

Redox potential tuning by redox-inactive cations in nature's water oxidizing complex and synthetic analogues

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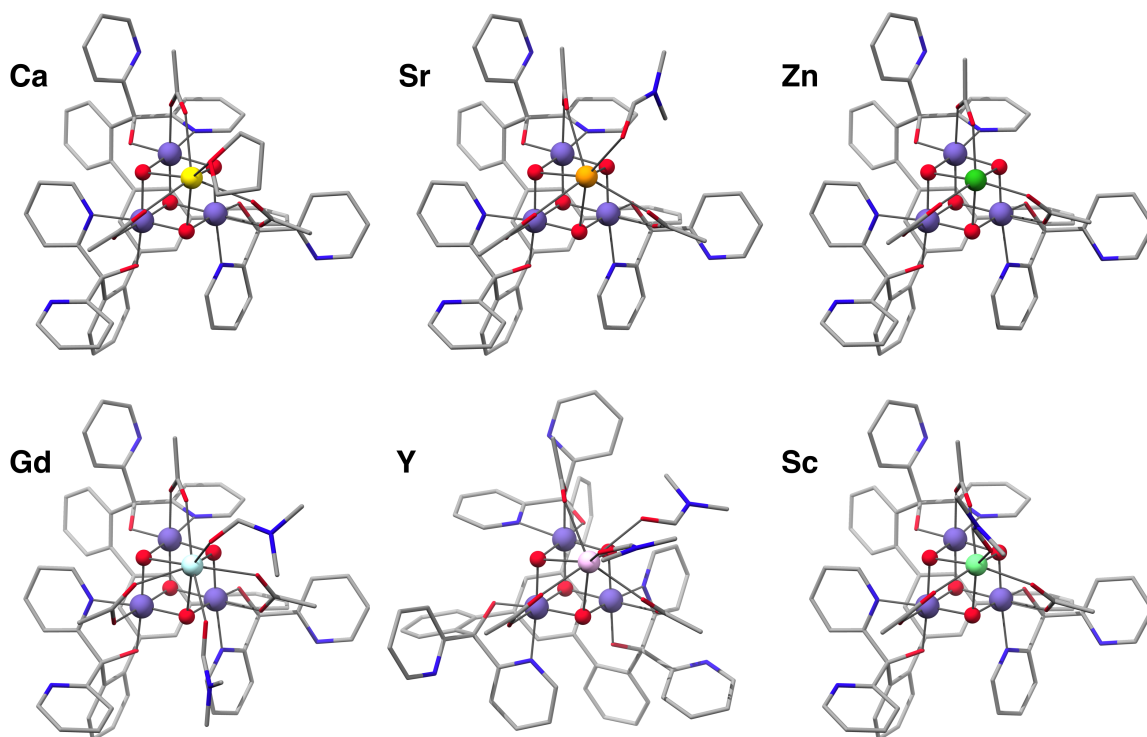


Figure S1. Optimized geometries of the Mn(IV)_3 cubane models with different A^{n+} . Color code: Mn purple, O red, N blue, C grey, H white, Ca yellow, Sr orange, Zn green, Gd pale blue, Y rose, Sc light green.

Table S1. Ionic radii of A^{n+} (coordination number 6) and O^{2-} (coordination number 4) in $\text{\AA}^1$ and deviation of A^{n+} - μ_2 -O bond length in $\text{\AA}$ from sum of atomic radii for the cubane model complexes.

	Ca^{2+}	Gd^{3+}	Sc^{3+}	Sr^{2+}	Y^{3+}	Zn^{2+}	O^{2-}
Ionic radii	1.000	0.935	0.745	1.180	0.900	0.740	1.380
Dev. for $\text{Mn(IV)}_3\text{A}$	0.017	0.081	0.054	0.021	0.082	0.049	
Dev. for $\text{Mn(III)Mn(IV)}_2\text{A}$	0.001	0.057	0.032	0.001	0.059	0.041	

¹ R. Shannon, *Acta Crystallogr., Sect. A*, 1976, **32**, 751-767.

Table S2. Selected interatomic distances in Å for the cubane models.

	Ca ²⁺	Gd ³⁺	Sc ³⁺	Sr ²⁺	Y ³⁺	Zn ²⁺
Mn(IV)₃Aⁿ⁺O₄						
A-Mn1	3.21	3.24	3.06	3.40	3.27	2.94
A-Mn2	3.22	3.25	3.05	3.41	3.21	2.93
A-Mn3	3.21	3.30	3.06	3.39	3.20	2.94
Mn1-Mn2	2.81	2.83	2.82	2.81	2.81	2.81
Mn1-Mn3	2.81	2.81	2.82	2.81	2.81	2.81
Mn2-Mn3	2.81	2.81	2.82	2.81	2.83	2.81
A-O1	3.79	3.83	3.58	4.00	3.78	3.47
A-O2	2.40	2.36	2.18	2.60	2.38	2.17
A-O3	2.39	2.41	2.18	2.56	2.38	2.17
A-O4	2.40	2.42	2.18	2.59	2.32	2.16
Mn1-O1	1.91	1.91	1.91	1.91	1.91	1.92
Mn1-O2	1.83	1.85	1.86	1.83	1.87	1.83
Mn1-O3	1.87	1.88	1.89	1.87	1.84	1.86
Mn2-O1	1.91	1.91	1.91	1.91	1.90	1.92
Mn2-O2	1.87	1.88	1.89	1.86	1.85	1.86
Mn2-O4	1.83	1.84	1.86	1.83	1.88	1.83
Mn3-O1	1.91	1.91	1.91	1.91	1.91	1.92
Mn3-O3	1.83	1.85	1.86	1.84	1.87	1.83
Mn3-O4	1.86	1.88	1.89	1.86	1.86	1.86
Mn(III)Mn(IV)₂Aⁿ⁺O₄						
A-Mn1	3.19	3.24	3.02	3.38	3.23	2.93
A-Mn2	3.19	3.19	3.02	3.36	3.18	2.94
A-Mn3	3.19	3.26	3.06	3.36	3.18	2.92
Mn1-Mn2	2.94	2.92	2.77	2.90	2.75	2.92
Mn1-Mn3	2.90	2.76	2.96	2.75	2.91	2.75
Mn2-Mn3	2.75	2.95	2.91	2.94	2.97	2.96
A-O1	3.81	3.84	3.60	4.02	3.80	3.51
A-O2	2.37	2.33	2.16	2.57	2.37	2.16
A-O3	2.38	2.42	2.15	2.55	2.35	2.18
A-O4	2.39	2.36	2.16	2.56	2.29	2.14
Mn1-O1	2.27	1.84	1.84	1.84	1.84	1.84
Mn1-O2	1.89	1.84	1.86	1.82	1.88	1.83
Mn1-O3	1.89	1.88	1.87	1.87	1.84	1.86
Mn2-O1	1.84	2.24	1.84	2.27	1.83	2.29

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Mn2-O2	1.85	1.91	1.90	1.88	1.85	1.88
Mn2-O4	1.84	1.90	1.86	1.88	1.86	1.88
Mn3-O1	1.84	1.84	2.25	1.84	2.26	1.84
Mn3-O3	1.83	1.85	1.92	1.84	1.89	1.83
Mn3-O4	1.87	1.86	1.91	1.84	1.93	1.85

Table S3. Mayer bond orders > 0.10 for the A^{n+} - μ_2 -O bonds in the Mn_3AO_4 cubanes, and Mulliken spin populations of the Mn ions in all complexes.

a) Mayer bond orders		Ca ²⁺	Sr ²⁺	Zn ²⁺	Gd ³⁺	Y ³⁺	Sc ³⁺
		<0.10	0.22	0.22	<0.10	0.30	0.37
Mn(IV) ₃ A		0.10	0.20	0.22	0.18	0.28	0.38
		<0.10	0.26	0.22	0.21	0.34	0.38
Mn(III)Mn(IV) ₂ A		0.11	0.24	0.26	<0.10	0.29	0.38
		0.12	0.21	0.19	0.18	0.31	0.45
		<0.10	0.29	0.27	0.22	0.40	0.42
b) Mulliken spin populations		Ca ²⁺	Sr ²⁺	Zn ²⁺	Gd ³⁺	Y ³⁺	Sc ³⁺
Mn(IV) ₃ A	Mn1	2.82	2.86	2.84	2.83	2.84	2.82
	Mn2	2.83	2.85	2.84	2.83	2.83	2.82
	Mn3	2.82	2.86	2.84	2.83	2.83	2.82
Mn(III)Mn(IV) ₂ A	Mn1	3.87	2.86	2.84	2.82	2.83	2.82
	Mn2	2.83	3.88	2.83	3.88	2.83	3.88
	Mn3	2.81	2.87	3.89	2.82	3.87	2.83

Table S4. Relative redox potentials ΔE (eV) for the cubane model complexes for all functionals tested.

