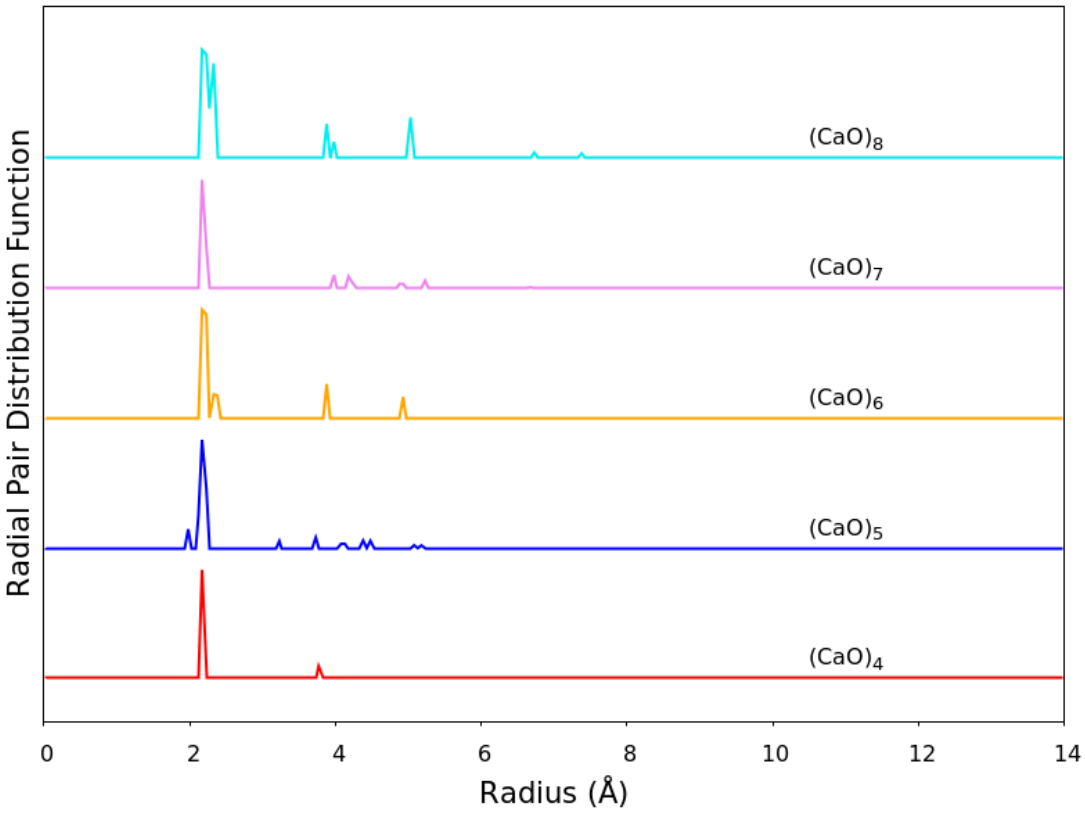

Radial Pair Distribution Function
(CaO)18
(CaO)17
(CaO)16
(CaO)15
(CaO)14
0
2
4
6
8
10
12
14
Radius (Å)

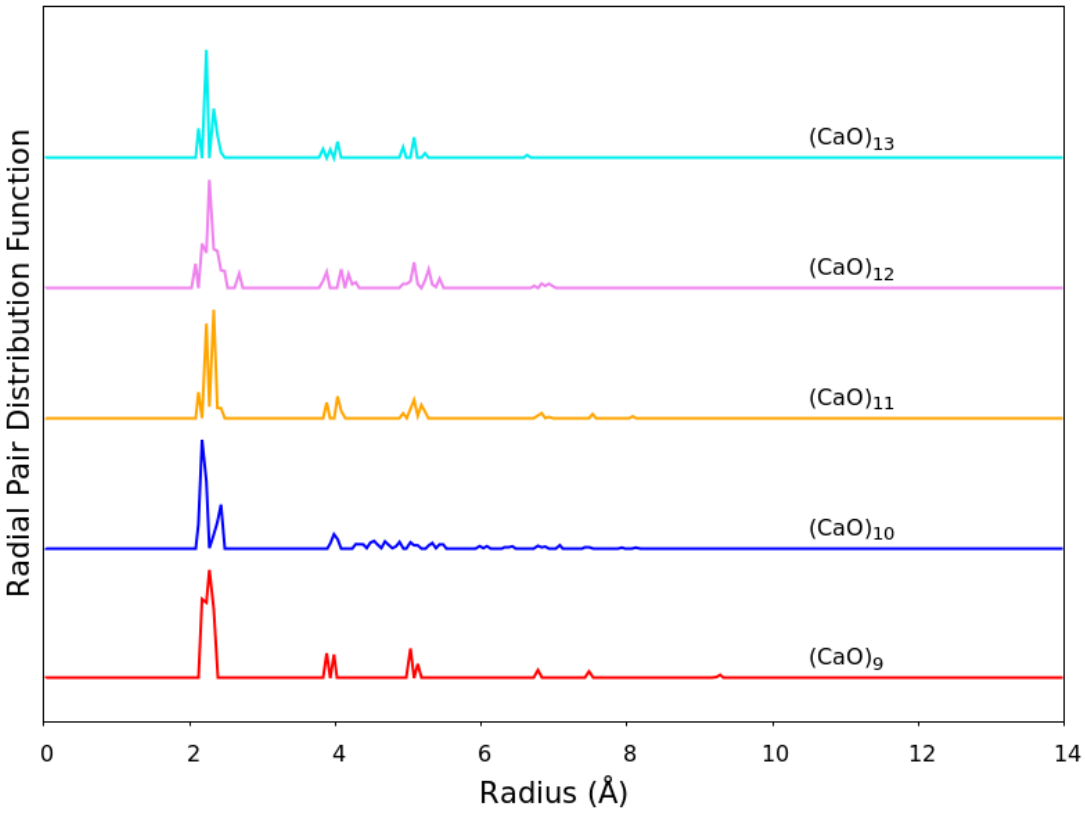

Radial Pair Distribution Function
(CaO)23
(CaO)22
(CaO)21
(CaO)20
(CaO)19
0
2
4
6
8
10
12
14
Radius (Å)

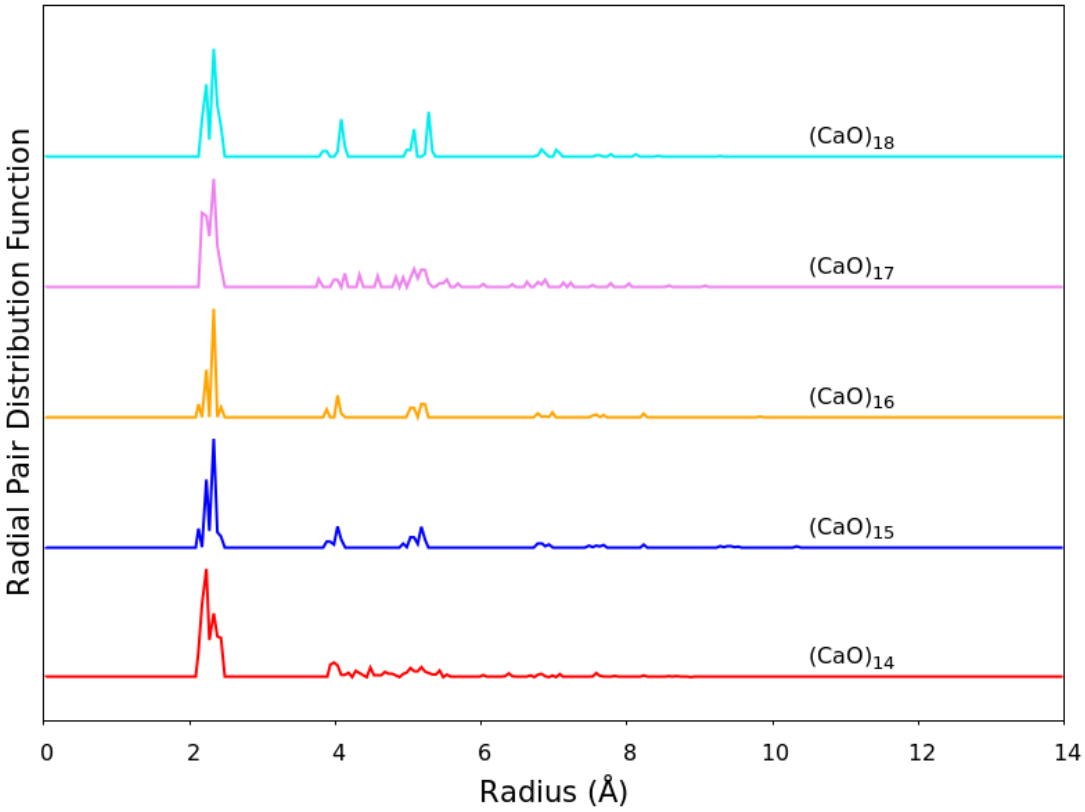

Radial Pair Distribution Function
(CaO)28
(CaO)27
(CaO)26
(CaO)25
(CaO)24
0
2
4
6
8
10
12
14
Radius (Å)

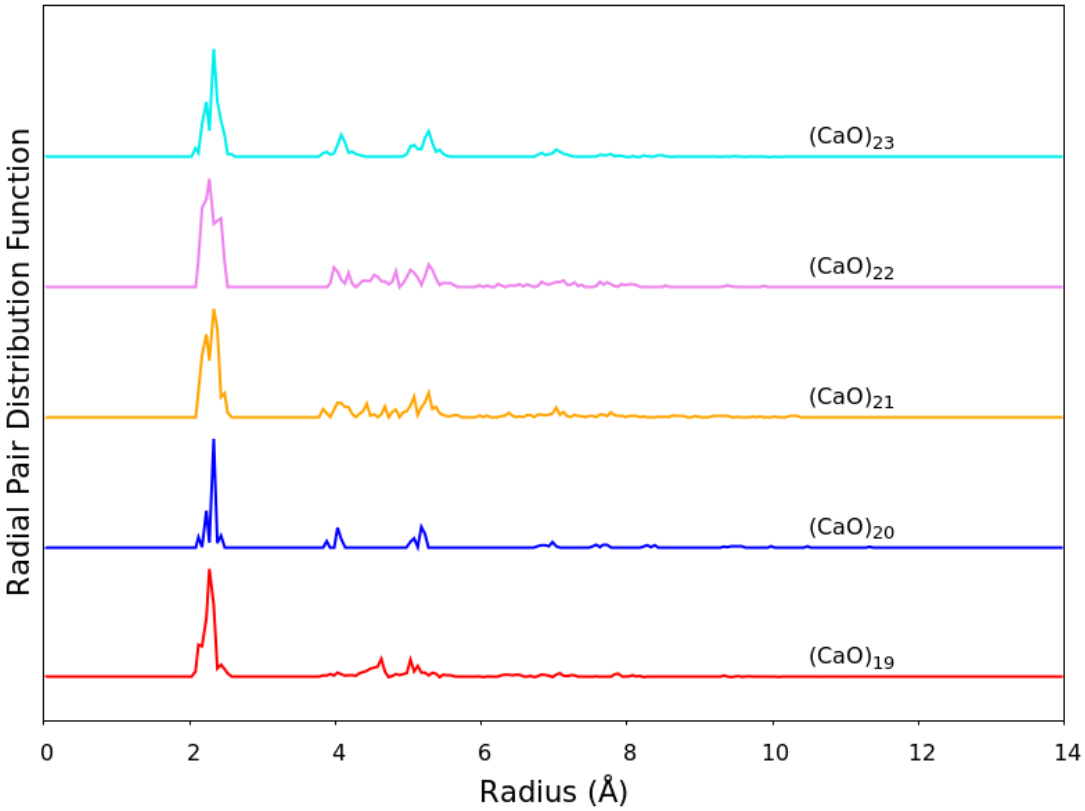

Radial Pair Distribution Function
(CaO)40
(CaO)36
(CaO)32
(CaO)30
0
2
4
6
8
10
12
14
Radius (Å)

(b)


Radial Pair Distribution Function
(CaO)8
(CaO)7
(CaO)6
(CaO)5
(CaO)4
0
2
4
6
8
10
12
14
Radius (Å)


Radial Pair Distribution Function
(CaO)13
(CaO)12
(CaO)11
(CaO)10
(CaO)9
0
2
4
6
8
10
12
14
Radius (Å)


Radial Pair Distribution Function
(CaO)18
(CaO)17
(CaO)16
(CaO)15
(CaO)14
0
2
4
6
8
10
12
14
Radius (Å)


Radial Pair Distribution Function
(CaO)23
(CaO)22
(CaO)21
(CaO)20
(CaO)19
0
2
4
6
8
10
12
14
Radius (Å)

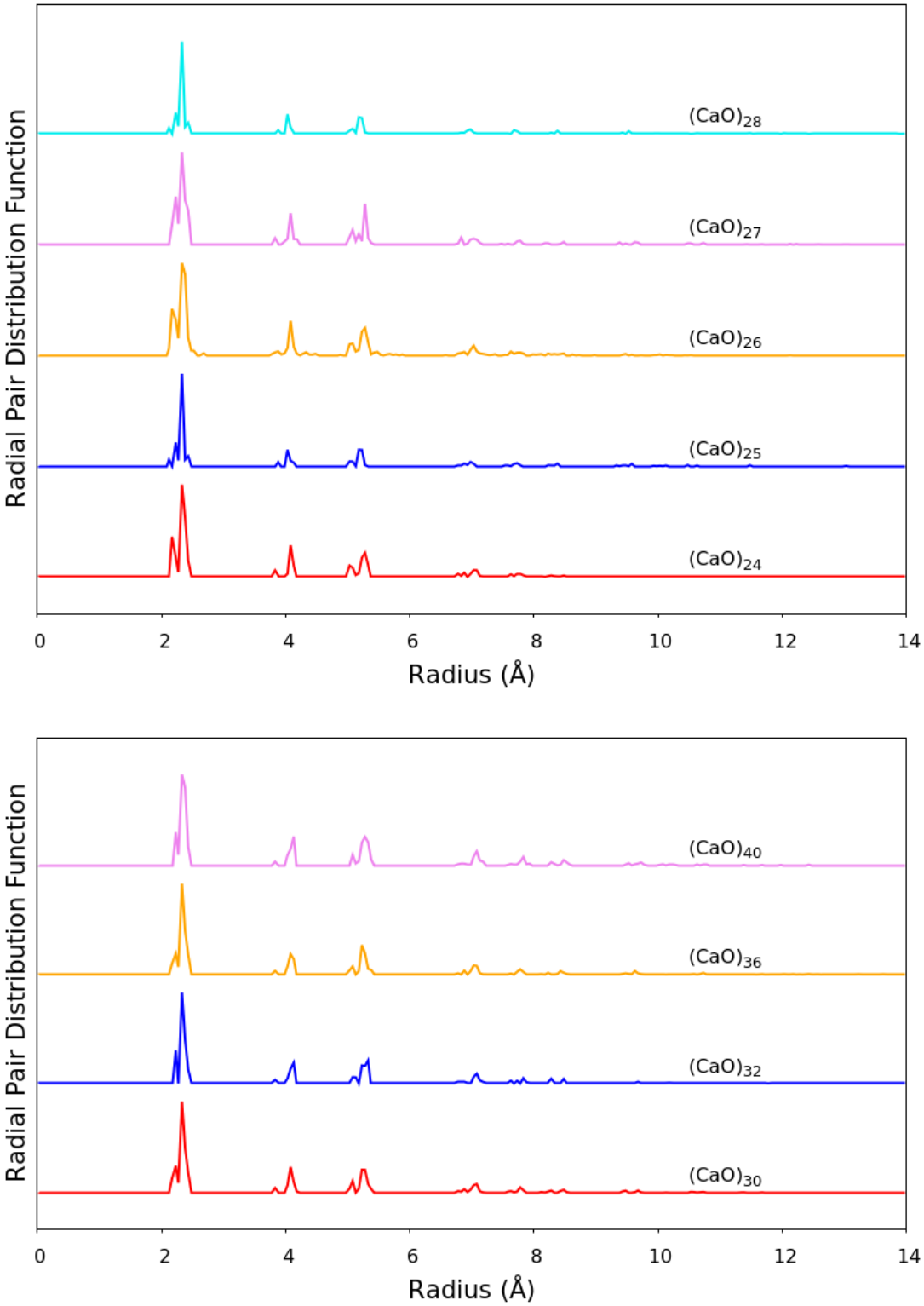


Figure S3. Predicted radial pair distribution function for (a) Ca-Ca and (b) Ca-O for the lowest energy $(CaO)_n$, $n \leq 40$.

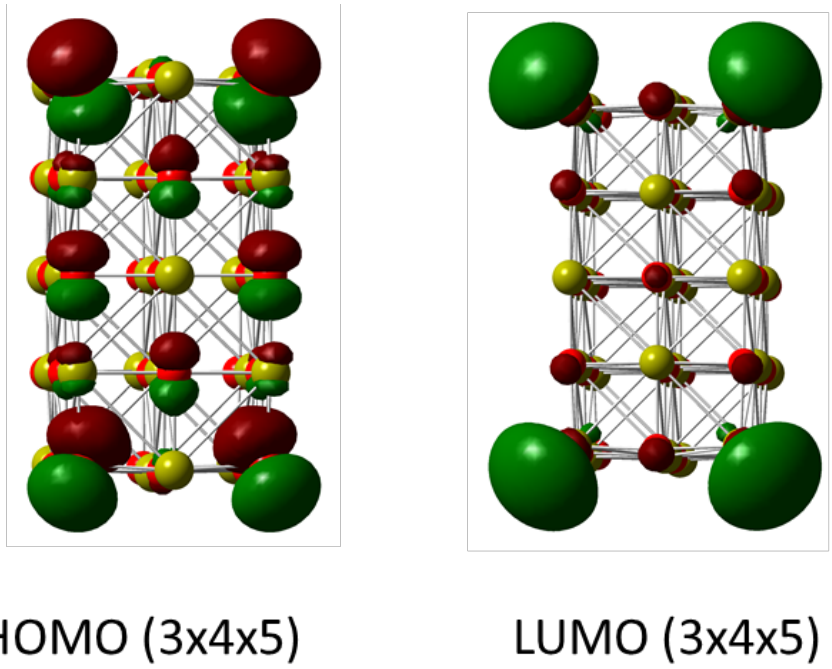
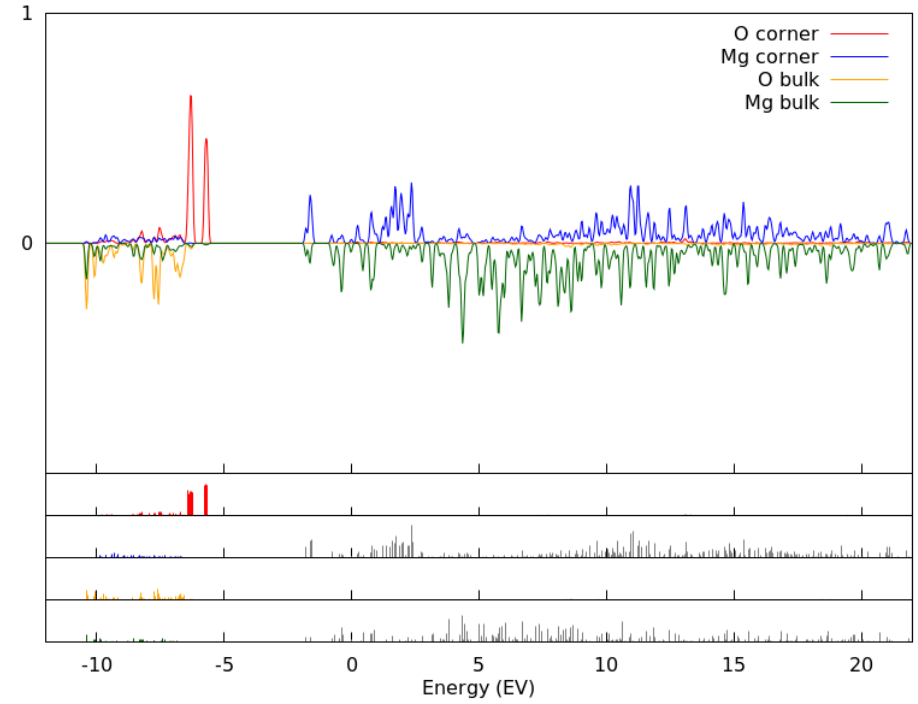
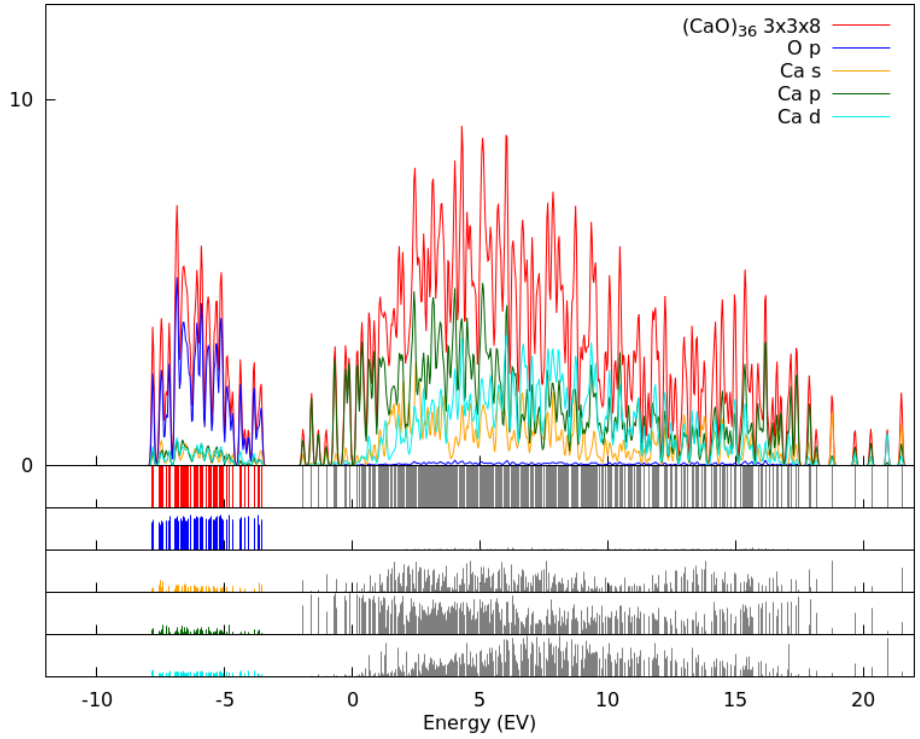


Figure S4. MO isodensity for HOMO and LUMO of 3×4×5 $(CaO)_{30}$.

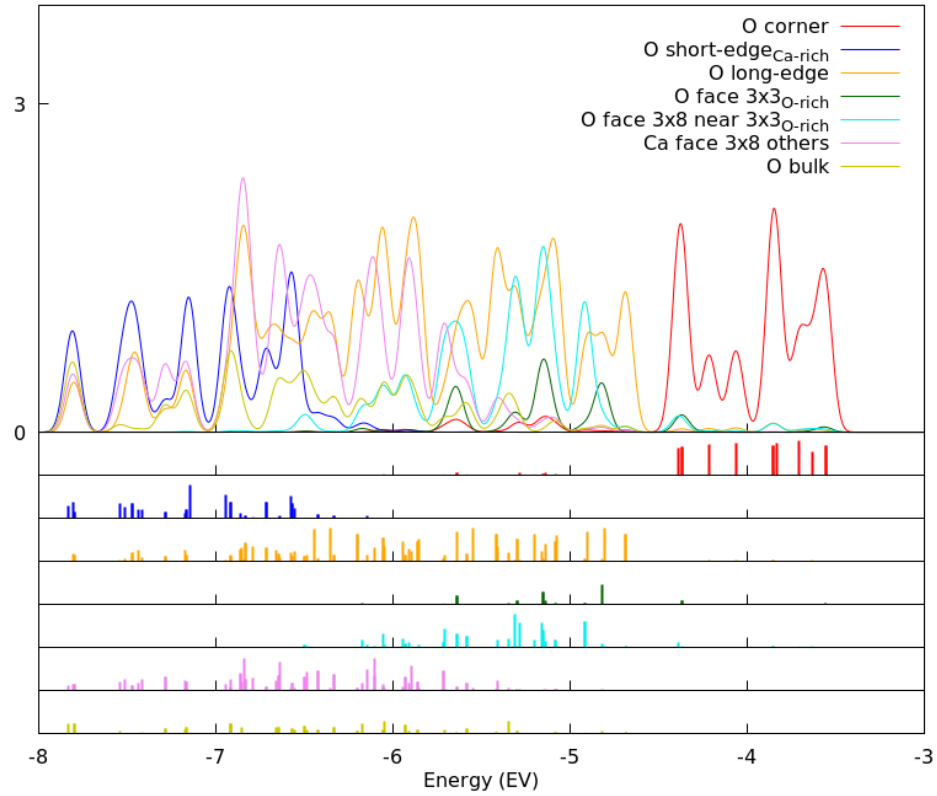
(a)


1
0
O corner
Mg corner
O bulk
Mg bulk
-10
-5
0
5
10
15
20
Energy (EV)

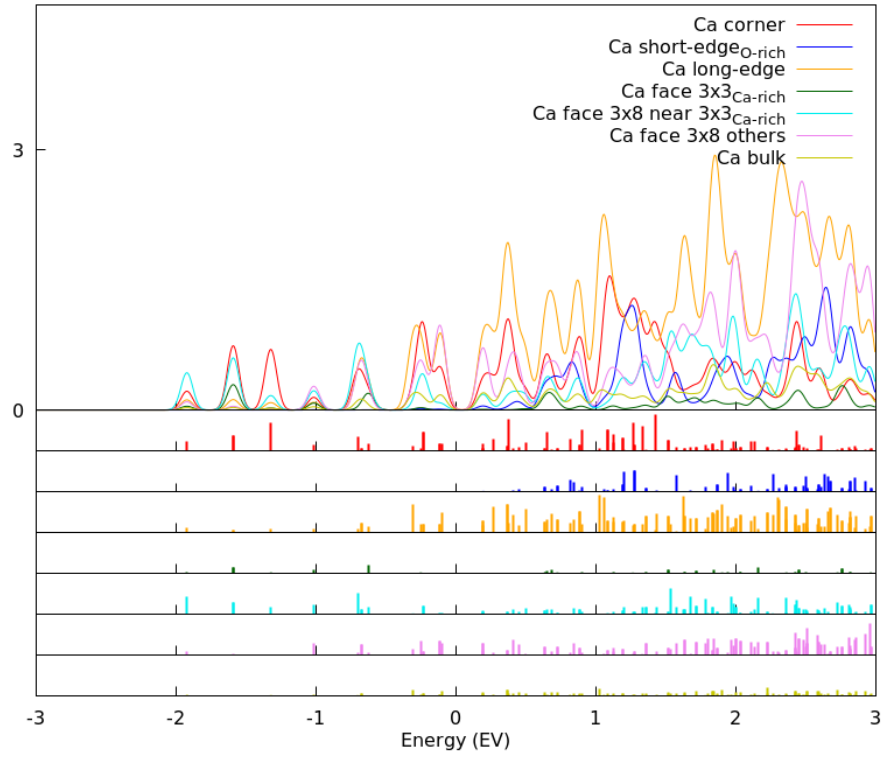
(b)


10
0
(CaO)36 3x3x8
O p
Ca s
Ca p
Ca d
-10
-5
0
5
10
15
20
Energy (EV)

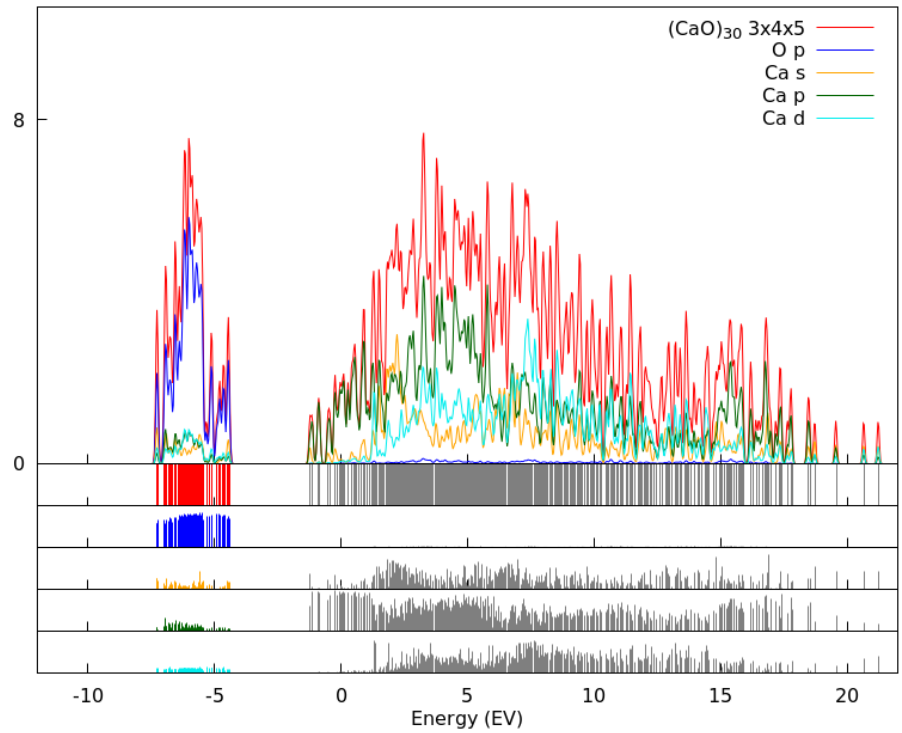
(c)


O corner
O short-edge$_{Ca\text{-}rich}$
O long-edge
O face 3x3$_{O\text{-}rich}$
O face 3x8 near 3x3$_{O\text{-}rich}$
Ca face 3x8 others
O bulk
3
0
-8
-7
-6
-5
-4
-3
Energy (EV)

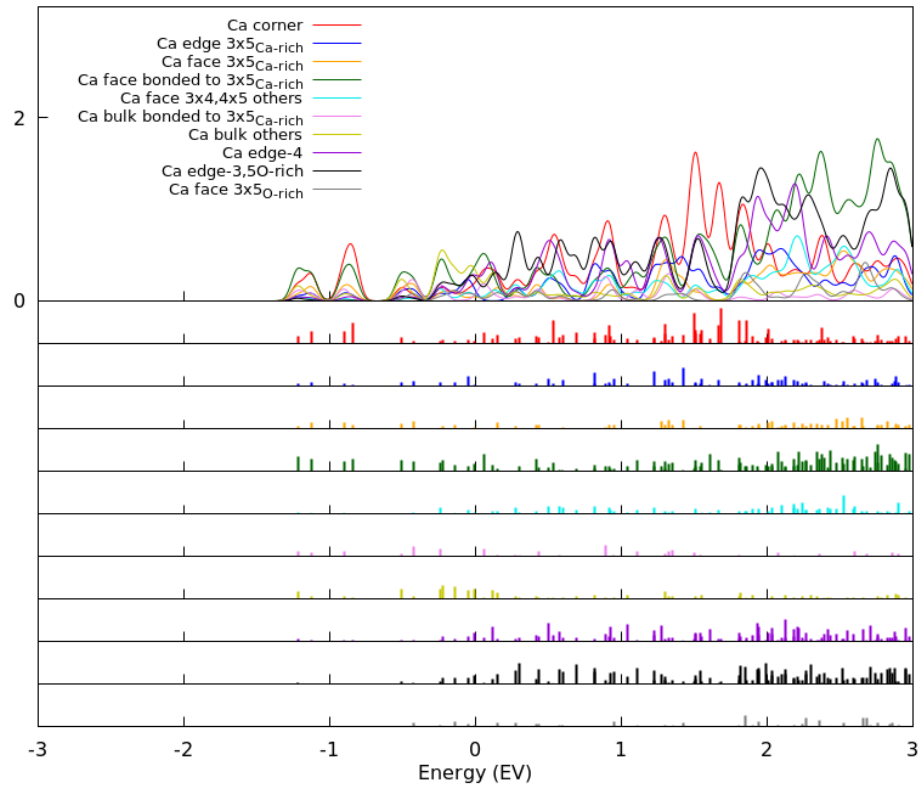
(d)


Ca corner
Ca short-edge$_{O\text{-}rich}$
Ca long-edge
Ca face 3x3$_{Ca\text{-}rich}$
Ca face 3x8 near 3x3$_{Ca\text{-}rich}$
Ca face 3x8 others
Ca bulk
3
0
-3
-2
-1
0
1
2
3
Energy (EV)