	TPSS	TPSSh	M06L	M06	PBE	PBE0	B3LYP	B2PLYP
Ca ²⁺	2.50	2.77	3.03	3.79	2.67	3.46	3.28	3.09
Gd ³⁺	3.06	3.39	3.64	4.38	3.21	4.04	3.85	3.51
Sc ³⁺	3.16	3.46	3.75	4.51	3.31	4.16	3.97	3.78
Sr ²⁺	2.51	2.79	3.02	3.76	2.68	3.46	3.28	3.09
Y ³⁺	3.02	3.32	3.59	4.37	3.18	4.01	3.82	3.62
Zn ²⁺	2.75	3.01	3.27	4.01	2.91	3.71	3.53	3.33

Table S5. Differentiation between energy contributions in eV for the relative redox potentials of the cubane model complexes calculated with the TPSS density functional: relative redox potentials ΔE , vertical ionization energies IE , geometry relaxation energies E_{opt} , and the differences in solvent-solute bulk electrostatic interaction energy ΔE_{diel} and cavity-dispersion solvent structure energy ΔE_{CDS} between the oxidized and reduced species.

	ΔE (eV)	IE (eV)	E_{opt} (eV)	ΔE_{diel} (eV)	ΔE_{CDS} (eV)
Ca^{2+}	2.50	3.56	-1.06	1.37	0.01
Gd^{3+}	3.06	4.14	-1.08	-0.74	0.02
Sc^{3+}	3.16	4.19	-1.02	-0.69	0.02
Sr^{2+}	2.51	3.64	-1.13	1.38	0.01
Y^{3+}	3.02	4.05	-1.04	-0.65	0.01
Zn^{2+}	2.75	3.84	-1.10	1.41	0.02

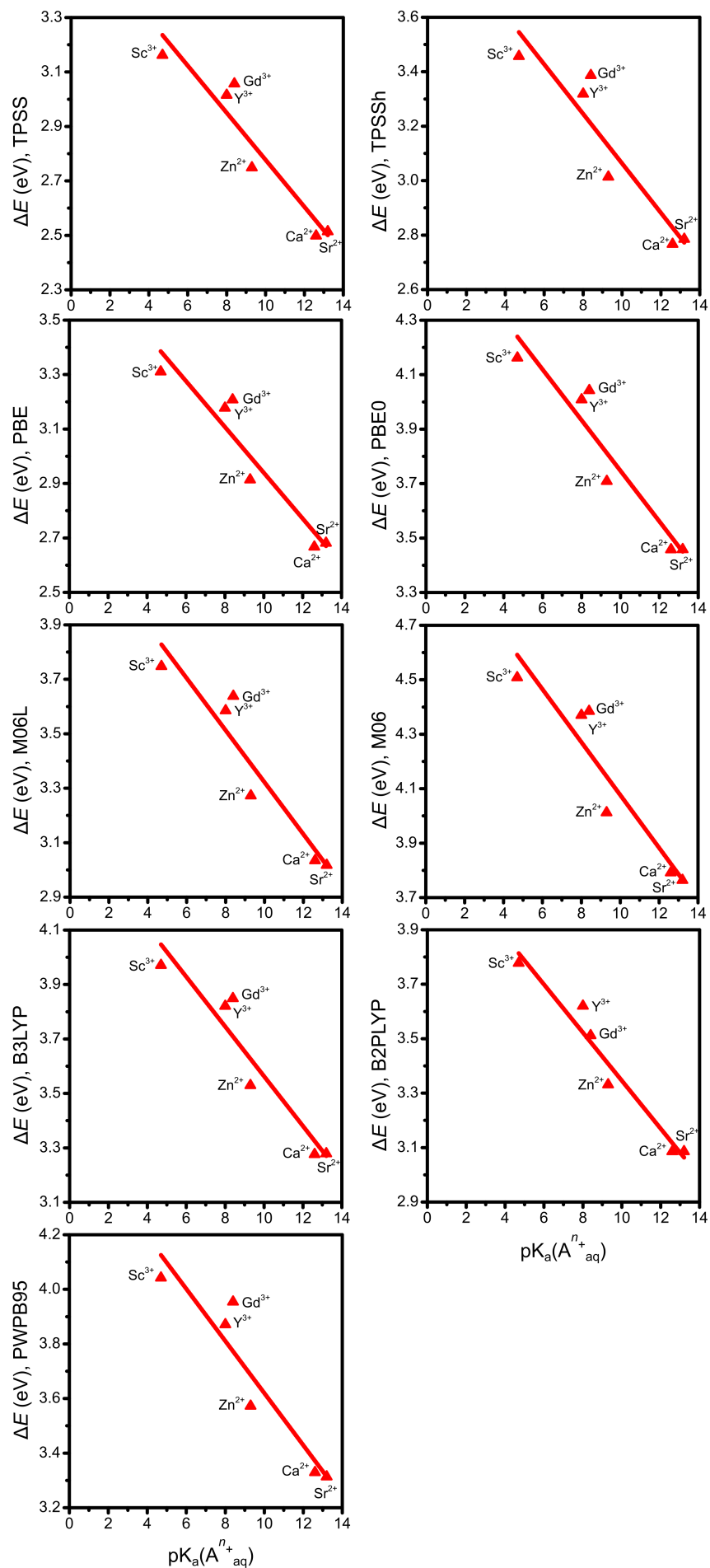


Figure S2. Linear correlations of computed ΔE (eV) vs. literature-based $pK_a(A^{n+}_{aq})$ for all density functionals.

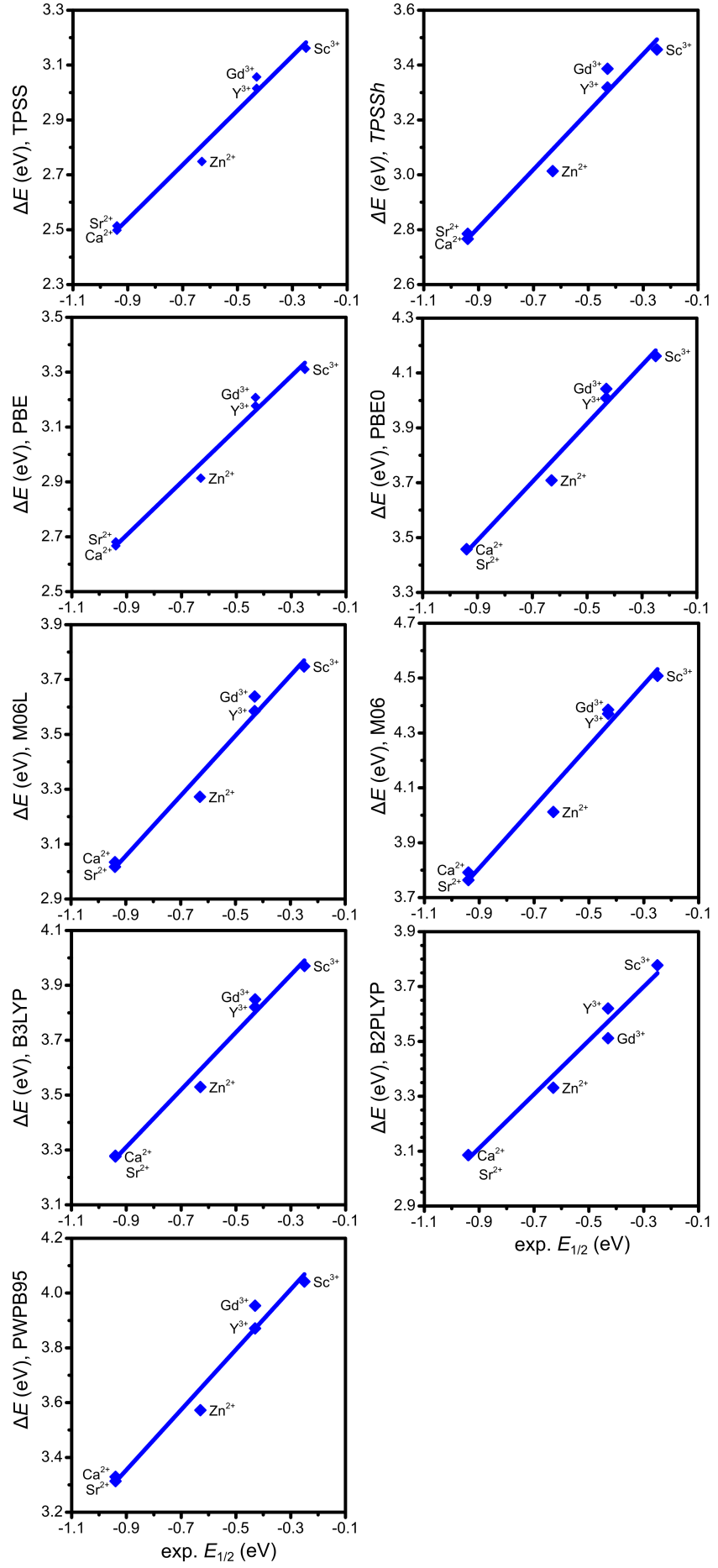


Figure S3. Linear correlations of computed ΔE (eV) vs. exp. redox potential $E_{1/2}$ (eV) for all density functionals.

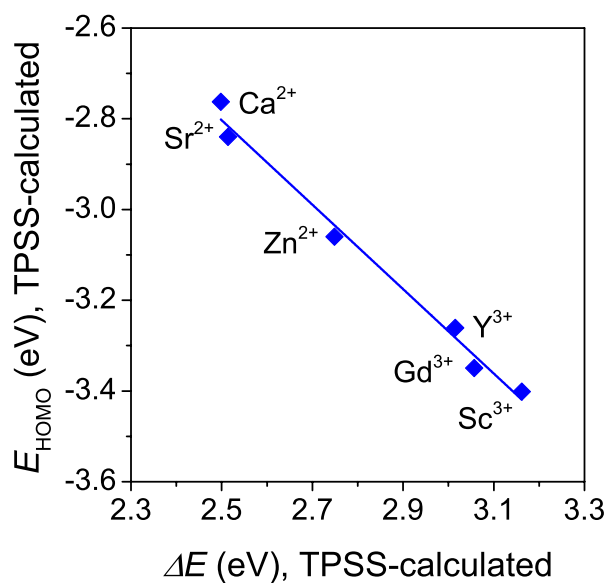


Figure S4. Correlation between the relative redox potential and the energy of the redox active orbital; $y = -0.93x - 0.48$, $R^2 = 0.99$.

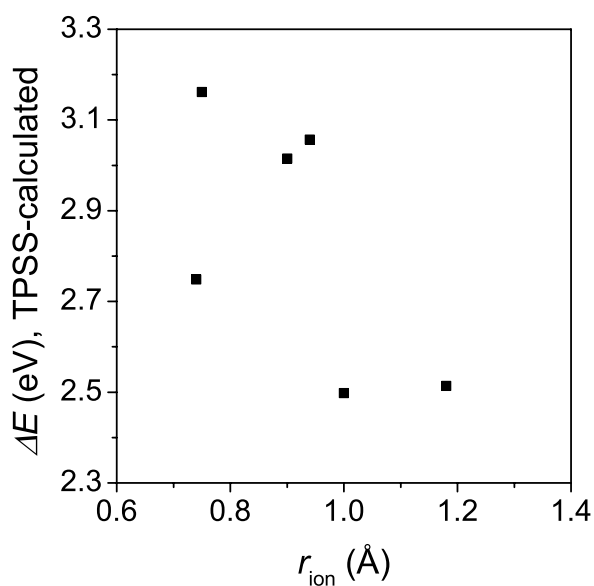


Figure S5. Attempt to correlate the relative redox potential and the ionic radii of the cations.

Table S6. Mayer bond orders > 0.05 , ordered by increasing $\text{A}^{n+}(\text{H}_2\text{O})$ bond order.

	Na^+	Sr^{2+}	Ca^{2+}	Mg^{2+}	Cd^{2+}	Gd^{3+}	Y^{3+}	Zn^{2+}	Sc^{3+}
$\text{A}^{n+}(\text{H}_2\text{O})$	0.08	0.20	0.28	0.45	0.56	0.61	0.71	0.75	0.98
$\text{A}^{n+}(\text{OH})$	0.54	0.62	0.94	1.07	1.15	1.28	1.50	1.34	1.66

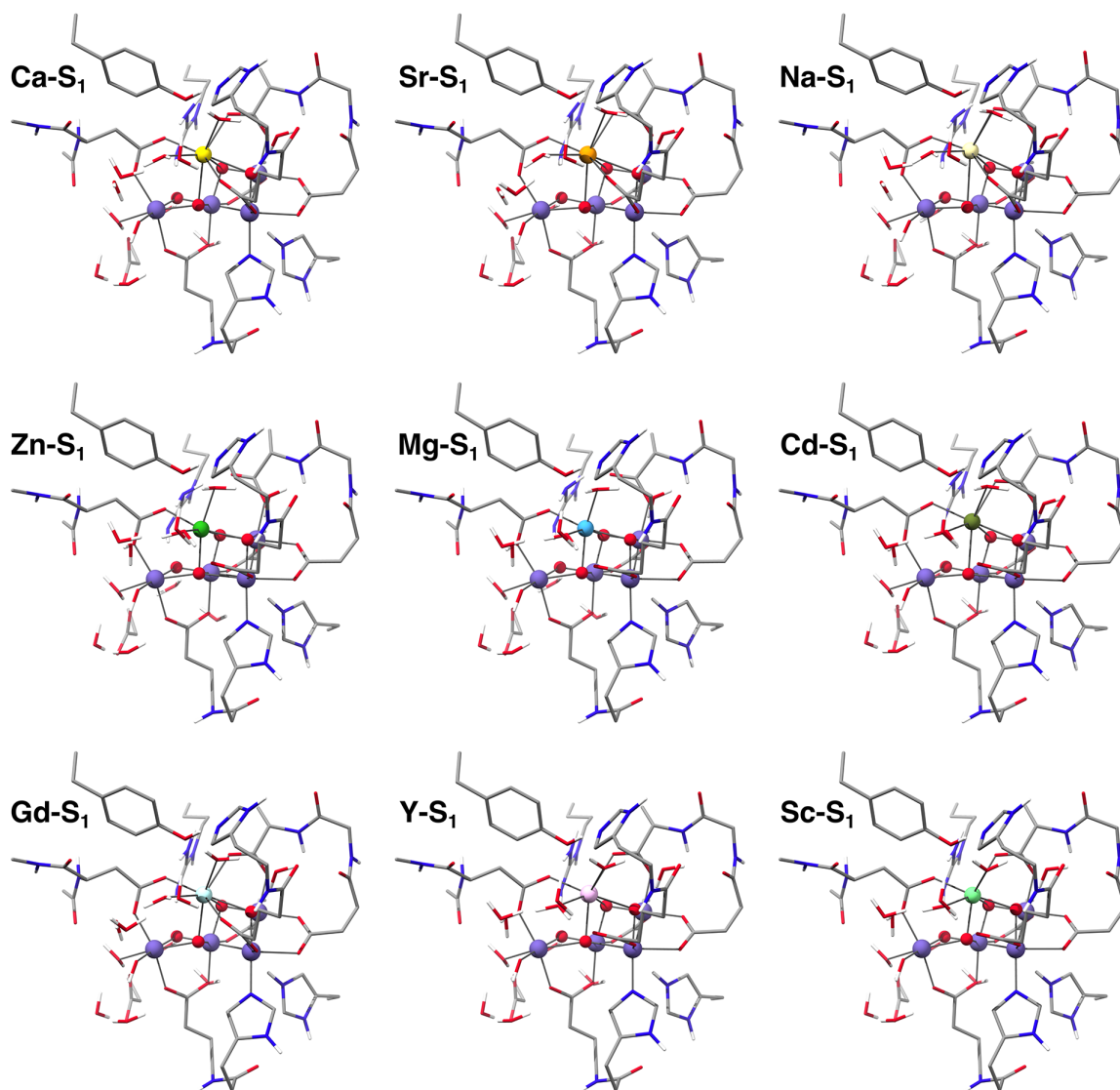


Figure S6. Structures of the optimized S_1 models. Color code: Mn purple, O red, N blue, C grey, H white, Ca yellow, Sr orange, Na light yellow, Zn green, Mg sky blue, Cd olive, Gd pale blue, Y rose, Sc light green.