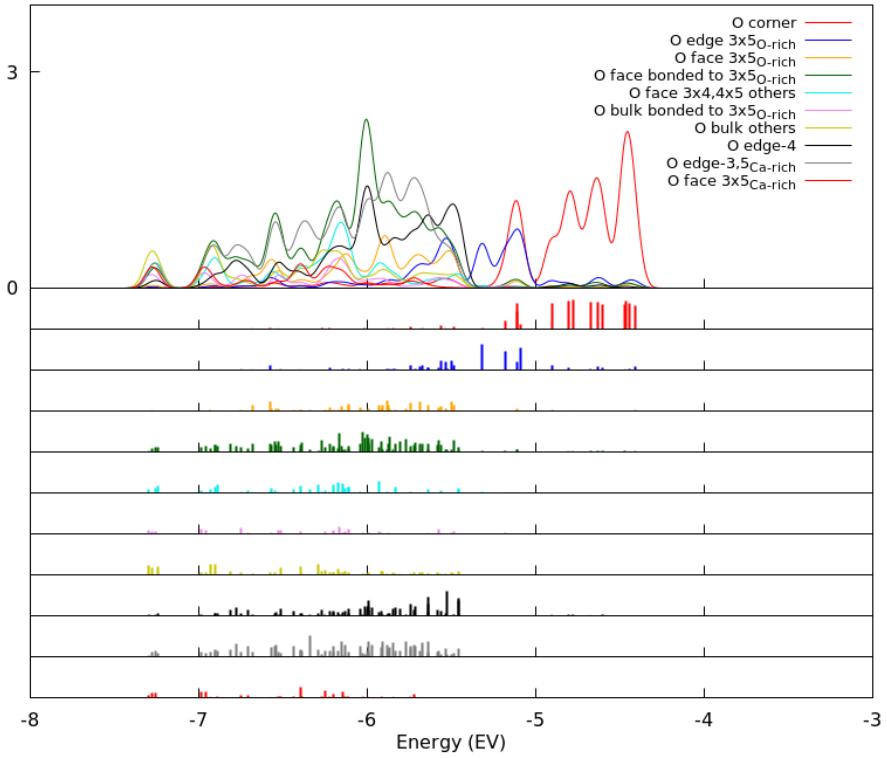
(e)


(CaO)30 3x4x5
O p
Ca s
Ca p
Ca d
8
0
-10
-5
0
5
10
15
20
Energy (EV)

(f)


Ca corner
Ca edge 3x5Ca-rich
Ca face 3x5Ca-rich
Ca face bonded to 3x5Ca-rich
Ca face 3x4,4x5 others
Ca bulk bonded to 3x5Ca-rich
Ca bulk others
Ca edge-4
Ca edge-3,5O-rich
Ca face 3x5O-rich
2
0
-3
-2
-1
0
1
2
3
Energy (EV)

(g)



(h)

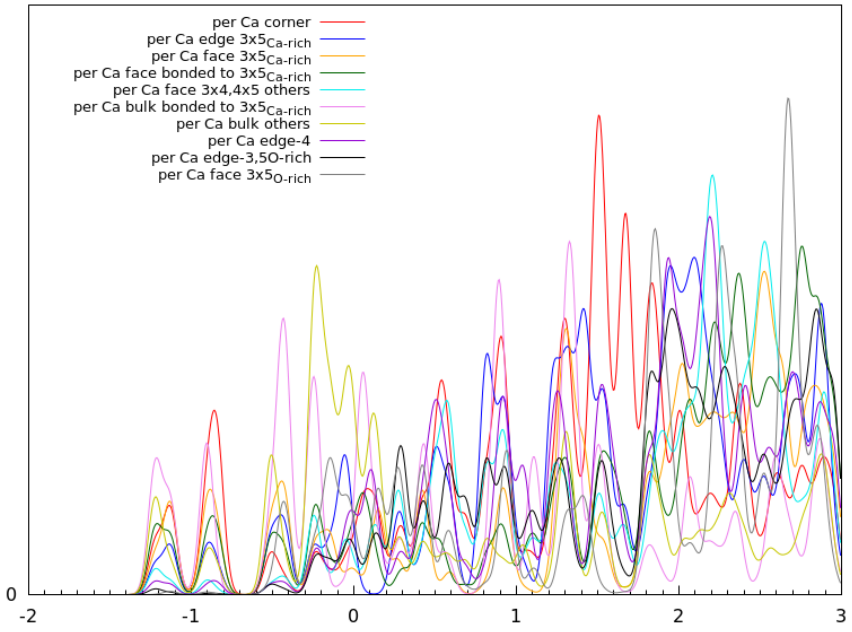


Figure S5. (a): PDOS for $(MgO)_{40}$ (4×4×5) projected to the corner and bulk atoms at B3LYP/cc-pVDZ level. (b), (c), (d): PDOS for $(MgO)_{36}$ (3×3×8). (e), (f), (g), (h): PDOS for $(MgO)_{30}$ (3×4×5).

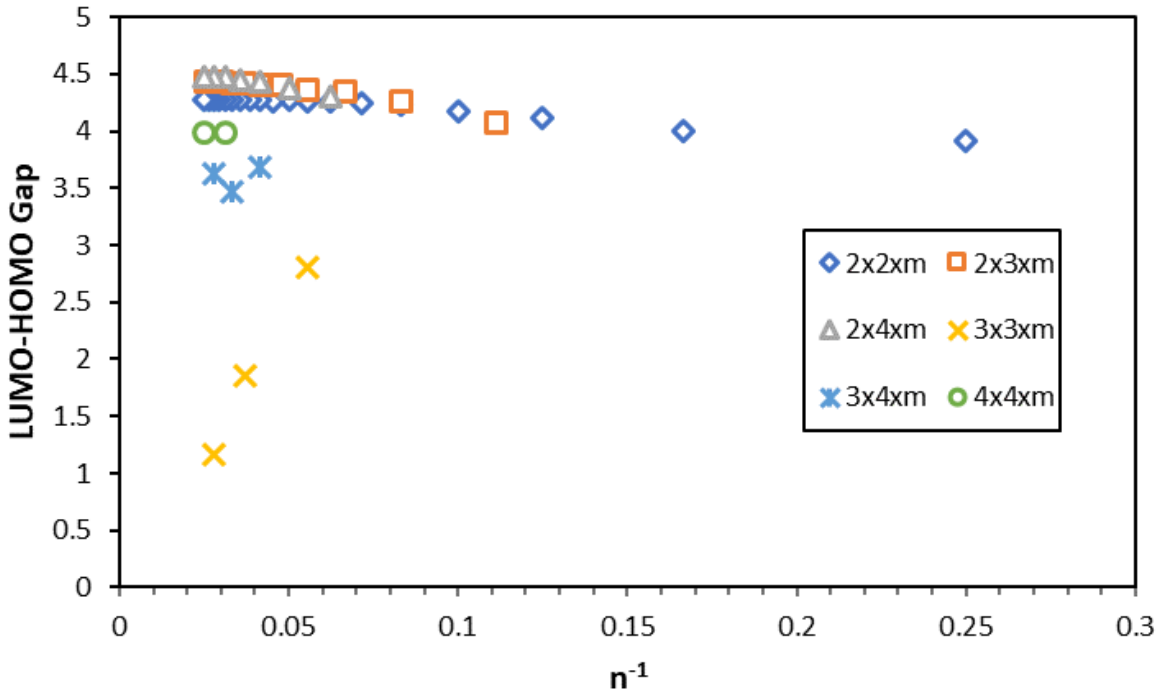
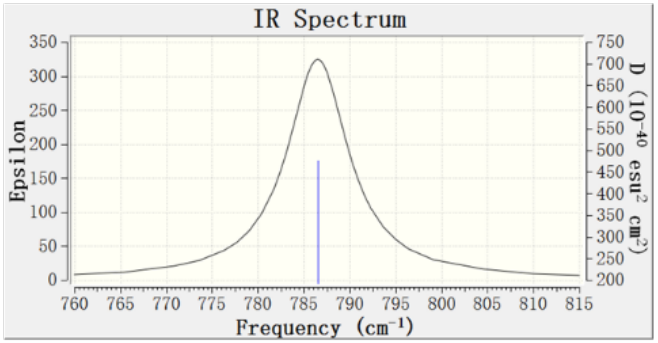
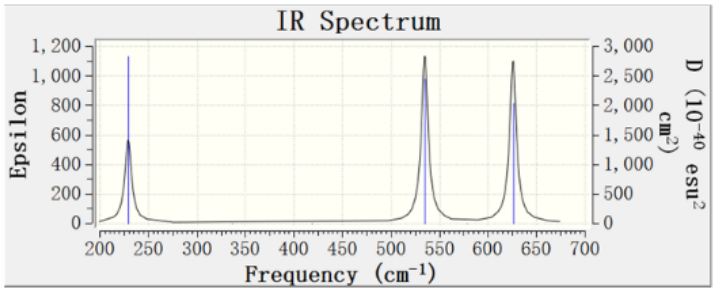


Figure S6. Calculated HOMO-LUMO for the cubic $(MgO)_n$ at the B3LYP/DZVP level.

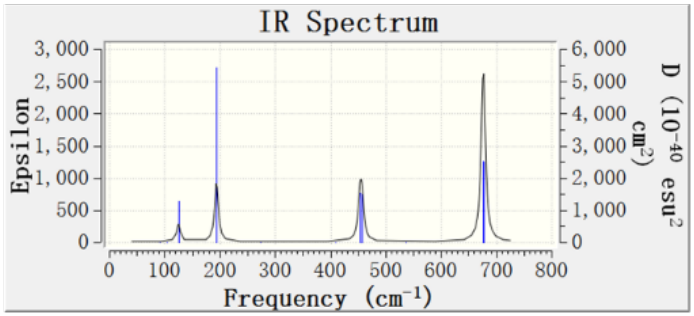
1


IR Spectrum
Epsilon
D (10^{-40} esu^2 cm^2)
Frequency (cm^{-1})

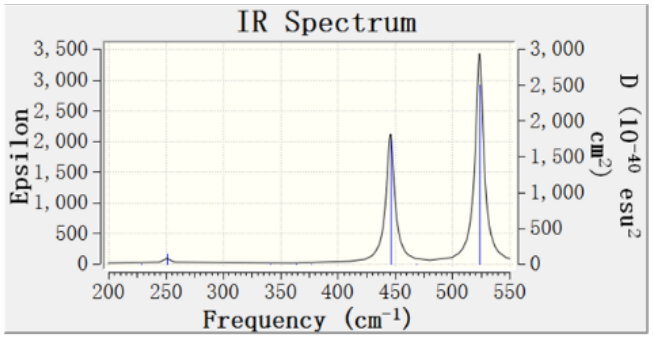
2


IR Spectrum
Epsilon
D (10^{-40} esu^2 cm^2)
Frequency (cm^{-1})

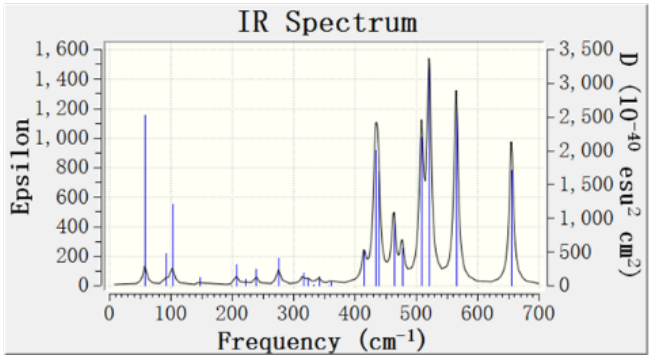
3


IR Spectrum
Epsilon
D (10^{-40} esu^2 cm^2)
Frequency (cm^{-1})

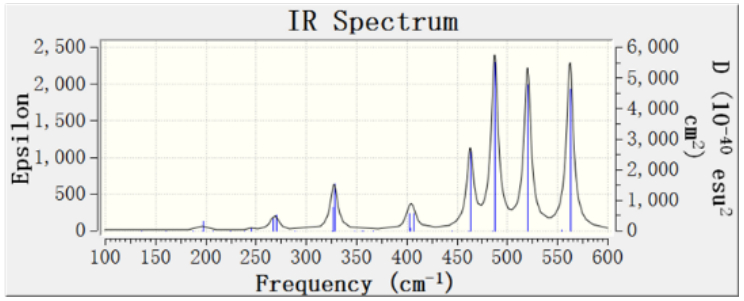
4


IR Spectrum
Epsilon
D (10^{-40} esu^2 cm^2)
Frequency (cm^{-1})

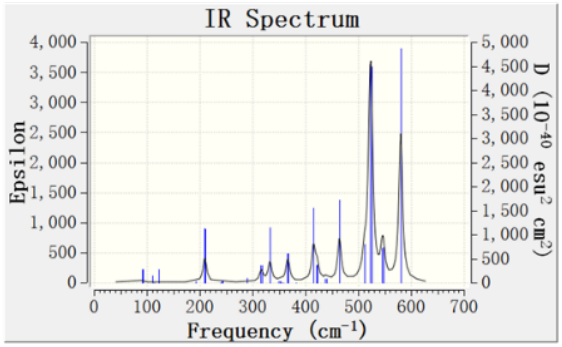
5


IR Spectrum
Epsilon
D (10^{-40} esu^2 cm^2)
Frequency (cm^{-1})

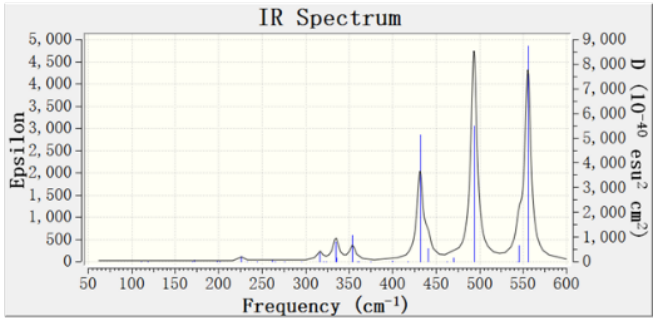
6


IR Spectrum
Epsilon
D (10^{-40} esu^2 cm^2)
Frequency (cm^{-1})

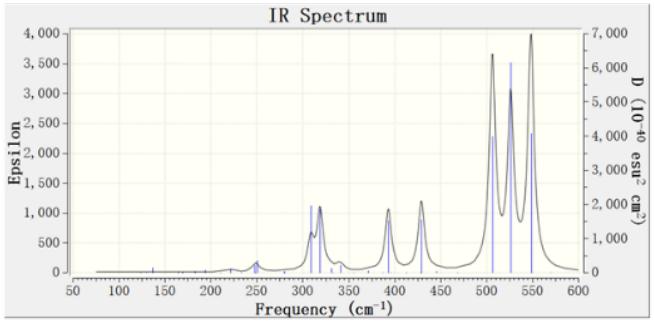
7


IR Spectrum
Epsilon
D (10-40 esu2 cm2)
Frequency (cm-1)

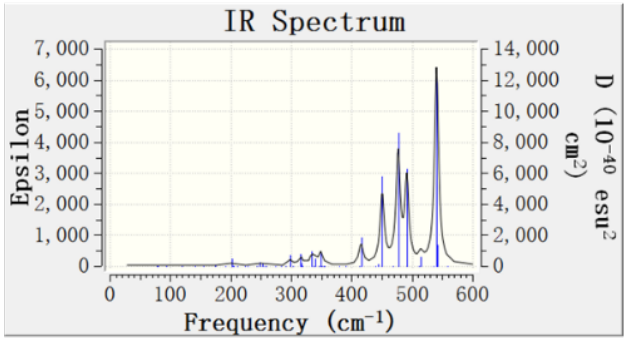
8


IR Spectrum
Epsilon
D (10-40 esu2 cm2)
Frequency (cm-1)

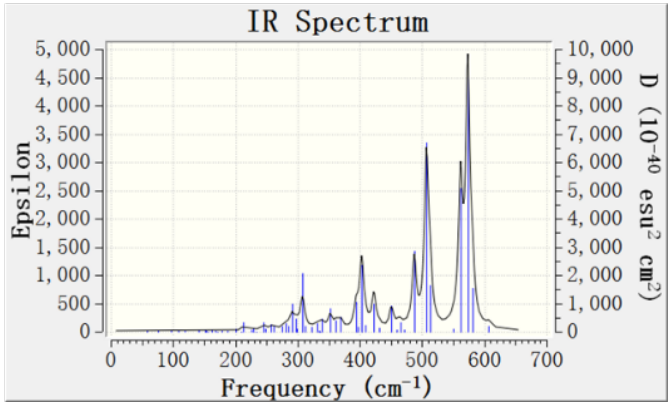
9


IR Spectrum
Epsilon
D (10-40 esu2 cm2)
Frequency (cm-1)