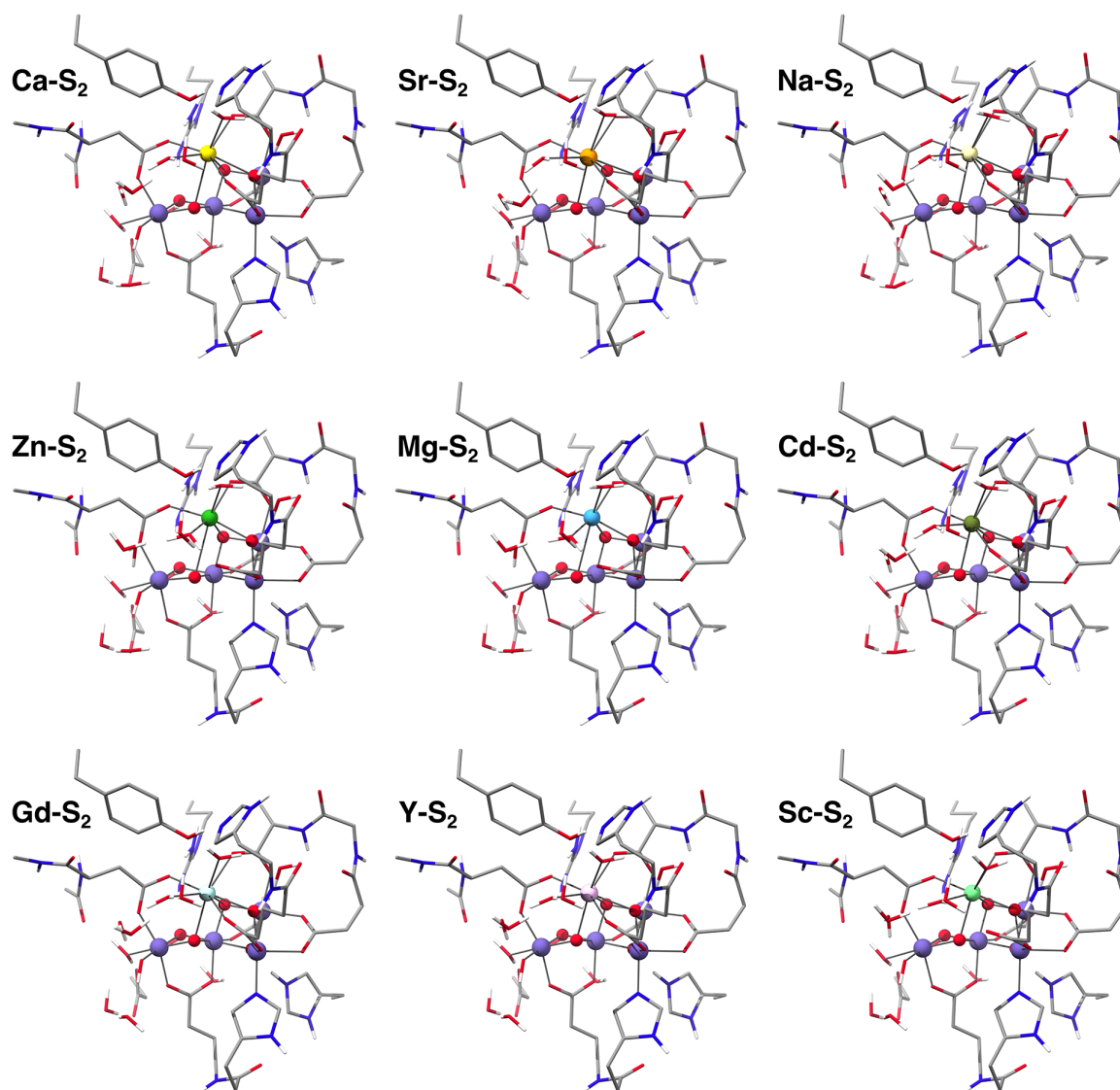


Figure S7. Structures of the optimized S_2 models. Color code: Mn purple, O red, N blue, C grey, H white, Ca yellow, Sr orange, Na light yellow, Zn green, Mg sky blue, Cd olive, Gd pale blue, Y rose, Sc light green.

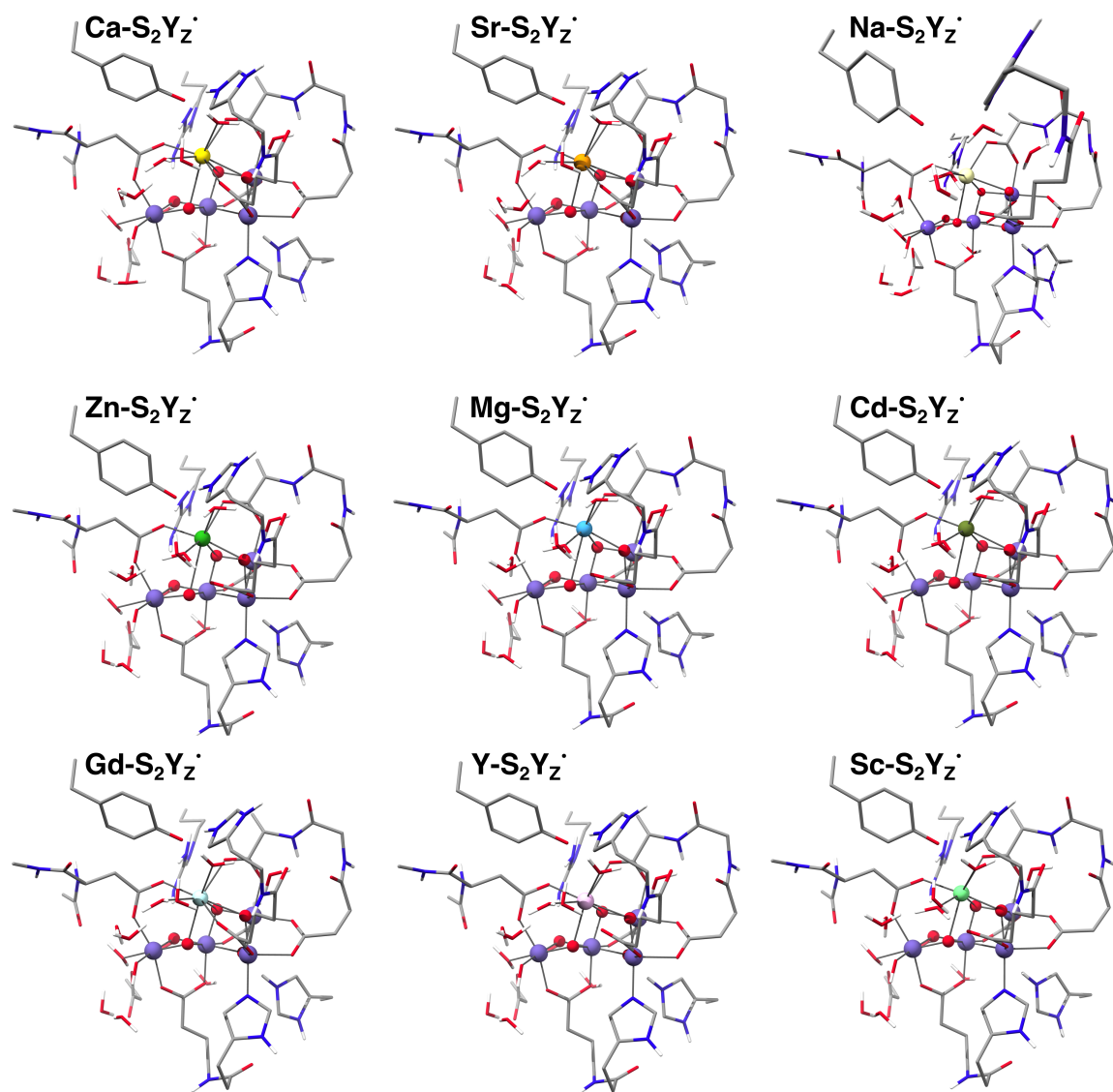


Figure S8. Structures of the optimized S_2YZ' models. Color code: Mn purple, O red, N blue, C grey, H white, Ca yellow, Sr orange, Na light yellow, Zn green, Mg sky blue, Cd olive, Gd pale blue, Y rose, Sc light green.

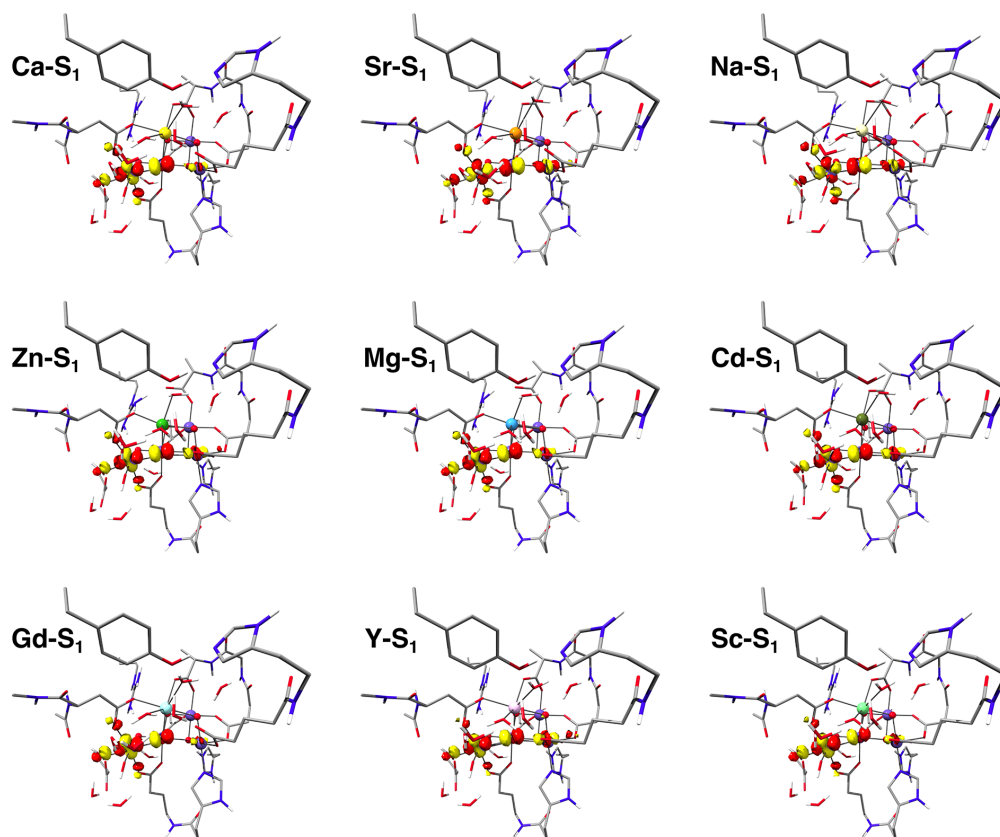


Figure S9. Redox active orbitals of the S_1 models. Color code: Mn purple, O red, N blue, C grey, H white, Ca yellow, Sr orange, Na light yellow, Zn green, Mg sky blue, Cd olive, Gd pale blue, Y rose, Sc light green.

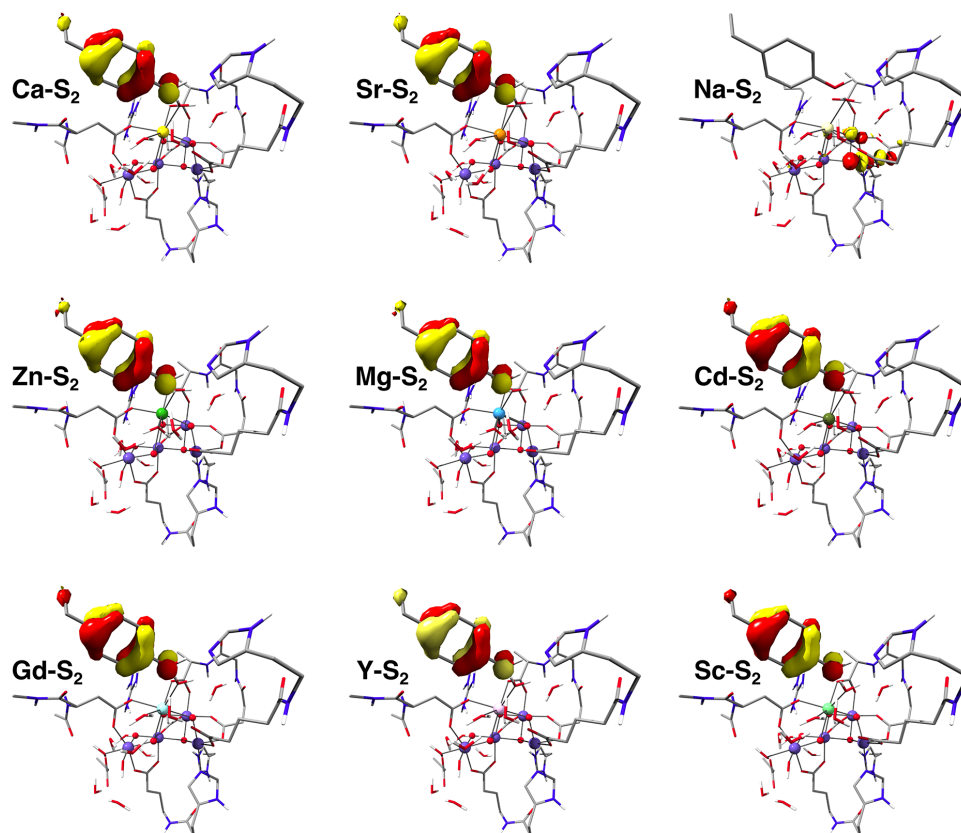


Figure S10. Redox active orbitals of the S_2 models. Color code as in Figure S9.

Table S7. Selected interatomic distances in Å in the S_1 , S_2 and $S_2Y_Z^*$ states of the OEC. Atomic labels as in Figure 1b.

Distance (Å)	Ca ²⁺	Sr ²⁺	Gd ³⁺	Cd ²⁺	Zn ²⁺	Mg ²⁺	Sc ³⁺	Na ⁺	Y ³⁺
S_1									
Mn1-Mn2	2.80	2.76	2.82	2.79	2.80	2.81	2.82	2.78	2.79
Mn1-Mn3	3.18	3.10	3.23	3.06	3.10	3.13	3.18	3.07	3.10
Mn1-Mn4	4.78	4.74	4.94	4.53	4.68	4.70	4.84	4.48	4.82
Mn2-Mn3	2.76	2.76	2.77	2.76	2.78	2.77	2.76	2.75	2.76
Mn2-Mn4	5.22	5.24	5.33	5.17	5.25	5.24	5.32	5.10	5.36
Mn3-Mn4	2.80	2.82	2.85	2.80	2.84	2.83	2.87	2.76	2.91
M-Mn1	3.52	3.49	3.51	3.39	3.22	3.23	3.30	3.51	3.33
M-Mn2	3.32	3.47	3.31	3.22	3.09	3.06	3.10	3.32	3.21
M-Mn3	3.35	3.51	3.28	3.30	2.95	2.99	3.09	3.49	3.20
M-Mn4	3.76	3.83	3.83	3.68	3.45	3.52	3.76	3.73	3.81
Mn1-O1	1.86	1.85	1.90	1.86	1.85	1.86	1.89	1.84	1.88
Mn1-O3	1.94	1.92	1.94	1.94	1.94	1.94	1.95	1.94	1.94
Mn1-O5	2.62	2.50	2.69	2.35	2.41	2.48	2.54	2.39	2.40
Mn2-O1	1.87	1.85	1.88	1.86	1.86	1.87	1.88	1.84	1.87
Mn2-O2	1.80	1.79	1.83	1.81	1.82	1.81	1.84	1.78	1.84
Mn2-O3	1.89	1.89	1.89	1.89	1.89	1.90	1.88	1.90	1.87
Mn3-O2	1.85	1.85	1.87	1.86	1.88	1.88	1.87	1.84	1.87
Mn3-O3	1.99	1.98	2.00	1.98	1.98	1.99	2.00	1.97	1.99
Mn3-O4	1.81	1.81	1.80	1.81	1.80	1.81	1.79	1.82	1.80
Mn3-O5	1.79	1.79	1.81	1.80	1.80	1.79	1.81	1.79	1.81
Mn4-O4	1.88	1.87	1.89	1.88	1.89	1.90	1.90	1.88	1.89
Mn4-O5	2.19	2.25	2.32	2.20	2.29	2.25	2.38	2.10	2.47
Mn4-W1	2.32	2.32	2.22	2.27	2.28	2.29	2.21	2.41	2.21
Mn4-W2	1.87	1.87	1.85	1.86	1.86	1.86	1.85	1.88	1.85
M-O1	2.44	2.55	2.39	2.37	2.29	2.22	2.19	2.47	2.31
M-O2	2.45	2.65	2.39	2.36	2.11	2.12	2.18	2.52	2.31
M-O5	2.49	2.63	2.33	2.53	2.13	2.16	2.15	2.76	2.30
M-W3	2.38	2.57	2.35	2.25	2.03	2.04	2.12	2.39	2.26
M-W4	2.45	2.64	2.42	2.43	2.19	2.17	2.26	2.55	2.36
M-Ala344	2.54	2.69	2.47	2.52	4.00	3.44	2.34	2.83	2.39
M-Asp170	2.39	2.57	2.37	2.30	2.10	2.08	2.18	2.41	2.29
M-Glu189	3.19	2.84	3.03	4.05	3.99	4.05	3.91	3.31	3.86