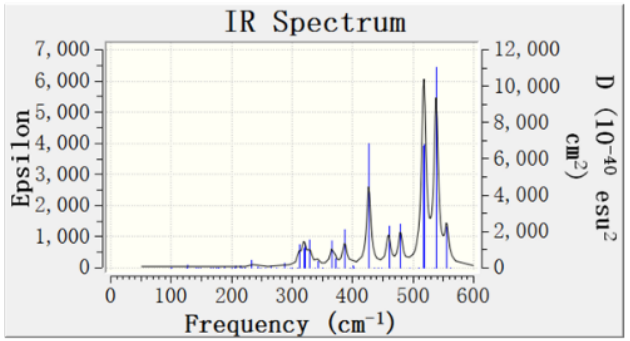
10


IR Spectrum
Epsilon
D (10-40 esu2 cm2)
Frequency (cm-1)

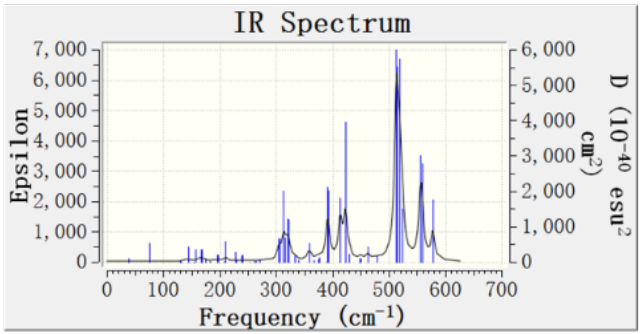
11


IR Spectrum
Epsilon
D (10-40 esu2 cm2)
Frequency (cm-1)

12


IR Spectrum
Epsilon
D (10-40 esu2 cm2)
Frequency (cm-1)

13



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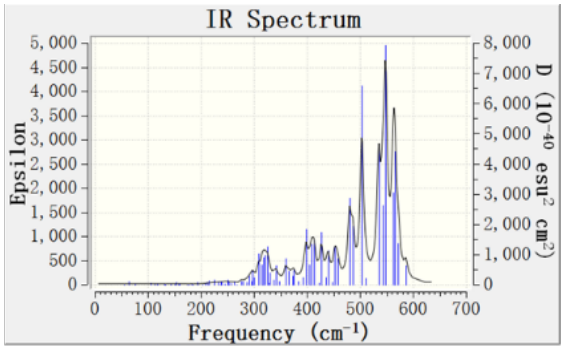

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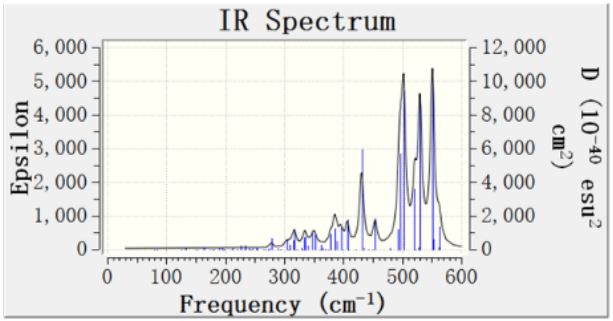

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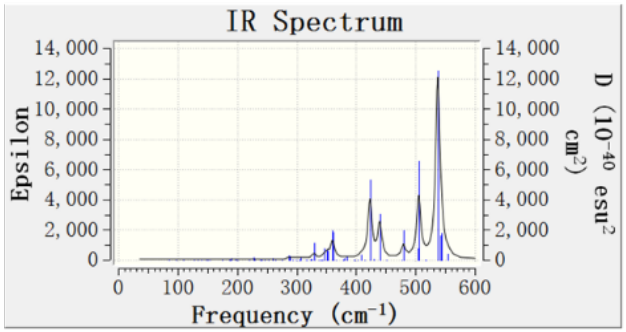
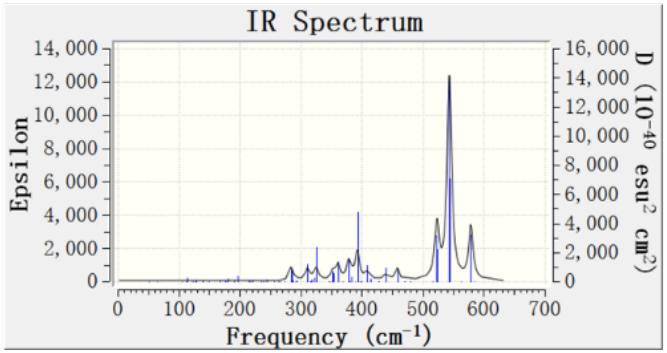


17



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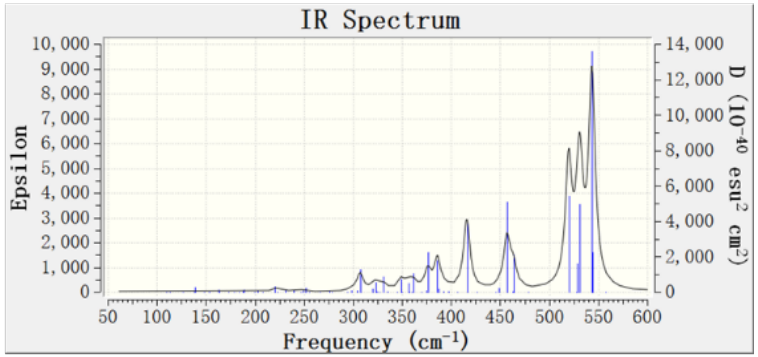

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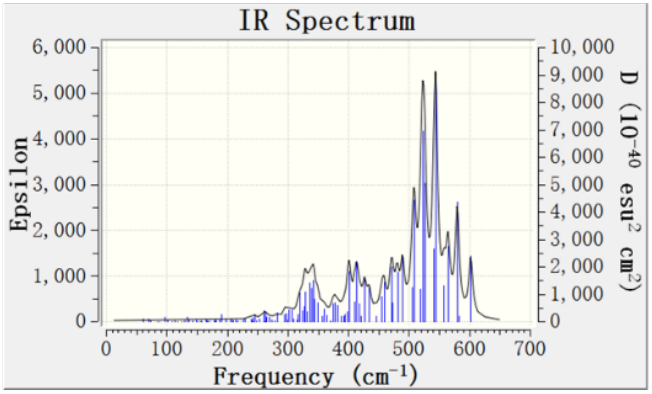

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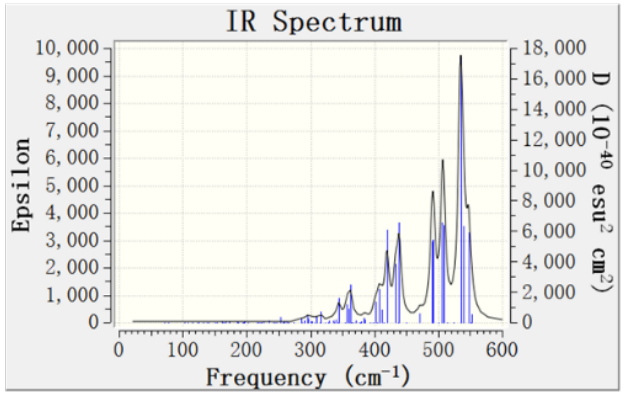

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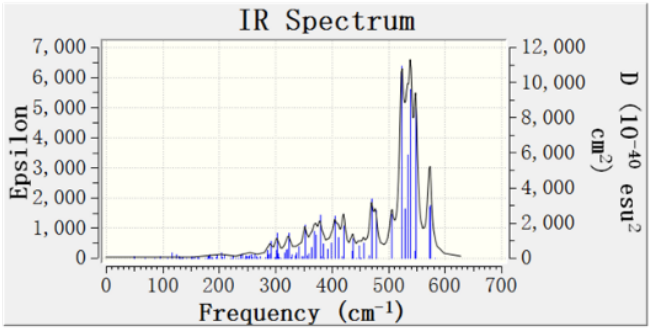

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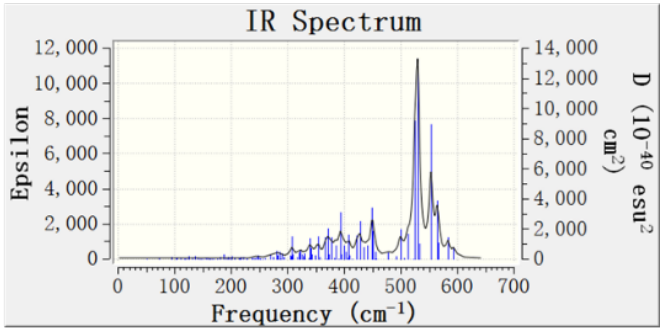

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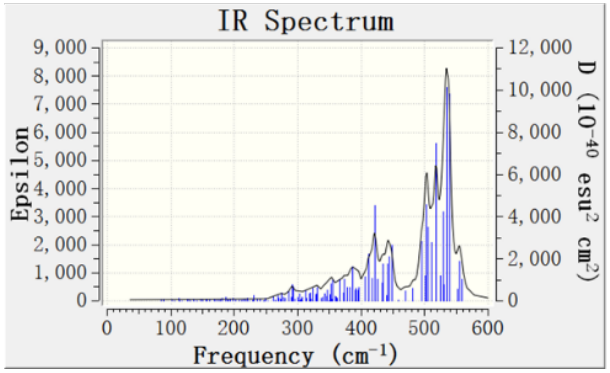

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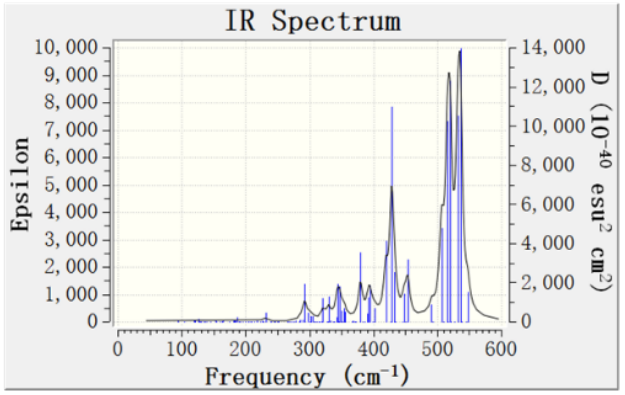

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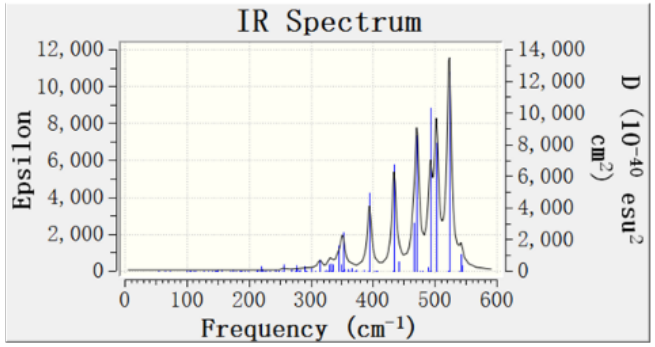

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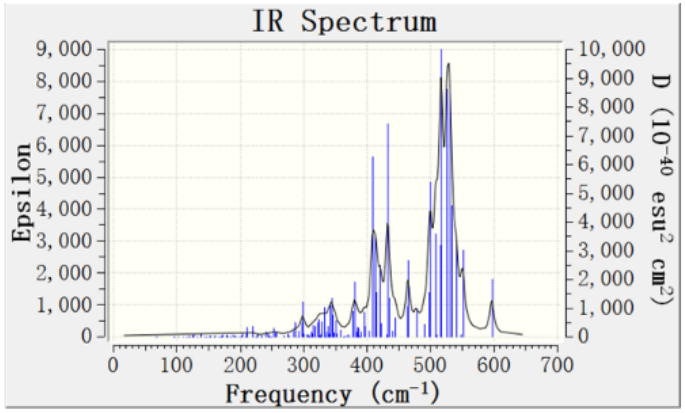

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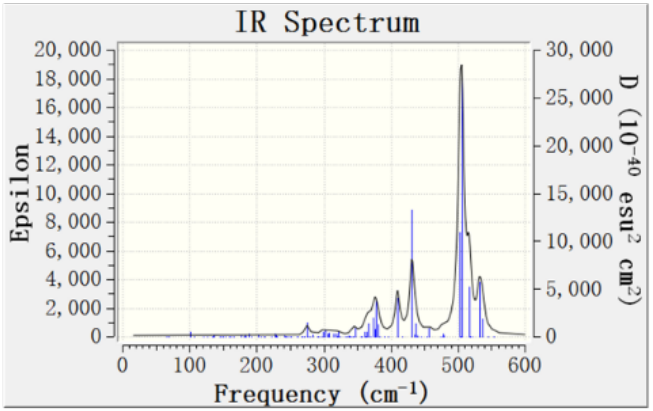

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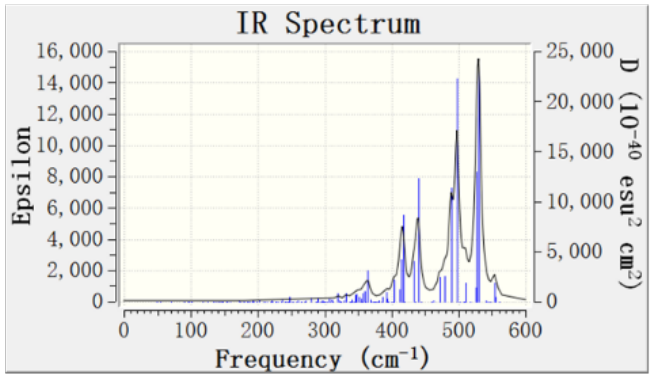

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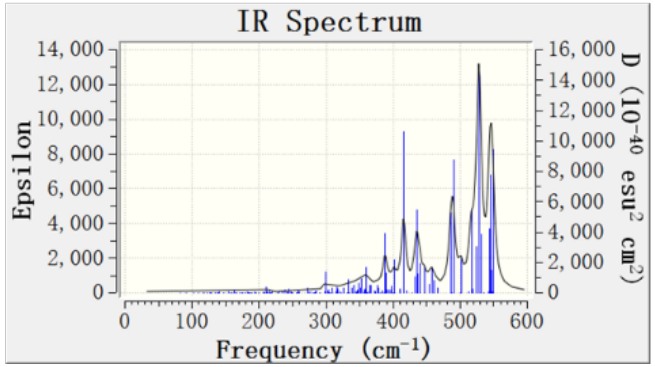

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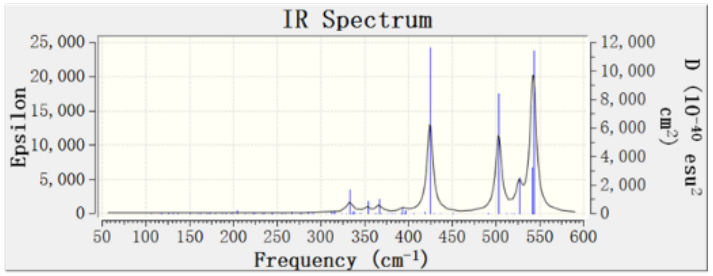

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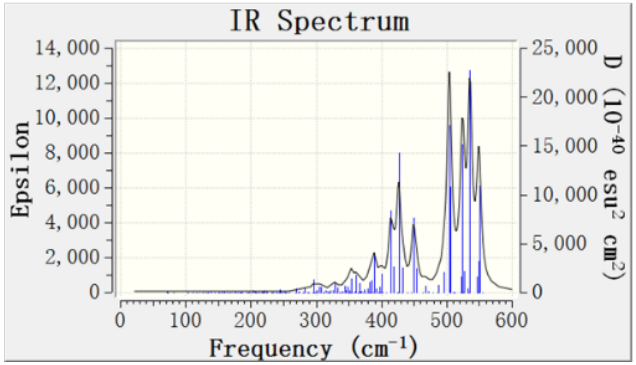

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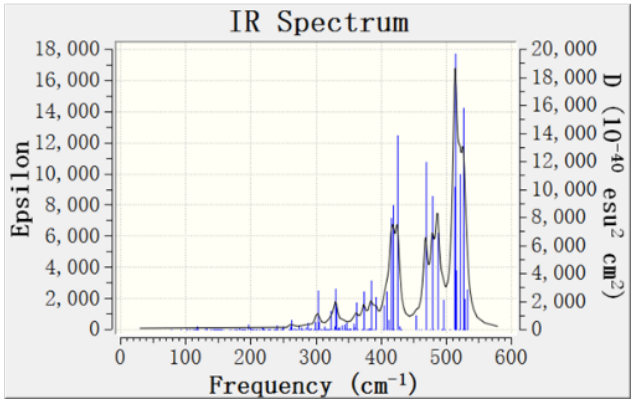

Figure S7. Calculated vibrational spectra for $(CaO)_n$, n≤40, at the B3LYP/DZVP level.