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S2									
Mn1-Mn2	2.79	2.76	2.82	2.76	2.75	2.75	2.78	2.75	2.81
Mn1-Mn3	3.35	3.37	3.39	3.31	3.32	3.32	3.37	3.33	3.39
Mn1-Mn4	4.92	5.02	5.02	4.84	4.84	4.82	4.94	4.90	5.02
Mn2-Mn3	2.77	2.78	2.78	2.76	2.77	2.77	2.75	2.77	2.77
Mn2-Mn4	5.24	5.20	5.21	5.19	5.18	5.17	5.23	5.15	5.20
Mn3-Mn4	2.84	2.74	2.75	2.82	2.79	2.80	2.86	2.72	2.75
M-Mn1	3.67	3.63	3.60	3.55	3.64	3.61	3.51	3.66	3.58
M-Mn2	3.34	3.48	3.31	3.29	3.07	3.09	3.11	3.34	3.27
M-Mn3	3.57	3.58	3.38	3.44	3.42	3.47	3.25	3.52	3.33
M-Mn4	4.00	3.95	3.85	3.81	4.00	4.04	3.77	3.93	3.82
Mn1-O1	1.86	1.84	1.89	1.86	1.86	1.87	1.90	1.83	1.89
Mn1-O3	1.93	1.92	1.94	1.92	1.92	1.92	1.93	1.92	1.94
Mn1-O5	3.10	3.18	3.17	3.02	3.01	3.00	3.09	3.10	3.18
Mn2-O1	1.86	1.85	1.88	1.86	1.85	1.86	1.89	1.83	1.88
Mn2-O2	1.82	1.81	1.83	1.81	1.83	1.82	1.84	1.80	1.83
Mn2-O3	1.91	1.91	1.90	1.91	1.90	1.90	1.89	1.91	1.89
Mn3-O2	1.83	1.83	1.85	1.83	1.85	1.85	1.86	1.82	1.85
Mn3-O3	1.99	2.00	2.01	1.98	1.99	2.00	1.99	1.99	2.00
Mn3-O4	1.81	1.81	1.79	1.81	1.81	1.81	1.79	1.82	1.79
Mn3-O5	1.88	1.84	1.85	1.88	1.84	1.84	1.88	1.82	1.85
Mn4-O4	1.97	1.89	1.90	1.94	1.95	1.96	2.02	1.89	1.90
Mn4-O5	1.85	1.86	1.91	1.85	1.83	1.83	1.92	1.83	1.91
Mn4-W1	2.41	2.03	1.99	2.40	2.39	2.39	2.36	2.07	1.99
Mn4-W2	1.82	1.84	1.82	1.82	1.82	1.82	1.79	1.86	1.82
M-O1	2.43	2.56	2.36	2.35	2.29	2.23	2.16	2.50	2.33
M-O2	2.52	2.67	2.42	2.46	2.16	2.23	2.21	2.55	2.37
M-O5	2.80	2.72	2.49	2.62	2.95	2.97	2.39	2.79	2.44
M-W3	2.34	2.55	2.31	2.26	2.00	2.02	2.10	2.37	2.26
M-W4	2.39	2.59	2.38	2.35	2.21	2.17	2.22	2.46	2.34
M-Ala344	2.45	2.67	2.43	2.58	2.25	2.18	2.28	2.82	2.41
M-Asp170	2.40	2.58	2.36	2.40	2.17	2.14	2.21	2.46	2.32
M-Glu189	3.06	2.80	2.98	3.10	4.07	4.12	3.61	3.18	3.09
S₂Y_Z'									
Mn1-Mn2	2.79	2.76	2.82	2.77	2.75	2.75	2.78	2.76	2.81
Mn1-Mn3	3.34	3.37	3.39	3.29	3.31	3.31	3.33	3.34	3.39
Mn1-Mn4	4.91	5.02	5.02	4.76	4.81	4.80	4.81	4.89	5.02

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Mn2-Mn3	2.77	2.78	2.78	2.77	2.78	2.77	2.77	2.77	2.77
Mn2-Mn4	5.24	5.20	5.22	5.17	5.18	5.17	5.22	5.13	5.21
Mn3-Mn4	2.84	2.74	2.75	2.80	2.79	2.80	2.85	2.73	2.75
A-Mn1	3.67	3.63	3.61	3.63	3.65	3.61	3.46	3.60	3.59
A-Mn2	3.33	3.47	3.30	3.20	3.06	3.07	3.08	3.15	3.25
A-Mn3	3.55	3.57	3.36	3.44	3.34	3.42	3.27	3.29	3.31
A-Mn4	4.00	3.94	3.84	3.88	3.92	4.01	3.82	3.75	3.81
Mn1-O1	1.87	1.84	1.90	1.86	1.86	1.87	1.89	1.84	1.90
Mn1-O3	1.93	1.91	1.94	1.92	1.92	1.92	1.92	1.92	1.94
Mn1-O5	3.09	3.18	3.17	2.94	2.99	2.98	2.97	3.08	3.18
Mn2-O1	1.86	1.85	1.89	1.86	1.85	1.86	1.89	1.84	1.89
Mn2-O2	1.82	1.81	1.84	1.82	1.84	1.83	1.85	1.80	1.84
Mn2-O3	1.91	1.91	1.90	1.90	1.90	1.90	1.88	1.91	1.89
Mn3-O2	1.83	1.83	1.85	1.84	1.86	1.85	1.87	1.82	1.85
Mn3-O3	1.99	2.00	2.01	1.98	1.99	2.00	2.01	1.99	2.00
Mn3-O4	1.81	1.81	1.79	1.81	1.80	1.80	1.79	1.81	1.79
Mn3-O5	1.88	1.84	1.86	1.86	1.85	1.85	1.87	1.83	1.86
Mn4-O4	1.97	1.89	1.89	1.95	1.95	1.96	2.03	1.89	1.90
Mn4-O5	1.85	1.87	1.92	1.85	1.83	1.84	1.91	1.84	1.92
Mn4-W1	2.41	2.03	1.98	2.37	2.38	2.39	2.34	2.05	1.98
Mn4-W2	1.82	1.84	1.82	1.81	1.81	1.81	1.79	1.85	1.82
A-O1	2.42	2.55	2.36	2.37	2.33	2.24	2.14	2.42	2.32
A-O2	2.50	2.65	2.40	2.35	2.09	2.18	2.18	2.32	2.36
A-O5	2.79	2.71	2.47	2.77	2.87	2.92	2.50	2.59	2.42
A-W3	2.37	2.57	2.33	2.24	2.04	2.05	2.09	2.30	2.28
A-W4	2.39	2.60	2.40	2.42	2.20	2.20	2.23	3.89	2.36
A-Ala344	2.44	2.66	2.43	2.39	2.33	2.19	2.23	2.38	2.39
A-Asp170	2.39	2.57	2.36	2.29	2.13	2.14	2.16	2.31	2.32
A-Glu189	3.10	2.82	3.02	4.09	4.11	4.13	3.93	4.04	3.16

Table S8. Mayer bond orders > 0.05 of A^{n+} -O interactions for the OEC models.