Table S1. Benchmarks for the Normalized Clustering Energies (DFT/T Compared with CCSD(T)/T) in kcal/mol for $(CaO)_n$, n = 2 - 8. [a]

CCSD(T)/T	ΔMP2/T	ΔM11/T	ΔM06/T	ΔB3LYP/T	ΔBP86/T	ΔPW91/T	ΔCAM-B3LYP/T	ΔωB97XD/T
61.5	-3.2	1.6	-2.7	-4.8	-8.6	-7.4	-1.0	-2.3
76.3	-3.2	1.5	-4.1	-6.7	-12.2	-11.0	-2.0	-2.5
97.3	-5.4	3.4	-4.7	-9.0	-14.5	-12.7	-3.0	-4.0
96.3	-5.1	3.2	-4.9	-9.0	-14.8	-13.0	-3.0	-3.6
107	-5.7	4.2	-5.5	-10.4	-16.6	-14.7	-3.6	-4.2
106.4	-5.8	3.2	-5.4	-10.1	-16.5	-14.7	-3.5	-3.9
112.2	-6.0	4.3	-6.0	-11.2	-17.8	-15.7	-4.1	-4.5

[a] For the CCSD(T)/T calculations, cc-pVTZ on Ca and aug-cc-pVTZ on O were used. For the MP2 and DFT/T calculations, cc-pVTZ on both Ca and O was used-

Table S2. Comparison of HOMO-LUMO Energy Gap E_g (in eV) Using HF, DFT, and TDDFT Methods for $(CaO)_8$.

	TD-B3LYP/D[a]	TD-ωB97XD/D	HF/D	B3LYP/DZVP	B3LYP/D	BP86/D	CAM-B3LYP/D	M06/D	M11/D	PW91/D	ωB97XD/D
HOMO			-8.15	-4.90	-4.87	-3.98	-6.42	-4.82	-7.51	-3.95	-6.82
LUMO			0.59	-0.91	-1.01	-1.21	-0.29	-1.12	-0.59	-1.44	0.49
E_g	3.18[b]	3.90[b]	8.74	3.99	3.85	2.77	6.14	3.71	6.92	2.50	7.31

[a] 'D' denotes cc-pVDZ

[b] first excitation energy calculated using TD-DFT method.

Table S3. First Excitation Energy and HOMO-LUMO Energy Gaps (in eV) at the B3LYP/cc-pVDZ Level for Lowest Energy Isomer for $(CaO)_n$, n ≤ 40.

n	First Excitation Energy	HOMO-LUMO Gap	LUMO	HOMO
1	1.70	2.49	-4.68	-2.20
2	2.41	3.22	-4.67	-1.45
3	2.78	3.60	-4.81	-1.21
4	3.19	3.92	-4.95	-1.03
5	2.46	3.21	-4.69	-1.47
6	3.14	3.80	-4.84	-1.04
7	3.11	3.83	-4.88	-1.05
8	3.18	3.85	-4.87	-1.01
9	3.08	3.66	-4.75	-1.09
10	3.18	3.84	-4.84	-1.00
11	3.01	3.58	-4.73	-1.15
12	3.17	3.74	-4.77	-1.03
13	1.88	2.28	-4.63	-2.35
14	3.12	3.67	-4.75	-1.08
15	3.17	3.73	-4.76	-1.03
16	3.25	3.84	-4.83	-0.99
17	3.16	3.54	-4.60	-1.06
18	2.51	2.84	-4.23	-1.40
19	2.86	3.50	-4.71	-1.21
20	3.26	3.84	-4.82	-0.98
21	2.29	2.60	-4.08	-1.49
22	2.57	2.90	-4.29	-1.40
23	2.35	2.85	-4.41	-1.56
24	3.07	3.46	-4.55	-1.09
25	3.27	3.83	-4.81	-0.98
26	3.01	3.44	-4.55	-1.11
27	2.00	2.22	-3.87	-1.66
28	3.26	3.84	-4.81	-0.97
29	2.86	3.40	-4.64	-1.24
30	2.88	3.19	-4.41	-1.22
32	3.29	3.71	-4.69	-0.98
36	3.00	3.35	-4.49	-1.14
40	3.29	3.68	-4.66	-0.98

Table S4. First Excitation Energy and HOMO-LUMO Energy Gaps (in eV) at the B3LYP/cc-pVDZ Level for Cubic $(CaO)_n$.

n	*a*×*b*×*c*	First Excitation Energy	HOMO-LUMO Gap	HOMO	LUMO
	2×2×m				
4	2×2×2	3.19	3.92	-4.95	-1.03
6	2×2×3	3.13	3.79	-4.83	-1.04
8	2×2×4	3.18	3.84	-4.85	-1.01
10	2×2×5	3.19	3.86	-4.85	-1.00
12	2×2×6	3.19	3.86	-4.84	-0.99
14	2×2×7	3.18	3.85	-4.83	-0.98
16	2×2×8	3.18	3.86	-4.83	-0.97
18	2×2×9	3.18	3.86	-4.82	-0.97
20	2×2×10	3.18	3.85	-4.81	-0.96
22	2×2×11	3.18	3.84	-4.79	-0.96
24	2×2×12	3.18	3.84	-4.79	-0.95
26	2×2×13	3.18	3.82	-4.77	-0.95
28	2×2×14	3.18	3.81	-4.76	-0.95
30	2×2×15	3.19	3.81	-4.76	-0.95
32	2×2×16	3.18	3.80	-4.75	-0.94
34	2×2×17	3.18	3.80	-4.74	-0.94
36	2×2×18	3.18	3.79	-4.73	-0.94
38	2×2×19	3.18	3.78	-4.72	-0.94
40	2×2×20	3.18	3.78	-4.72	-0.94
	2×3×m				
6	2×3×2	3.13	3.79	-4.83	-1.04
9	2×3×3	3.08	3.66	-4.75	-1.09
12	2×3×4	3.17	3.74	-4.77	-1.03
15	2×3×5	3.17	3.73	-4.76	-1.03
18	2×3×6	3.19	3.76	-4.76	-1.01
27	2×3×9	3.18	3.76	-4.75	-0.99
30	2×3×10	3.19	3.78	-4.76	-0.98
33	2×3×11	3.19	3.77	-4.75	-0.98
36	2×3×12	3.18	3.77	-4.75	-0.98
39	2×3×13	3.20	3.79	-4.76	-0.98
	2×4×m				
8	2×4×2	3.18	3.84	-4.85	-1.01
12	2×4×3	3.17	3.74	-4.77	-1.03
16	2×4×4	3.25	3.84	-4.83	-0.99
20	2×4×5	3.26	3.84	-4.82	-0.98
32	2×4×8	3.26	3.85	-4.81	-0.96
36	2×4×9	3.26	3.85	-4.81	-0.96

40	2×4×10	3.26	3.85	-4.80	-0.95
	2×5×m				
10	2×5×2	3.19	3.86	-4.85	-1.00
15	2×5×3	3.17	3.73	-4.76	-1.03
20	2×5×4	3.26	3.84	-4.82	-0.98
25	2×5×5	3.27	3.83	-4.81	-0.98
30	2×5×6	3.27	3.84	-4.82	-0.97
35	2×5×7	2.38	2.70	-4.81	-2.12
40	2×5×8	3.27	3.86	-4.82	-0.96
	3×3×m				
9	3×3×2	3.08	3.66	-4.75	-1.09
18	3×3×4	2.51	2.84	-4.23	-1.40
27	3×3×6	2.00	2.22	-3.87	-1.66
36	3×3×8	1.47	1.64	-3.56	-1.92
45	3×3×10	1.24	1.38	-3.41	-2.03
54	3×3×12	1.01	1.12	-3.27	-2.15
63	3×3×14	0.87	0.97	-3.18	-2.21
72	3×3×16	0.77	0.85	-3.12	-2.27
81	3×3×18	0.70	0.78	-3.09	-2.31
	3×4×m				
12	3×4×2	3.17	3.74	-4.77	-1.03
18	3×4×3	2.51	2.84	-4.23	-1.40
24	3×4×4	3.07	3.46	-4.55	-1.09
30	3×4×5	2.87	3.19	-4.41	-1.22
36	3×4×6	3.02	3.37	-4.50	-1.13
	3×5×m				
15	3×5×2	3.17	3.73	-4.76	-1.03
30	3×5×4	2.87	3.19	-4.41	-1.22
45	3×5×6	2.57	2.78	-4.19	-1.41
60	3×5×8	2.48	2.64	-4.09	-1.45
	4×4×m				
16	4×4×2	3.25	3.84	-4.83	-0.99
24	4×4×3	3.07	3.46	-4.55	-1.09
32	4×4×4	3.29	3.71	-4.69	-0.98
40	4×4×5	3.29	3.68	-4.66	-0.98
	4×5×m				
20	4×5×2	3.26	3.84	-4.82	-0.98
30	4×5×3	2.87	3.19	-4.41	-1.22
40	4×5×4	3.29	3.68	-4.66	-0.98
50	4×5×5	3.18	3.50	-4.52	-1.02
	5×5×m				
25	5×5×2	3.27	3.83	-4.81	-0.98

50	5×5×4	3.18	3.50	-4.52	-1.02

Table S5. Cartesian Coordinates and Electronic Energy at the B3LYP/DZVP Level for Optimized lowest energy $(CaO)_n$ clusters.

1

E = -752.733803 Hartree

O	0.000000	0.000000	-1.298808
Ca	0.000000	0.000000	0.519523

2

E = -1505.650072 Hartree

O	-0.000565	-1.409737	-0.000004
Ca	-1.485771	0.000197	0.000002
Ca	1.485796	-0.000209	0.000002
O	0.000505	1.409767	-0.000004

3

E = -2258.538777 Hartree

O	1.277174	1.551389	-0.001375
Ca	-0.737601	1.958080	0.000338
O	-1.992364	0.329751	0.000644
Ca	2.073619	-0.342298	0.000125
O	0.706084	-1.877725	0.001201
Ca	-1.332374	-1.617149	-0.000651

4

E = -3011.505262 Hartree

Ca	1.111491	1.111491	-1.111491
O	1.065651	1.065651	1.065651
Ca	-1.111491	1.111491	1.111491
O	-1.065651	1.065651	-1.065651
O	-1.065651	-1.065651	1.065651
O	1.065651	-1.065651	-1.065651
Ca	-1.111491	-1.111491	-1.111491
Ca	1.111491	-1.111491	1.111491

5

E = -3764.373853 Hartree

Ca	2.461137	0.764085	-0.000048
O	-2.661489	1.408288	-0.000041
Ca	-3.009664	-0.540147	0.000052
O	-1.053958	-1.372690	0.000062
O	2.022775	-1.356577	0.000040
Ca	0.528535	-1.137451	1.553883
O	0.904933	0.981889	1.498759
O	0.904920	0.981768	-1.498857

Ca	-0.555394	1.794017	-0.000075
Ca	0.528513	-1.137575	-1.553799

6

E = -4517.339783 Hartree

Ca	-0.000045	-0.005309	-1.711210
O	-2.224042	-0.002179	-1.488681
O	-0.000033	1.609875	-0.000566
O	-2.224244	0.003099	1.488512
Ca	-2.225495	-1.558684	0.002835
Ca	-2.223561	1.560434	-0.002998
O	2.223941	-0.001861	-1.488724
Ca	2.223486	1.560475	-0.002778
O	2.224345	0.002862	1.488484
Ca	2.225568	-1.558636	0.002518
Ca	0.000048	0.002249	1.711301
O	0.000031	-1.613117	0.001808

7

E = -5270.225890 Hartree

O	-1.097406	-0.473089	-1.987688
Ca	-2.132227	1.310441	-1.237897
Ca	-2.137548	-1.727114	-0.515928
O	-3.319684	0.004586	-0.002743
O	-1.100492	-1.486448	1.402769
Ca	-2.136352	0.417027	1.752560
O	-1.097876	1.959041	0.585012
O	2.086720	1.267965	-1.198142
Ca	1.060634	2.024074	0.605643
O	2.083808	0.402777	1.697557
O	2.082613	-1.672933	-0.499281
Ca	1.059457	-1.535796	1.450506
Ca	1.059979	-0.487788	-2.053454
Ca	3.370983	-0.001604	-0.000423

8

E = -6023.178068 Hartree

O	1.151183	1.134154	-1.130693
Ca	1.129303	-1.183970	-1.186507
Ca	3.373283	1.104621	-1.102121
O	3.356914	-1.054830	-1.057568
O	3.356935	1.054800	1.057558
Ca	1.129317	1.183995	1.186520
Ca	3.373278	-1.104648	1.102109

O	1.151179	-1.134115	1.130725
Ca	-3.373282	1.102096	1.104646
O	-3.356934	1.057541	-1.054819
O	-3.356915	-1.057569	1.054825
O	-1.151179	-1.130706	-1.134135
Ca	-1.129304	-1.186513	1.183967
Ca	-3.373278	-1.102121	-1.104637
Ca	-1.129316	1.186534	-1.183978
O	-1.151183	1.130740	1.134106

9

E = -6776.109359 Hartree

O	0.000000	-3.148876	-1.041957
O	0.000000	0.000000	-1.268880
Ca	1.647760	-1.647760	-1.259821
O	0.000000	3.148876	-1.041957
Ca	0.000000	3.158516	1.064097
Ca	1.647760	1.647760	-1.259821
O	1.628339	1.628339	1.117552
O	3.148876	0.000000	-1.041957
Ca	3.158516	0.000000	1.064097
Ca	-1.647760	-1.647760	-1.259821
O	-3.148876	0.000000	-1.041957
Ca	0.000000	-3.158516	1.064097
O	1.628339	-1.628339	1.117552
O	-1.628339	-1.628339	1.117552
Ca	-3.158516	0.000000	1.064097
Ca	0.000000	0.000000	1.169496
Ca	-1.647760	1.647760	-1.259821
O	-1.628339	1.628339	1.117552

10

E = -7529.013740 Hartree

Ca	4.502019	-1.561345	0.001134
O	2.281609	-1.601669	-0.000474
Ca	-0.000068	-1.653267	-0.001544
O	-2.281332	-1.601216	0.000011
Ca	-4.501490	-1.561836	0.001455
O	4.493551	-0.000429	-1.489627
Ca	2.267220	-0.000067	-1.682943
O	0.000000	0.000617	-1.583930
Ca	-2.267222	0.000694	-1.682942
O	-4.493555	-0.001386	-1.489626
O	4.492445	-0.000649	1.491845

Ca	2.265889	0.000345	1.682414
O	0.000001	0.000967	1.580977
Ca	-2.265886	0.001162	1.682406
O	-4.492442	-0.000670	1.491850
Ca	4.502646	1.560263	0.001107
O	2.282065	1.601862	-0.000317
Ca	0.000070	1.654386	-0.001838
O	-2.282344	1.602313	-0.000816
Ca	-4.503178	1.559770	0.000793

11

E = -8281.928426 Hartree

Ca	-0.994146	-3.264312	-1.052496
Ca	-0.600611	-0.000604	-1.135647
O	-2.403163	-1.593441	-1.095093
O	-2.423198	1.571971	-1.094672
Ca	-1.033921	3.259833	-1.052983
Ca	-3.923328	-0.020104	-1.085124
Ca	-2.475571	1.607500	1.263045
O	-3.964573	-0.020287	1.046633
O	-1.003878	3.251448	1.069683
Ca	-2.454105	-1.627628	1.263689
Ca	2.929638	-1.866825	-1.124358
O	3.987637	0.014164	-1.147233
O	-0.964072	-3.255085	1.070057
O	0.733509	-1.911253	-1.132845
Ca	2.903917	1.882287	-1.127935
O	0.707904	1.924510	-1.134208
O	-0.655881	-0.000680	1.273589
Ca	0.777371	-1.899064	1.296874
Ca	0.752236	1.911481	1.296840
O	2.951081	1.815853	1.047942
Ca	4.141665	0.017460	1.075773
O	2.976774	-1.797259	1.051957

12

E = -9034.888578 Hartree

Ca	-1.651586	3.149343	2.232429
O	-1.675090	-0.045732	0.000000
Ca	-1.651586	-0.039693	2.342613
Ca	-3.336155	1.566871	0.000000
Ca	0.064086	1.664339	0.000000
O	-1.653744	3.231032	0.000000
O	-0.048898	1.615972	2.313474

O	-3.121255	1.627292	2.233408
Ca	-1.651586	3.149343	-2.232429
Ca	-1.651586	-0.039693	-2.342613
O	-0.048898	1.615972	-2.313474
O	-3.121255	1.627292	-2.233408
Ca	1.651586	0.039693	2.342613
O	1.653744	-3.231032	0.000000
Ca	1.651586	-3.149343	2.232429
Ca	-0.064086	-1.664339	0.000000
Ca	3.336155	-1.566871	0.000000
O	1.675090	0.045732	0.000000
O	3.121255	-1.627292	2.233408
O	0.048898	-1.615972	2.313474
Ca	1.651586	0.039693	-2.342613
Ca	1.651586	-3.149343	-2.232429
O	3.121255	-1.627292	-2.233408
O	0.048898	-1.615972	-2.313474

13

E = -9787.764018 Hartree

O	-3.038889	-1.956497	1.146696
O	-1.614049	-0.992592	-1.695709
Ca	-3.334721	-0.181227	-0.080741
Ca	-1.890202	1.024901	-2.685475
O	-3.281522	1.713153	-1.338014
O	-1.713122	0.886895	1.199207
O	-0.173390	3.614529	1.126101
Ca	-1.868441	2.829477	0.016205
Ca	-0.052990	1.906873	2.588943
Ca	1.510680	2.975021	-0.099368
Ca	3.385348	0.203388	0.011451
O	3.221079	-1.646933	1.135961
O	3.121338	1.975480	-1.351180
O	1.623403	1.047424	1.193119
Ca	1.830653	1.103211	-2.694645
Ca	1.680900	-0.887505	2.594003
Ca	-0.001008	-0.000231	-0.156342
O	0.007880	0.011605	3.709147
O	1.655862	-0.904917	-1.700880
O	0.095857	-1.919966	1.204544
Ca	-1.609507	-0.991687	2.599436
Ca	1.824842	-2.794136	-0.081995
Ca	-1.516896	-3.033191	0.031611
O	0.150823	-3.700848	-1.325936

O	-0.054025	1.876493	-1.707193
Ca	0.040844	-2.156424	-2.681427

14
E = -10540.706482 Hartree

O	4.750994	-1.508835	1.098315
O	4.537251	0.558892	-1.094056
O	-1.788603	-0.154653	1.219807
Ca	-2.503322	2.039812	1.221092
O	-0.360420	2.731040	1.061516
Ca	0.542658	0.509322	1.178845
Ca	-4.672547	1.293664	-1.022480
Ca	1.625613	3.620205	1.003487
O	2.590646	1.649612	1.110175
O	-2.581599	2.002289	-1.120265
O	1.604579	3.566892	-1.126182
Ca	-0.438688	2.746972	-1.239422
Ca	2.591157	1.589685	-1.311090
Ca	4.548055	0.645107	1.083001
Ca	-1.814393	-0.167586	-1.182535
O	-4.049909	-0.842398	-1.067204
O	0.482009	0.505730	-1.231726
Ca	-3.382585	-2.960797	-1.021397
Ca	4.840217	-1.571438	-1.126313
Ca	-4.052759	-0.832528	1.294111
O	-4.615264	1.315615	1.096385
O	-3.343905	-2.942229	1.098376
Ca	0.957060	-1.826485	-1.226225
O	2.987436	-2.677918	-1.071450
Ca	2.968066	-2.722064	1.114104
O	0.990117	-1.781158	1.129963
O	-1.240099	-2.394939	-1.094883
Ca	-1.193826	-2.375047	1.231314

15
E = -11293.669364 Hartree

Ca	-1.226997	-4.629527	0.000000
O	-1.031725	-4.521097	2.232297
O	1.113471	-2.302121	2.318699
Ca	1.084185	-4.529090	2.234429
Ca	1.197007	-2.271572	0.000000
O	1.147745	0.000205	0.000000
O	1.136812	-4.593674	0.000000
O	1.113471	-2.302121	-2.318699

Ca	1.084185	-4.529090	-2.234429
Ca	1.120544	-0.000200	-2.354406
O	-1.031725	-4.521097	-2.232297
Ca	-1.209307	-2.302569	-2.337245
Ca	1.120544	-0.000200	2.354406
Ca	-1.209307	-2.302569	2.337245
O	-1.231979	-2.310270	0.000000
O	-1.129612	-0.000419	2.327483
O	1.111679	2.302189	2.312808
Ca	-1.213675	2.300900	2.332242
Ca	1.083495	4.529220	2.235753
Ca	1.197842	2.274371	-0.000000
O	-1.030967	4.520049	2.233047
O	-1.234747	2.310559	-0.000000
O	-1.030967	4.520049	-2.233047
Ca	-1.213675	2.300900	-2.332242
Ca	-1.223516	4.630935	-0.000000
O	-1.129612	-0.000419	-2.327483
Ca	-1.283309	-0.001175	-0.000000
O	1.137698	4.597090	-0.000000
Ca	1.083495	4.529220	-2.235753
O	1.111679	2.302189	-2.312808

16

E = -12046.613255 Hartree

Ca	3.319360	-3.474529	1.091372
O	3.296374	-3.454153	-1.031662
Ca	3.463817	-1.234298	-1.179564
Ca	1.071102	-3.520630	-1.174979
O	1.146173	-1.200952	-1.185910
O	-1.249679	-3.440200	-1.131468
O	-3.454236	-3.296890	1.030584
Ca	-1.235038	-3.465269	1.178905
O	1.091216	-3.489306	1.137812
Ca	3.475948	3.318174	-1.091646
O	3.451766	3.298733	1.031440
O	3.494562	1.091559	-1.127557
Ca	3.518239	1.072923	1.177931
Ca	1.178301	1.124701	-1.235969
O	3.439695	-1.249329	1.124995
Ca	1.125061	-1.177962	1.236533
O	-1.198455	-1.145111	1.181257
O	-3.493500	-1.090413	-1.135341
Ca	-1.175580	-1.124588	-1.234768

Ca	-3.475417	-3.316739	-1.092180
O	1.200288	1.146712	1.186159
Ca	-1.123474	1.177865	1.237308
O	1.249397	3.435201	-1.136503
O	-3.297740	3.452949	-1.031978
Ca	-1.072874	3.518630	-1.177132
Ca	-3.319295	3.474017	1.090671
Ca	-3.464249	1.233209	-1.176721
O	-1.144043	1.199028	-1.179183
Ca	1.232812	3.466014	1.176134
O	-1.091712	3.493408	1.134094
O	-3.440499	1.249029	1.132222
Ca	-3.518556	-1.071623	1.174520

17

E = -12799.481642 Hartree

Ca	3.211656	2.239114	2.221567
Ca	-1.329693	-2.244407	-2.225043
Ca	0.921192	-2.371194	0.009599
Ca	3.211696	-2.239070	-2.221568
O	3.331150	-2.329447	0.009208
Ca	3.211695	-2.221543	2.239100
O	3.331133	0.009235	2.329451
O	1.041483	-2.312322	-2.294061
O	3.331109	2.329470	-0.009245
Ca	0.921144	2.371167	-0.009585
Ca	3.211655	2.221586	-2.239095
O	-1.323750	-0.011895	-2.825274
Ca	-1.329731	2.225071	-2.244392
O	1.041451	2.294053	-2.312330
Ca	0.921153	-0.009582	-2.371154
O	1.101473	-0.000011	-0.000001
Ca	3.387321	0.000024	0.000011
O	3.331121	-0.009219	-2.329463
Ca	-1.329706	-2.225054	2.244367
O	1.041492	-2.294057	2.312314
O	-1.323729	0.011900	2.825287
O	1.041461	2.312323	2.294049
Ca	0.921156	0.009598	2.371163
O	-1.323693	-2.825395	0.011896
O	-3.568677	2.024646	-2.042130
Ca	-3.552188	2.797893	-0.011423
O	-1.323729	2.825344	-0.011899
Ca	-1.329746	2.244392	2.225045

O	-3.568666	2.042161	2.024599
Ca	-3.552196	-0.011436	-2.797742
Ca	-3.552192	0.011419	2.797757
O	-3.568643	-2.024645	2.042093
O	-3.568653	-2.042179	-2.024577
Ca	-3.552150	-2.797963	0.011426

18

E = -13552.481954 Hartree

Ca	2.238207	2.238207	3.371405
Ca	2.343627	2.343627	-1.235441
O	0.000000	0.000000	1.149649
O	0.000000	0.000000	-3.586386
Ca	0.000000	2.405233	1.076356
Ca	0.000000	2.339776	-3.568056
Ca	2.405233	-0.000000	1.076356
Ca	2.339776	-0.000000	-3.568056
Ca	0.000000	0.000000	3.497545
Ca	0.000000	0.000000	-1.249143
O	2.318154	-0.000000	3.464127
O	2.376036	-0.000000	-1.188073
O	0.000000	2.318154	3.464127
O	0.000000	2.376036	-1.188073
O	2.319887	2.319887	1.205473
O	2.231181	2.231181	-3.388255
Ca	2.238207	-2.238207	3.371405
Ca	2.343627	-2.343627	-1.235441
Ca	-0.000000	-2.405233	1.076356
Ca	-0.000000	-2.339776	-3.568056
O	-0.000000	-2.318154	3.464127
O	-0.000000	-2.376036	-1.188073
O	2.319887	-2.319887	1.205473
O	2.231181	-2.231181	-3.388255
Ca	-2.238207	2.238207	3.371405
Ca	-2.343627	2.343627	-1.235441
Ca	-2.405233	0.000000	1.076356
Ca	-2.339776	0.000000	-3.568056
O	-2.318154	0.000000	3.464127
O	-2.376036	0.000000	-1.188073
O	-2.319887	2.319887	1.205473
O	-2.231181	2.231181	-3.388255
Ca	-2.238207	-2.238207	3.371405
Ca	-2.343627	-2.343627	-1.235441
O	-2.319887	-2.319887	1.205473

O	-2.231181	-2.231181	-3.388255

19

E = -14305.339863 Hartree

Ca	4.783824	1.721765	-1.011206
O	4.714799	1.605008	1.098608
O	4.938959	-0.123021	-2.078839
O	5.181915	-1.980040	1.105300
O	3.020964	-2.350217	-1.122805
Ca	5.227440	-2.000097	-1.048388
O	-0.450340	3.405354	-1.122840
Ca	1.662271	3.924195	-1.059408
Ca	0.090247	1.139315	-1.144261
O	2.471872	1.781543	-1.236211
O	0.469904	-0.817703	-2.251628
Ca	2.717981	-0.387941	-2.282698
Ca	-2.698737	2.957094	-1.225625
Ca	-1.829985	-1.231840	-2.360014
O	-1.485340	-3.177190	-1.170480
Ca	0.774809	-2.786468	-1.181137
Ca	2.977272	-2.426390	1.178776
O	-2.213977	0.698864	-1.204533
Ca	-4.562152	0.198747	-1.206122
O	-4.016734	-1.693681	-2.213646
Ca	-3.707093	-3.531941	-1.174934
O	-4.850101	2.424290	-1.060819
O	-4.544375	0.236993	1.142289
O	-3.752841	-3.436976	0.991707
Ca	-4.096648	-1.682894	2.158923
Ca	-1.488494	-3.223819	1.124813
Ca	0.421797	-0.804638	2.301549
O	0.061241	1.151768	1.192156
Ca	2.447195	1.757294	1.306651
Ca	-0.496864	3.417534	1.214325
O	1.647634	3.867030	1.034099
O	-2.736756	2.927599	1.104202
Ca	-2.222448	0.662237	1.135361
O	-1.890269	-1.296189	2.276203
Ca	-4.886376	2.452021	1.051693
O	2.672320	-0.453924	2.322518
Ca	4.899400	-0.175170	2.261384
O	0.727526	-2.717018	1.095513

20

E = -15058.334397 Hartree

Ca	-1.135491	1.196957	4.645962
O	-1.187345	-1.111679	4.619585
O	-1.157698	1.210054	2.325800
Ca	-1.160237	1.244981	-0.000000
Ca	-3.414536	-1.040471	4.546581
Ca	-1.170067	-1.211746	-2.304783
O	-3.491987	-1.075730	-2.315087
O	-1.205801	-1.154961	-0.000000
Ca	-3.529007	-1.095588	-0.000000
Ca	-1.170067	-1.211746	2.304783
O	-3.491987	-1.075730	2.315087
O	-3.469605	1.160672	-0.000000
Ca	-3.481400	1.239658	-2.311296
O	-3.362374	1.078046	4.537870
Ca	-3.481400	1.239658	2.311296
Ca	-1.135491	1.196957	-4.645962
O	-3.362374	1.078046	-4.537870
Ca	-3.414536	-1.040471	-4.546581
O	-1.187345	-1.111679	-4.619585
O	-1.157698	1.210054	-2.325800
O	1.157698	-1.210054	2.325800
Ca	1.160237	-1.244981	-0.000000
O	1.157698	-1.210054	-2.325800
O	3.469605	-1.160672	-0.000000
Ca	3.481400	-1.239658	-2.311296
O	3.362374	-1.078046	-4.537870
Ca	1.135491	-1.196957	-4.645962
O	3.491987	1.075730	-2.315087
O	1.187345	1.111679	-4.619585
Ca	3.414536	1.040471	-4.546581
O	3.362374	-1.078046	4.537870
Ca	3.414536	1.040471	4.546581
Ca	1.135491	-1.196957	4.645962
Ca	3.529007	1.095588	-0.000000
Ca	3.481400	-1.239658	2.311296
O	3.491987	1.075730	2.315087
O	1.187345	1.111679	4.619585
Ca	1.170067	1.211746	-2.304783
Ca	1.170067	1.211746	2.304783
O	1.205801	1.154961	-0.000000

21

E = -15811.229998 Hartree

O	-2.731172	-0.313629	2.319725
Ca	-3.580759	1.648181	2.244186
Ca	-1.529410	2.575485	0.000000
O	-1.629007	2.645639	-2.335782
O	-3.669125	1.702439	0.000000
O	-0.505771	0.492362	0.000000
Ca	-2.803067	-0.476488	0.000000
Ca	-3.580759	1.648181	-2.244186
O	-2.098247	-2.577397	0.000000
O	-1.629007	2.645639	2.335782
O	1.553825	4.693819	2.256098
Ca	-0.574878	4.583115	2.255625
Ca	1.712313	4.954737	0.000000
O	1.553825	4.693819	-2.256098
Ca	-0.574878	4.583115	-2.255625
Ca	2.780484	2.925919	-2.260150
O	-0.569043	4.671713	0.000000
O	2.874392	2.991800	0.000000
O	1.830412	0.970668	-2.343268
Ca	-0.460287	0.469598	-2.409230
Ca	2.780484	2.925919	2.260150
Ca	-0.460287	0.469598	2.409230
Ca	3.063366	-3.539960	0.000000
O	2.908645	-3.426475	-2.233991
O	2.908645	-3.426475	2.233991
O	0.812337	-4.176335	0.000000
Ca	0.817669	-4.191222	2.325693
Ca	2.397613	-1.325058	2.359494
Ca	0.161725	-1.917070	0.000000
O	0.150686	-1.812724	-2.373845
Ca	-2.028258	-2.567874	-2.381462
Ca	2.397613	-1.325058	-2.359494
Ca	-1.445742	-4.814581	0.000000
O	2.428797	-1.267963	0.000000
O	0.150686	-1.812724	2.373845
Ca	1.848937	0.893864	0.000000
Ca	0.817669	-4.191222	-2.325693
O	-1.359174	-4.627241	-2.239308
O	-1.359174	-4.627241	2.239308
O	-2.731172	-0.313629	-2.319725
Ca	-2.028258	-2.567874	2.381462
O	1.830412	0.970668	2.343268