	Ca^{2+}	Sr^{2+}	Gd^{3+}	Cd^{2+}	Zn^{2+}	Mg^{2+}	Sc^{3+}	Na^{+}	Y^{3+}
S ₁									
A ⁿ⁺ -O1	<0.05	0.15	0.05	0.16	0.12	<0.05	0.27	<0.05	0.25
A ⁿ⁺ -O2	0.09	0.17	0.20	0.16	0.20	0.13	0.35	<0.05	0.31
A ⁿ⁺ -O5	0.11	0.22	0.24	0.12	0.21	0.12	0.45	<0.05	0.37
A ⁿ⁺ -W3	0.07	0.17	0.24	0.29	0.45	0.41	0.51	<0.05	0.41
A ⁿ⁺ -W4	0.15	0.28	0.35	0.28	0.38	0.32	0.42	0.11	0.32
A ⁿ⁺ -Asp170	0.08	0.20	0.24	0.21	0.28	0.25	0.32	<0.05	0.30
A ⁿ⁺ -Glu189	<0.05	0.09	0.06	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
A ⁿ⁺ -Ala344	0.14	0.21	0.30	0.18	<0.05	<0.05	0.36	<0.05	0.33
S ₂									
A ⁿ⁺ -O1	0.05	0.15	0.05	0.17	0.11	<0.05	0.30	<0.05	0.27
A ⁿ⁺ -O2	0.08	0.16	0.18	0.13	0.19	0.09	0.34	<0.05	0.29
A ⁿ⁺ -O5	0.07	0.17	0.14	0.10	<0.05	<0.05	0.26	<0.05	0.28
A ⁿ⁺ -W3	0.10	0.19	0.27	0.26	0.39	0.35	0.46	<0.05	0.36
A ⁿ⁺ -W4	0.17	0.30	0.36	0.28	0.42	0.33	0.44	0.10	0.35
A ⁿ⁺ -Asp170	0.07	0.20	0.25	0.17	0.21	0.19	0.34	<0.05	0.32
A ⁿ⁺ -Glu189	<0.05	0.09	0.07	<0.05	<0.05	<0.05	<0.05	<0.05	0.08
A ⁿ⁺ -Ala344	0.16	0.22	0.32	0.18	0.31	0.29	0.41	<0.05	0.34

Table S9. ΔE , IE and E_{relax} in eV in eV calculated with the TPSS density functional for the OEC.

	ΔE (eV)	IE (eV)	E_{relax} (eV)
S ₁ –S ₂			
Ca ²⁺	4.24	4.79	0.55
Sr ²⁺	3.93	4.72	0.80
Gd ³⁺	4.81	5.60	0.79
Cd ²⁺	4.43	4.80	0.37
Zn ²⁺	4.40	4.93	0.53
Mg ²⁺	4.28	4.91	0.63
Sc ³⁺	5.46	5.68	0.21
Na ⁺	3.24	3.98	0.74
Y ³⁺	4.66	5.63	0.97
S ₂ –S ₂ Y _Z [•]			
Ca ²⁺	5.43	6.08	0.65
Sr ²⁺	5.42	6.08	0.66
Gd ³⁺	5.78	6.50	0.72
Cd ²⁺	5.19	6.08	0.88
Zn ²⁺	5.29	6.04	0.75
Mg ²⁺	5.32	6.05	0.73
Sc ³⁺	5.49	6.47	0.97
Na ⁺	4.57	5.67	1.10
Y ³⁺	5.77	6.50	0.72

Coordinates of all structures

Mn(IV)₃CaO₄

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Ca	19.727022	3.086733	14.953951
Mn	17.732144	3.537011	12.477796
Mn	19.613176	5.575031	12.910556
Mn	17.420351	5.300843	14.640344
O	17.716993	5.425635	12.758418
O	19.546654	3.728084	12.649032
O	17.456293	3.494415	14.322782
O	19.278953	5.431022	14.708647
O	19.547438	7.449642	12.862244
O	17.707882	3.741702	10.612862
O	15.565120	5.484764	14.431245
O	21.550241	5.606052	13.115448
O	21.904720	3.912965	14.572360
O	17.805958	1.595763	12.314872
O	19.231096	1.002144	13.970289
O	17.234937	5.107867	16.570860
O	18.773411	3.523760	17.066430
O	21.147861	1.627210	16.361870
N	20.071071	5.910774	10.924588
N	15.722882	3.253813	12.102476
N	17.199319	7.307717	15.066910
N	22.647516	8.509777	11.433276
N	16.057191	0.847662	9.323075
N	14.392792	7.012027	17.440551
C	20.170121	4.965465	9.976283
H	19.963421	3.958831	10.311879
C	20.496684	5.287431	8.666633
H	20.552542	4.506475	7.916308
C	20.742887	6.621783	8.341879
H	20.993552	6.903790	7.323976
C	20.669614	7.589623	9.339473
H	20.859468	8.634961	9.126842
C	20.326632	7.197642	10.629783
C	20.224062	8.121478	11.832550
C	21.649973	8.470858	12.325441
C	21.841431	8.763848	13.678127
H	21.001284	8.709631	14.357901
C	23.112696	9.108509	14.119135
H	23.287265	9.342243	15.165358
C	24.161385	9.142515	13.197224
H	25.172374	9.398061	13.498150
C	23.878788	8.834619	11.871472
H	24.663801	8.846267	11.118399
C	19.449105	9.415772	11.501437
C	20.126573	10.640280	11.446303
H	21.203817	10.660475	11.568682
C	19.456466	11.847745	11.253522
H	20.017677	12.777280	11.217585
C	18.070615	11.847453	11.124862
H	17.524805	12.776910	10.988230
C	17.385959	10.635007	11.157900
H	16.306684	10.624216	11.029889
C	18.046661	9.406427	11.325120
C	14.760990	3.161398	13.034704
H	15.102839	3.265349	14.055067
C	13.432393	2.966444	12.685035
H	12.672961	2.913454	13.457320
C	13.101215	2.847101	11.335010
H	12.069175	2.700463	11.031996
C	14.110224	2.912301	10.378413
H	13.892709	2.819682	9.320998
C	15.419993	3.120999	10.798852
C	16.635000	3.199144	9.888799
C	17.021083	1.770097	9.434848
C	18.357148	1.500354	9.127099
H	19.097501	2.280864	9.243716
C	18.703649	0.229379	8.686923
H	19.734865	-0.004759	8.439119
C	17.705985	-0.741793	8.575113
H	17.931671	-1.750164	8.243152
C	16.403865	-0.385116	8.905992
H	15.594592	-1.108859	8.837276
C	16.375613	4.092358	8.655543
C	16.284685	3.514228	7.383020
H	16.327961	2.435485	7.282225
C	16.155211	4.284663	6.228124

H	16.088951	3.798302	5.258933
C	16.127863	5.672281	6.331795
H	16.042162	6.294534	5.445268
C	16.197151	6.260129	7.592400
H	16.148304	7.342082	7.683548
C	16.302284	5.499521	8.769153
C	18.202532	8.184285	15.234379
H	19.194095	7.772480	15.107912
C	17.955184	9.517498	15.528673
H	18.783377	10.208458	15.641224
C	16.633839	9.942658	15.669638
H	16.410320	10.981230	15.892985
C	15.602675	9.018780	15.526548
H	14.564596	9.310087	15.634083
C	15.922184	7.699624	15.220403
C	14.922221	6.566986	15.052219
C	14.435618	6.112220	16.450159
C	14.034984	4.785103	16.624319
H	14.096064	4.097644	15.790886
C	13.579286	4.377452	17.871330
H	13.260999	3.351444	18.031992
C	13.543365	5.305781	18.913867
H	13.204037	5.029487	19.907101
C	13.958701	6.605392	18.648853
H	13.947731	7.362931	19.429650
C	13.718474	6.985162	14.180494
C	12.453820	7.134458	14.763249
H	12.343931	7.021518	15.836129
C	11.317780	7.410301	14.003159
H	10.353649	7.518166	14.492117
C	11.432386	7.529209	12.621207
H	10.559414	7.729851	12.006282
C	12.687387	7.402961	12.030465
H	12.789213	7.522464	10.954963
C	13.846939	7.150698	12.782558
C	15.118581	7.112246	12.003227
C	15.231709	6.211766	10.936700
H	14.436556	5.493555	10.773948
C	16.299099	6.284479	10.037910
C	17.261281	7.286796	10.213372
H	18.045607	7.391757	9.472907
C	17.173826	8.197820	11.269053
C	16.093451	8.101720	12.154808
H	15.983710	8.854334	12.926888
C	22.299943	4.841325	13.833824
C	23.782666	5.128188	13.710455
H	24.315286	4.777052	14.596546
H	23.961752	6.193781	13.554600
H	24.174255	4.590842	12.838280
C	18.473682	0.738963	13.009897
C	18.260019	-0.702294	12.592721
H	19.136102	-1.305644	12.840044
H	18.038180	-0.772017	11.526357
H	17.401742	-1.105000	13.144181
C	17.859730	4.319541	17.377849
C	17.386019	4.387586	18.816150
H	18.230704	4.259183	19.497532
H	16.684191	3.564209	18.992433
H	16.869819	5.326209	19.022035
C	22.113735	0.782642	15.663151
H	21.831080	-0.263391	15.829486
H	23.916040	1.970431	15.760399
H	24.164595	0.267903	16.212238
H	22.050046	1.001745	14.594885
C	23.471694	1.111428	16.272459
C	23.097099	1.487031	17.712844
H	22.922589	0.587119	18.312722
H	23.858985	2.093103	18.210448
C	21.797930	2.256105	17.508146
H	21.104374	2.202937	18.349332
H	21.992717	3.307289	17.263661