22

E = -16564.171877 Hartree

Ca	0.835063	-1.029713	1.913384
Ca	-0.344379	-3.548938	0.000000
Ca	3.193843	-3.176854	1.880896
O	0.982696	-3.426238	1.949666
O	3.121829	-0.960312	1.922353
Ca	-0.773420	-3.449977	3.268185
Ca	3.193843	-3.176854	-1.880896
Ca	3.878035	3.727133	0.000000
O	-0.587212	-1.216622	0.000000
O	4.088347	1.452581	0.000000
Ca	2.942197	1.418477	1.979504
O	2.728549	3.617024	1.801172
Ca	4.331747	-0.813171	0.000000
O	4.195570	-3.127820	0.000000
O	-2.168283	-3.640146	1.594283
Ca	-2.446778	-1.258823	1.664189
O	-0.927956	-1.273069	3.380604
O	0.666885	1.243839	1.948279
Ca	0.503261	3.642195	1.920140
O	-1.233369	3.324352	3.260026
O	-2.573523	1.004931	1.629818
Ca	-1.104863	1.164101	3.413414
O	-2.168283	-3.640146	-1.594283
O	0.982696	-3.426238	-1.949666
O	2.728549	3.617024	-1.801172
Ca	2.942197	1.418477	-1.979504
O	3.121829	-0.960312	-1.922353
Ca	0.835063	-1.029713	-1.913384
Ca	-3.667202	-3.690213	0.000000
O	-3.999771	-1.518328	0.000000
Ca	-2.446778	-1.258823	-1.664189
Ca	-4.196419	0.938186	0.000000
Ca	-2.730952	3.378696	-1.630882
Ca	-1.104863	1.164101	-3.413414
O	-1.233369	3.324352	-3.260026
Ca	0.503261	3.642195	-1.920140
O	0.666885	1.243839	-1.948279
O	-2.573523	1.004931	-1.629818
O	-0.927956	-1.273069	-3.380604
Ca	-0.773420	-3.449977	-3.268185
Ca	-2.730952	3.378696	1.630882
O	-0.928346	3.530967	0.000000
Ca	-0.739204	1.206772	0.000000

O	-4.210455	3.108525	0.000000

23

E = -17317.101915 Hartree

Ca	-4.931600	1.036913	0.198042
Ca	0.378636	2.206890	-1.912684
O	-0.965283	4.064273	-1.576557
O	-4.829925	0.508018	2.398387
Ca	-3.499931	-0.357772	-2.394118
Ca	-2.915387	2.817568	-1.771181
O	-4.642721	1.467674	-1.931378
O	-2.976095	2.475371	0.683049
O	2.246308	3.464115	-1.611516
O	-0.320402	-1.416310	-0.132775
O	-3.577990	-0.828143	-0.079195
Ca	-2.288584	-2.701502	-0.458014
O	-2.165567	-2.274897	-2.723287
Ca	-0.259614	-0.933864	-2.507383
O	-1.614945	0.932572	-2.094663
O	1.656374	0.310276	-2.195796
O	0.976866	-2.872247	-2.802151
O	-2.229860	-3.168598	1.825609
Ca	-3.606670	-1.336717	2.180436
O	-0.922165	-4.573430	-0.806246
Ca	-0.863937	-4.035516	-2.974657
Ca	-1.607014	0.528658	0.247992
Ca	2.986970	-1.551279	-2.562021
Ca	1.091552	-3.334726	-0.534743
Ca	-0.924481	-4.907355	1.393113
Ca	1.000193	5.245762	-1.376264
Ca	-3.246070	1.770886	2.815516
Ca	-0.977516	3.849179	0.644900
O	-1.721820	0.109589	2.633096
O	0.856952	4.996196	0.703003
O	0.265727	1.851823	0.592981
O	3.622167	1.186431	0.381731
Ca	2.279935	3.222177	0.929650
O	1.624403	-0.666067	2.440345
Ca	3.683968	0.673608	2.651575
O	2.271371	2.342976	3.000013
Ca	0.482359	1.206247	2.885535
Ca	1.680764	-0.088257	0.133682
Ca	3.629570	1.631380	-1.865675
O	2.954935	-2.061419	-0.275257

Ca	2.965216	-2.509910	2.023619
Ca	-0.314186	-1.885897	2.215864
O	0.915893	-3.785108	1.738561
O	4.710219	-0.280156	-2.189918
O	4.713308	-1.233236	2.157639
Ca	4.916726	-0.766356	-0.017455

24

E = -18070.106333 Hartree

Ca	-0.556367	4.781026	2.229399
O	-0.198392	1.670041	0.000000
Ca	-2.111001	3.106194	0.000000
O	-1.978565	3.108727	-2.316593
Ca	-3.486081	1.228866	-2.346973
O	-1.655830	-0.202608	-2.382114
Ca	-0.556367	4.781026	-2.229399
O	-0.575432	4.915136	0.000000
Ca	-0.191661	1.632363	-2.416043
Ca	0.191661	-1.632363	-2.416043
O	3.507273	-1.272306	0.000000
Ca	4.944406	0.589990	0.000000
O	1.213867	3.494833	2.313235
Ca	3.107752	2.043132	2.332075
O	4.728213	0.577674	2.230900
O	3.113886	2.080968	0.000000
O	1.978565	-3.108727	-2.316593
O	1.655830	0.202608	-2.382114
O	4.728213	0.577674	-2.230900
Ca	3.486081	-1.228866	-2.346973
Ca	1.323839	3.520830	0.000000
Ca	1.646829	0.196560	0.000000
Ca	3.107752	2.043132	-2.332075
O	1.213867	3.494833	-2.313235
O	-1.978565	3.108727	2.316593
Ca	-0.191661	1.632363	2.416043
O	1.655830	0.202608	2.382114
O	-1.655830	-0.202608	2.382114
Ca	-3.486081	1.228866	2.346973
O	-4.728213	-0.577674	2.230900
Ca	-3.107752	-2.043132	2.332075
O	-4.728213	-0.577674	-2.230900
Ca	-4.944406	-0.589990	0.000000
Ca	-1.646829	-0.196560	0.000000
O	-3.507273	1.272306	0.000000

O	-3.113886	-2.080968	0.000000
Ca	-3.107752	-2.043132	-2.332075
O	0.198392	-1.670041	0.000000
Ca	0.556367	-4.781026	-2.229399
O	0.575432	-4.915136	0.000000
Ca	-1.323839	-3.520830	0.000000
O	-1.213867	-3.494833	-2.313235
Ca	2.111001	-3.106194	0.000000
O	-1.213867	-3.494833	2.313235
Ca	0.191661	-1.632363	2.416043
O	1.978565	-3.108727	2.316593
Ca	0.556367	-4.781026	2.229399
Ca	3.486081	-1.228866	2.346973

25

E = -18822.988062 Hartree

Ca	0.000000	6.433237	1.081273
O	-1.634185	4.916083	1.122043
Ca	-3.300718	3.300718	1.139954
O	-4.916083	1.634185	1.122043
Ca	-6.433237	0.000000	1.081273
O	1.634185	4.916083	1.122043
Ca	0.000000	3.267417	1.221350
O	-1.662363	1.662363	1.170480
Ca	-3.267417	0.000000	1.221350
O	-4.916083	-1.634185	1.122043
Ca	3.300718	3.300718	1.139954
O	1.662363	1.662363	1.170480
Ca	0.000000	0.000000	1.201650
O	-1.662363	-1.662363	1.170480
Ca	-3.300718	-3.300718	1.139954
O	4.916083	1.634185	1.122043
Ca	3.267417	-0.000000	1.221350
O	1.662363	-1.662363	1.170480
Ca	-0.000000	-3.267417	1.221350
O	-1.634185	-4.916083	1.122043
Ca	6.433237	-0.000000	1.081273
O	4.916083	-1.634185	1.122043
Ca	3.300718	-3.300718	1.139954
O	1.634185	-4.916083	1.122043
Ca	-0.000000	-6.433237	1.081273
O	0.000000	6.415219	-1.037639
Ca	-1.658136	4.928290	-1.197844
O	-3.280405	3.280405	-1.111763

Ca	-4.928290	1.658136	-1.197844
O	-6.415219	0.000000	-1.037639
Ca	1.658136	4.928290	-1.197844
O	0.000000	3.299909	-1.213572
Ca	-1.649526	1.649526	-1.251800
O	-3.299909	0.000000	-1.213572
Ca	-4.928290	-1.658136	-1.197844
O	3.280405	3.280405	-1.111763
Ca	1.649526	1.649526	-1.251800
O	0.000000	0.000000	-1.161385
Ca	-1.649526	-1.649526	-1.251800
O	-3.280405	-3.280405	-1.111763
Ca	4.928290	1.658136	-1.197844
O	3.299909	-0.000000	-1.213572
Ca	1.649526	-1.649526	-1.251800
O	-0.000000	-3.299909	-1.213572
Ca	-1.658136	-4.928290	-1.197844
O	6.415219	-0.000000	-1.037639
Ca	4.928290	-1.658136	-1.197844
O	3.280405	-3.280405	-1.111763
Ca	1.658136	-4.928290	-1.197844
O	-0.000000	-6.415219	-1.037639

26

E = -19575.908860 Hartree

O	-2.817647	-3.307576	1.706175
O	-2.812356	3.310046	1.717404
O	-2.888730	-0.002278	1.741976
Ca	-4.399357	-1.638625	1.062011
Ca	-1.365718	1.631797	2.417400
O	0.136458	3.318104	2.984653
O	-0.407139	1.664876	0.195956
O	1.918845	3.345065	-1.247450
O	-1.013496	0.003256	-2.640362
Ca	-2.557708	-1.645039	-3.249371
Ca	-2.556160	1.652112	-3.246113
Ca	0.438795	4.837744	-1.816433
Ca	0.520990	1.667713	-2.006736
O	-3.921783	0.005187	-3.715700
O	-0.999116	3.333972	-2.552135
Ca	-1.946610	-0.000357	-0.448528
O	-3.483715	1.692219	-1.098656
Ca	-2.014115	3.333996	-0.462650
Ca	-4.996733	0.005953	-1.745451

O	-3.490427	-1.681291	-1.102147
Ca	-1.312631	4.809316	2.278462
Ca	-4.396900	1.649797	1.059112
O	-5.677943	0.007388	0.388766
O	-0.438043	4.944506	0.234219
Ca	1.175585	3.330861	0.908676
O	2.633080	1.672816	1.529851
Ca	1.690331	1.636829	3.680782
Ca	3.669516	1.809274	-0.718474
O	4.988462	1.481255	-2.496269
Ca	-1.365386	-1.632510	2.423568
O	0.188856	-0.001311	3.017461
O	-0.403096	-1.657982	0.195406
Ca	1.693491	-1.659600	3.668073
O	0.124785	-3.325637	2.987362
O	3.044172	-0.013083	4.177634
Ca	6.266415	-0.001483	-1.574042
O	2.630720	-1.687972	1.523117
Ca	4.107230	-0.003640	2.202992
Ca	1.157395	-3.330397	0.901192
O	5.015123	-0.006157	0.179622
O	-0.998658	-3.321369	-2.558073
Ca	-1.322195	-4.811946	2.270975
Ca	0.428170	-4.838514	-1.821979
Ca	-2.023820	-3.328025	-0.471116
O	-0.458979	-4.943388	0.223010
Ca	3.666393	-1.815023	-0.718682
Ca	0.522223	-1.665480	-2.007961
O	1.913079	-3.353037	-1.252312
O	4.988282	-1.478596	-2.503239
O	2.187630	-0.000644	-1.661043
Ca	1.157280	0.004262	0.829705
Ca	3.780173	0.001637	-3.405502

27

E = -20328.853205 Hartree

Ca	0.000000	3.157071	5.686103
Ca	0.000000	3.308562	1.084165
Ca	0.000000	3.311897	-3.555524
O	0.000000	0.000000	3.499743
O	0.000000	0.000000	-1.194774
O	0.000000	0.000000	-5.914257
Ca	-1.708269	1.708269	3.405468
Ca	-1.713711	1.713711	-1.241773

Ca	-1.655454	1.655454	-5.889144
Ca	1.708269	1.708269	3.405468
Ca	1.713711	1.713711	-1.241773
Ca	1.655454	1.655454	-5.889144
Ca	0.000000	0.000000	5.836311
Ca	0.000000	0.000000	1.079798
Ca	0.000000	0.000000	-3.568771
O	1.641468	1.641468	5.787666
O	1.683830	1.683830	1.147596
O	1.680830	1.680830	-3.509318
O	-1.641468	1.641468	5.787666
O	-1.683830	1.683830	1.147596
O	-1.680830	1.680830	-3.509318
O	0.000000	3.277045	3.510927
O	0.000000	3.286456	-1.135062
O	0.000000	3.152969	-5.714812
Ca	3.157071	-0.000000	5.686103
Ca	3.308562	-0.000000	1.084165
Ca	3.311897	-0.000000	-3.555524
Ca	1.708269	-1.708269	3.405468
Ca	1.713711	-1.713711	-1.241773
Ca	1.655454	-1.655454	-5.889144
O	1.641468	-1.641468	5.787666
O	1.683830	-1.683830	1.147596
O	1.680830	-1.680830	-3.509318
O	3.277045	-0.000000	3.510927
O	3.286456	-0.000000	-1.135062
O	3.152969	-0.000000	-5.714812
Ca	-3.157071	0.000000	5.686103
Ca	-3.308562	0.000000	1.084165
Ca	-3.311897	0.000000	-3.555524
Ca	-1.708269	-1.708269	3.405468
Ca	-1.713711	-1.713711	-1.241773
Ca	-1.655454	-1.655454	-5.889144
O	-1.641468	-1.641468	5.787666
O	-1.683830	-1.683830	1.147596
O	-1.680830	-1.680830	-3.509318
O	-3.277045	0.000000	3.510927
O	-3.286456	0.000000	-1.135062
O	-3.152969	0.000000	-5.714812
Ca	-0.000000	-3.157071	5.686103
Ca	-0.000000	-3.308562	1.084165
Ca	-0.000000	-3.311897	-3.555524
O	-0.000000	-3.277045	3.510927

O	-0.000000	-3.286456	-1.135062
O	-0.000000	-3.152969	-5.714812

28

E = -21081.777269 Hartree

Ca	3.411498	1.048790	6.858357
O	3.493049	1.092374	4.625763
Ca	3.529603	1.115715	2.308869
O	3.518481	1.083783	-0.000000
Ca	3.529603	1.115715	-2.308869
O	3.493049	1.092374	-4.625763
Ca	3.411498	1.048790	-6.858357
O	1.184046	1.116393	6.925857
Ca	1.166403	1.220991	4.612455
O	1.204668	1.170198	2.307579
Ca	1.191948	1.219226	-0.000000
O	1.204668	1.170198	-2.307579
Ca	1.166403	1.220991	-4.612455
O	1.184046	1.116393	-6.925857
Ca	-1.138257	1.194422	6.947664
O	-1.165290	1.195627	4.632193
Ca	-1.163317	1.237543	2.306512
O	-1.182548	1.185234	0.000000
Ca	-1.163317	1.237543	-2.306512
O	-1.165290	1.195627	-4.632193
Ca	-1.138257	1.194422	-6.947664
O	-3.365645	1.074419	6.841987
Ca	-3.490245	1.222567	4.616525
O	-3.478073	1.153027	2.300931
Ca	-3.508810	1.193495	0.000000
O	-3.478073	1.153027	-2.300931
Ca	-3.490245	1.222567	-4.616525
O	-3.365645	1.074419	-6.841987
O	3.365645	-1.074419	6.841987
Ca	3.490245	-1.222567	4.616525
O	3.478073	-1.153027	2.300931
Ca	3.508810	-1.193495	0.000000
O	3.478073	-1.153027	-2.300931
Ca	3.490245	-1.222567	-4.616525
O	3.365645	-1.074419	-6.841987
Ca	1.138257	-1.194422	6.947664
O	1.165290	-1.195627	4.632193
Ca	1.163317	-1.237543	2.306512
O	1.182548	-1.185234	0.000000

Ca	1.163317	-1.237543	-2.306512
O	1.165290	-1.195627	-4.632193
Ca	1.138257	-1.194422	-6.947664
O	-1.184046	-1.116393	6.925857
Ca	-1.166403	-1.220991	4.612455
O	-1.204668	-1.170198	2.307579
Ca	-1.191948	-1.219226	-0.000000
O	-1.204668	-1.170198	-2.307579
Ca	-1.166403	-1.220991	-4.612455
O	-1.184046	-1.116393	-6.925857
Ca	-3.411498	-1.048790	6.858357
O	-3.493049	-1.092374	4.625763
Ca	-3.529603	-1.115715	2.308869
O	-3.518481	-1.083783	-0.000000
Ca	-3.529603	-1.115715	-2.308869
O	-3.493049	-1.092374	-4.625763
Ca	-3.411498	-1.048790	-6.858357

29

E = -21834.667549 Hartree

Ca	-2.357078	4.627432	1.157892
O	-2.224087	4.508464	3.347517
O	0.000000	0.000000	-3.816623
Ca	2.232337	4.515343	-3.390020
O	0.000000	4.633932	-3.479132
Ca	0.000000	4.750021	-1.142631
O	2.313081	2.326902	-3.461324
Ca	2.340700	2.241087	-1.153841
O	2.331647	4.624013	-1.185331
O	0.000000	4.652561	1.170361
O	2.361853	2.248281	1.192565
Ca	2.357078	4.627432	1.157892
Ca	0.000000	2.354594	1.130604
Ca	0.000000	4.671432	3.496527
O	2.224087	4.508464	3.347517
Ca	2.312499	2.319639	3.493500
O	0.000000	2.252524	3.546038
Ca	-2.941755	0.000000	1.146422
O	-2.361853	2.248281	1.192565
Ca	-2.312499	2.319639	3.493500
O	-2.251324	0.000000	3.413642
O	-2.313081	2.326902	-3.461324
Ca	0.000000	2.225432	-3.503422
O	-2.830593	0.000000	-1.132462

Ca	-2.308222	0.000000	-3.440724
Ca	-2.232337	4.515343	-3.390020
O	-2.331647	4.624013	-1.185331
Ca	-2.340700	2.241087	-1.153841
O	0.000000	2.431182	-1.131504
O	2.251324	-0.000000	3.413642
O	-0.000000	-2.252524	3.546038
Ca	-2.312499	-2.319639	3.493500
Ca	-0.000000	-0.000000	3.983930
Ca	2.312499	-2.319639	3.493500
Ca	2.357078	-4.627432	1.157892
O	-2.331647	-4.624013	-1.185331
O	2.224087	-4.508464	3.347517
Ca	-0.000000	-2.354594	1.130604
O	-0.000000	-4.652561	1.170361
Ca	-0.000000	-4.671432	3.496527
O	-2.224087	-4.508464	3.347517
Ca	-2.357078	-4.627432	1.157892
Ca	-2.340700	-2.241087	-1.153841
O	-2.361853	-2.248281	1.192565
Ca	2.232337	-4.515343	-3.390020
O	2.331647	-4.624013	-1.185331
O	2.313081	-2.326902	-3.461324
Ca	2.340700	-2.241087	-1.153841
O	2.361853	-2.248281	1.192565
Ca	2.941755	-0.000000	1.146422
O	-0.000000	-2.431182	-1.131504
Ca	-0.000000	-2.225432	-3.503422
O	-0.000000	-4.633932	-3.479132
Ca	-2.232337	-4.515343	-3.390020
Ca	-0.000000	-4.750021	-1.142631
O	-2.313081	-2.326902	-3.461324
Ca	2.308222	-0.000000	-3.440724
O	2.830593	-0.000000	-1.132462

30

E = -22587.729011 Hartree

Ca	2.326961	-1.124861	-2.419742
Ca	-2.339629	3.547530	2.339527
O	-4.647670	-1.204309	-2.320981
O	-4.714867	1.182323	-0.000053
O	-2.354503	-1.179357	-0.000998
Ca	-4.740190	-1.106517	0.001009
O	-2.346292	-3.483596	-2.325288

O	-4.647403	-3.479929	0.001816
Ca	-4.563385	-3.389690	-2.232845
Ca	-2.306939	-3.551525	0.002091
O	-2.347182	-3.484881	2.325684
Ca	-4.564311	-3.390637	2.236390
Ca	-2.340171	1.214498	0.000468
O	-4.540760	3.387912	2.232459
Ca	-4.673493	3.556438	0.000733
Ca	-2.328325	-1.127413	2.415440
O	-4.651501	-1.207238	2.322911
O	-2.347362	1.187766	2.384914
Ca	-4.676544	1.217290	2.338241
Ca	-2.338982	3.551193	-2.335813
O	2.345534	1.189934	-2.385178
Ca	-0.000663	1.233125	-2.424180
O	0.000075	-3.553677	-0.004254
O	-2.332018	3.575460	0.001783
Ca	0.000485	3.632105	0.001654
O	0.000412	3.499794	-2.327945
Ca	-4.676179	1.219381	-2.339845
Ca	-2.328484	-1.124754	-2.418509
O	-2.346515	1.189406	-2.384876
Ca	-0.000549	-3.486137	-2.348995
O	-0.000761	-1.205312	-2.395129
O	-4.540594	3.390016	-2.230956
O	4.652663	-1.209010	2.323355
Ca	2.339711	1.213997	0.000995
O	2.333068	3.574611	0.002455
Ca	2.340374	3.547362	2.340226
Ca	4.674020	3.555365	0.002595
O	4.541319	3.387372	2.234351
O	4.541095	3.390043	-2.230596
Ca	2.339035	3.551024	-2.336148
O	4.713776	1.182481	0.000942
O	2.347895	1.186762	2.385539
Ca	4.676290	1.217131	2.340396
O	4.646572	-1.202130	-2.322227
Ca	-0.000297	-1.139835	-0.002375
O	0.000326	1.204709	-0.000730
O	2.354215	-1.179153	-0.001309
O	4.648061	-3.479246	-0.001660
Ca	4.675303	1.219038	-2.339968
Ca	4.739321	-1.105949	0.000732
O	2.348744	-3.485661	2.322831

Ca	4.565426	-3.392243	2.233645
Ca	4.562935	-3.386953	-2.235926
O	2.345855	-3.482925	-2.327400
Ca	2.307222	-3.552012	-0.000644
Ca	0.000015	-3.487601	2.342631
O	0.000552	3.496487	2.332337
Ca	0.000336	1.226934	2.423353
Ca	2.329416	-1.128813	2.415171
O	0.000497	-1.207324	2.387435

32

E = -24093.641456 Hartree

Ca	3.410022	3.410022	3.410022
O	1.201527	3.490290	3.490290
Ca	-1.181090	3.515884	3.515884
O	-3.379594	3.379594	3.379594
O	3.490290	1.201527	3.490290
Ca	1.164102	1.164102	3.595418
O	-1.183525	1.183525	3.561028
Ca	-3.515884	1.181090	3.515884
Ca	3.515884	-1.181090	3.515884
O	1.183525	-1.183525	3.561028
Ca	-1.164102	-1.164102	3.595418
O	-3.490290	-1.201527	3.490290
O	3.379594	-3.379594	3.379594
Ca	1.181090	-3.515884	3.515884
O	-1.201527	-3.490290	3.490290
Ca	-3.410022	-3.410022	3.410022
O	3.490290	3.490290	1.201527
Ca	1.164102	3.595418	1.164102
O	-1.183525	3.561028	1.183525
Ca	-3.515884	3.515884	1.181090
Ca	3.595418	1.164102	1.164102
O	1.193600	1.193600	1.193600
Ca	-1.181951	1.181951	1.181951
O	-3.561028	1.183525	1.183525
O	3.561028	-1.183525	1.183525
Ca	1.181951	-1.181951	1.181951
O	-1.193600	-1.193600	1.193600
Ca	-3.595418	-1.164102	1.164102
Ca	3.515884	-3.515884	1.181090
O	1.183525	-3.561028	1.183525
Ca	-1.164102	-3.595418	1.164102
O	-3.490290	-3.490290	1.201527

Ca	3.515884	3.515884	-1.181090
O	1.183525	3.561028	-1.183525
Ca	-1.164102	3.595418	-1.164102
O	-3.490290	3.490290	-1.201527
O	3.561028	1.183525	-1.183525
Ca	1.181951	1.181951	-1.181951
O	-1.193600	1.193600	-1.193600
Ca	-3.595418	1.164102	-1.164102
Ca	3.595418	-1.164102	-1.164102
O	1.193600	-1.193600	-1.193600
Ca	-1.181951	-1.181951	-1.181951
O	-3.561028	-1.183525	-1.183525
O	3.490290	-3.490290	-1.201527
Ca	1.164102	-3.595418	-1.164102
O	-1.183525	-3.561028	-1.183525
Ca	-3.515884	-3.515884	-1.181090
O	3.379594	3.379594	-3.379594
Ca	1.181090	3.515884	-3.515884
O	-1.201527	3.490290	-3.490290
Ca	-3.410022	3.410022	-3.410022
Ca	3.515884	1.181090	-3.515884
O	1.183525	1.183525	-3.561028
Ca	-1.164102	1.164102	-3.595418
O	-3.490290	1.201527	-3.490290
O	3.490290	-1.201527	-3.490290
Ca	1.164102	-1.164102	-3.595418
O	-1.183525	-1.183525	-3.561028
Ca	-3.515884	-1.181090	-3.515884
Ca	3.410022	-3.410022	-3.410022
O	1.201527	-3.490290	-3.490290
Ca	-1.181090	-3.515884	-3.515884
O	-3.379594	-3.379594	-3.379594

36

E = -27105.351364 Hartree

Ca	-3.312242	5.786605	2.234476
O	-3.445394	3.575764	2.325948
Ca	-3.499682	1.209254	2.344767
O	-3.511121	-1.080794	2.331884
Ca	-3.567703	-3.447071	2.342680
O	-3.455493	-5.643122	2.232998
O	-1.120387	5.835317	2.330910
Ca	-1.101513	3.509074	2.424865
O	-1.193115	1.184071	2.400163

Ca	-1.212441	-1.148063	2.427748
O	-1.225147	-3.485279	2.391432
Ca	-1.279203	-5.818655	2.346018
Ca	1.279203	5.818655	2.346018
O	1.225147	3.485279	2.391432
Ca	1.212441	1.148063	2.427748
O	1.193115	-1.184071	2.400163
Ca	1.101513	-3.509074	2.424865
O	1.120387	-5.835317	2.330910
O	3.455493	5.643122	2.232998
Ca	3.567703	3.447071	2.342680
O	3.511121	1.080794	2.331884
Ca	3.499682	-1.209254	2.344767
O	3.445394	-3.575764	2.325948
Ca	3.312242	-5.786605	2.234476
O	-3.387115	5.871282	0.000000
Ca	-3.517374	3.524466	0.000000
O	-3.543154	1.221582	0.000000
Ca	-3.618174	-1.119319	0.000000
O	-3.594731	-3.430858	0.000000
Ca	-3.608546	-5.774257	0.000000
Ca	-1.032595	5.921162	0.000000
O	-1.140038	3.536575	0.000000
Ca	-1.155148	1.182886	0.000000
O	-1.208407	-1.143826	0.000000
Ca	-1.232887	-3.481710	0.000000
O	-1.255197	-5.849442	0.000000
O	1.255197	5.849442	0.000000
Ca	1.232887	3.481710	0.000000
O	1.208407	1.143826	0.000000
Ca	1.155148	-1.182886	0.000000
O	1.140038	-3.536575	0.000000
Ca	1.032595	-5.921162	0.000000
Ca	3.608546	5.774257	0.000000
O	3.594731	3.430858	0.000000
Ca	3.618174	1.119319	0.000000
O	3.543154	-1.221582	0.000000
Ca	3.517374	-3.524466	0.000000
O	3.387115	-5.871282	0.000000
Ca	-3.312242	5.786605	-2.234476
O	-3.445394	3.575764	-2.325948
Ca	-3.499682	1.209254	-2.344767
O	-3.511121	-1.080794	-2.331884
Ca	-3.567703	-3.447071	-2.342680

O	-3.455493	-5.643122	-2.232998
O	-1.120387	5.835317	-2.330910
Ca	-1.101513	3.509074	-2.424865
O	-1.193115	1.184071	-2.400163
Ca	-1.212441	-1.148063	-2.427748
O	-1.225147	-3.485279	-2.391432
Ca	-1.279203	-5.818655	-2.346018
Ca	1.279203	5.818655	-2.346018
O	1.225147	3.485279	-2.391432
Ca	1.212441	1.148063	-2.427748
O	1.193115	-1.184071	-2.400163
Ca	1.101513	-3.509074	-2.424865
O	1.120387	-5.835317	-2.330910
O	3.455493	5.643122	-2.232998
Ca	3.567703	3.447071	-2.342680
O	3.511121	1.080794	-2.331884
Ca	3.499682	-1.209254	-2.344767
O	3.445394	-3.575764	-2.325948
Ca	3.312242	-5.786605	-2.234476

40

E = -30117.141157 Hartree

Ca	4.569762	4.820544	0.000000
O	2.353077	4.948625	0.000000
Ca	0.000000	4.975828	0.000000
O	-2.353077	4.948625	-0.000000
Ca	-4.569762	4.820544	-0.000000
O	4.659457	3.325335	1.611519
Ca	2.335922	3.362421	1.724247
O	0.000000	3.389344	1.662565
Ca	-2.335922	3.362421	1.724247
O	-4.659457	3.325335	1.611519
Ca	4.687370	1.652412	3.323339
O	2.354009	1.688569	3.357084
Ca	0.000000	1.703988	3.405165
O	-2.354009	1.688569	3.357084
Ca	-4.687370	1.652412	3.323339
O	4.559668	-0.000000	4.772829
Ca	2.352995	-0.000000	4.981867
O	0.000000	0.000000	4.933311
Ca	-2.352995	0.000000	4.981867
O	-4.559668	0.000000	4.772829
O	4.659457	3.325335	-1.611519
Ca	2.335922	3.362421	-1.724247

O	0.000000	3.389344	-1.662565
Ca	-2.335922	3.362421	-1.724247
O	-4.659457	3.325335	-1.611519
Ca	4.766513	1.645932	0.000000
O	2.369783	1.692617	0.000000
Ca	0.000000	1.684706	0.000000
O	-2.369783	1.692617	-0.000000
Ca	-4.766513	1.645932	-0.000000
O	4.736555	-0.000000	1.676012
Ca	2.352570	-0.000000	1.676533
O	0.000000	0.000000	1.703228
Ca	-2.352570	0.000000	1.676533
O	-4.736555	0.000000	1.676012
Ca	4.687370	-1.652412	3.323339
O	2.354009	-1.688569	3.357084
Ca	-0.000000	-1.703988	3.405165
O	-2.354009	-1.688569	3.357084
Ca	-4.687370	-1.652412	3.323339
Ca	4.687370	1.652412	-3.323339
O	2.354009	1.688569	-3.357084
Ca	0.000000	1.703988	-3.405165
O	-2.354009	1.688569	-3.357084
Ca	-4.687370	1.652412	-3.323339
O	4.736555	-0.000000	-1.676012
Ca	2.352570	0.000000	-1.676533
O	0.000000	0.000000	-1.703228
Ca	-2.352570	-0.000000	-1.676533
O	-4.736555	-0.000000	-1.676012
Ca	4.766513	-1.645932	-0.000000
O	2.369783	-1.692617	-0.000000
Ca	-0.000000	-1.684706	0.000000
O	-2.369783	-1.692617	0.000000
Ca	-4.766513	-1.645932	0.000000
O	4.659457	-3.325335	1.611519
Ca	2.335922	-3.362421	1.724247
O	-0.000000	-3.389344	1.662565
Ca	-2.335922	-3.362421	1.724247
O	-4.659457	-3.325335	1.611519
O	4.559668	0.000000	-4.772829
Ca	2.352995	0.000000	-4.981867
O	0.000000	0.000000	-4.933311
Ca	-2.352995	-0.000000	-4.981867
O	-4.559668	-0.000000	-4.772829
Ca	4.687370	-1.652412	-3.323339

O	2.354009	-1.688569	-3.357084
Ca	-0.000000	-1.703988	-3.405165
O	-2.354009	-1.688569	-3.357084
Ca	-4.687370	-1.652412	-3.323339
O	4.659457	-3.325335	-1.611519
Ca	2.335922	-3.362421	-1.724247
O	-0.000000	-3.389344	-1.662565
Ca	-2.335922	-3.362421	-1.724247
O	-4.659457	-3.325335	-1.611519
Ca	4.569762	-4.820544	-0.000000
O	2.353077	-4.948625	-0.000000
Ca	-0.000000	-4.975828	0.000000
O	-2.353077	-4.948625	0.000000
Ca	-4.569762	-4.820544	0.000000