Mn(III)Mn(IV)₂CaO₄

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Ca	19.675289	3.057624	14.874468
Mn	17.667605	3.425721	12.428168
Mn	19.586855	5.594569	12.942753
Mn	17.429019	5.311480	14.622689

O	17.749991	5.651136	12.844750	H	19.184909	7.800261	15.123519
O	19.515804	3.779789	12.617846	C	17.938375	9.544259	15.532970
O	17.415698	3.513365	14.296865	H	18.763198	10.242549	15.627904
O	19.288486	5.414335	14.748430	C	16.615029	9.964783	15.670126
O	19.652434	7.510444	12.932806	H	16.385919	11.005596	15.879622
O	17.645673	3.625979	10.532986	C	15.588770	9.033851	15.533589
O	15.545855	5.498595	14.431803	H	14.548548	9.322788	15.630154
O	21.585256	5.569059	13.127915	C	15.916363	7.711189	15.244556
O	21.908994	3.851994	14.567220	C	14.917158	6.576226	15.054334
O	17.815374	1.172612	12.388072	C	14.408819	6.119830	16.445351
O	19.386583	0.886098	13.987896	C	14.050939	4.779899	16.618598
O	17.226387	5.070822	16.597779	H	14.165957	4.096690	15.787335
O	18.729188	3.433611	17.037177	C	13.581974	4.360341	17.856125
O	21.139693	1.657592	16.426643	H	13.296833	3.323954	18.015036
N	20.043794	5.963798	10.949982	C	13.493505	5.289391	18.895620
N	15.655193	3.161485	12.048646	H	13.144357	5.004245	19.883215
N	17.194483	7.321413	15.109729	C	13.871991	6.600856	18.634758
N	22.690505	8.639513	11.389245	H	13.821685	7.358867	19.414104
N	15.854290	0.854835	9.132594	C	13.727585	7.016751	14.171320
N	14.315040	7.020273	17.433503	C	12.454656	7.177403	14.732629
C	20.060683	5.035007	9.981320	H	12.328523	7.066187	15.804272
H	19.789206	4.038945	10.304174	C	11.331596	7.459527	13.954891
C	20.370687	5.363501	8.668066	H	10.360036	7.573858	14.428221
H	20.352583	4.596505	7.901015	C	11.469244	7.576093	12.574752
C	20.689564	6.686587	8.360981	H	10.607630	7.782018	11.945229
H	20.931028	6.974082	7.341776	C	12.733236	7.438565	12.005111
C	20.691066	7.637652	9.377598	H	12.852903	7.553541	10.930713
H	20.928810	8.675861	9.178791	C	13.879559	7.176264	12.774229
C	20.355168	7.240070	10.670059	C	15.160147	7.117629	12.008182
C	20.290653	8.160060	11.882414	C	15.270290	6.207218	10.949154
C	21.734574	8.515823	12.320922	H	14.472419	5.490091	10.794675
C	21.989737	8.707319	13.681862	C	16.333309	6.271119	10.044209
H	21.180965	8.573488	14.388505	C	17.300898	7.272877	10.213552
C	23.275206	9.041095	14.088405	H	18.084106	7.369461	9.470292
H	23.497411	9.197007	15.140509	C	17.224098	8.187566	11.267634
C	24.279507	9.160282	13.124703	C	16.141828	8.100471	12.154299
H	25.300963	9.407281	13.397077	H	16.040643	8.853006	12.928046
C	23.937521	8.947496	11.794278	C	22.313079	4.788771	13.836238
H	24.686849	9.026499	11.008922	C	23.809878	5.044576	13.733299
C	19.492689	9.443703	11.546585	H	24.313287	4.763029	14.661790
C	20.138351	10.686382	11.535084	H	24.013545	6.090957	13.495696
H	21.210839	10.728334	11.691373	H	24.222266	4.426006	12.926372
C	19.447105	11.883153	11.346223	C	18.643547	0.475798	13.044615
H	19.986808	12.826466	11.348031	C	18.731085	-1.005121	12.674888
C	18.067501	11.852020	11.168486	H	19.710176	-1.420455	12.930064
H	17.502947	12.770025	11.028277	H	18.527712	-1.149400	11.610303
C	17.413128	10.622013	11.160974	H	17.972190	-1.562584	13.238781
H	16.338223	10.589156	11.001704	C	17.825183	4.238689	17.367405
C	18.092841	9.403677	11.333463	C	17.357297	4.249637	18.815752
C	14.693805	3.130076	12.986086	H	18.220820	4.282849	19.487629
H	15.054636	3.222007	14.002963	H	16.815299	3.319960	19.024403
C	13.351827	3.023256	12.647601	H	16.694852	5.092792	19.017255
H	12.594815	3.019091	13.424647	C	22.154949	0.842135	15.772060
C	13.003735	2.937413	11.298622	H	21.945265	-0.210365	16.000519
H	11.961709	2.858744	11.002629	H	23.873037	2.147774	15.781188
C	14.007080	2.961973	10.333161	H	24.240250	0.494557	16.335306
H	13.773473	2.907320	9.276155	H	22.069575	0.993115	14.694125
C	15.332063	3.085671	10.743908	C	23.493014	1.293111	16.348971
C	16.546840	3.149836	9.823372	C	23.100085	1.734499	17.765733
C	16.864694	1.712209	9.337905	H	22.986325	0.864479	18.422678
C	18.200608	1.355811	9.136031	H	23.821572	2.419412	18.220350
H	18.972650	2.086545	9.339810	C	21.751993	2.401830	17.517945
C	18.498333	0.069920	8.703660	H	21.066750	2.365150	18.367162
H	19.529166	-0.230819	8.537232	H	21.879459	3.443964	17.200637
C	17.452995	-0.833252	8.499122				
H	17.639088	-1.852311	8.174081				
C	16.154117	-0.394278	8.728698				
H	15.308158	-1.063678	8.584147				
C	16.306443	4.089298	8.617107				
C	16.190063	3.551304	7.329083				
H	16.175972	2.473845	7.205097				
C	16.111334	4.352450	6.190090				
H	16.025801	3.892625	5.209080				
C	16.158625	5.736414	6.326899				
H	16.111792	6.384554	5.455767				
C	16.250750	6.287571	7.602741				
H	16.257099	7.368421	7.718733				
C	16.310287	5.498485	8.764952				
C	18.191413	8.206484	15.258592				
				Mn(IV)₃SrO₄			
				146			
				Sr	11.377255	5.705810	12.854647
				Mn	9.336706	8.428452	12.958100
				Mn	8.593589	6.362216	14.707811
				Mn	8.130092	6.096773	11.952718
				O	7.777501	7.383297	13.314945
				O	10.067215	7.420282	14.297683
				O	9.621540	7.124949	11.648433
				O	8.901072	5.159021	13.364914
				C	12.213311	9.071992	12.584423
				C	13.178174	10.205946	12.296313
				H	13.290868	10.812706	13.201188

H	12.791127	10.858730	11.510446	C	8.767848	8.686510	16.675171
H	14.157712	9.813486	12.016704	H	9.599372	8.951782	16.036941
C	9.574464	3.968795	10.440707	C	9.849694	11.909725	13.704313
C	9.411020	2.982219	9.300352	C	10.627577	11.706616	14.847469
H	9.795952	3.442493	8.382769	H	10.332570	10.949262	15.562054
H	8.360631	2.735699	9.136503	C	11.763613	12.483174	15.035886
H	9.990255	2.076523	9.493788	H	12.380927	12.349617	15.919639
C	10.665842	4.699159	16.084565	C	12.100168	13.433059	14.068754
C	10.975385	3.982847	17.385287	H	12.982317	14.057159	14.170539
H	10.924053	2.901343	17.217583	C	11.274034	13.558428	12.958211
H	10.268582	4.252835	18.169995	H	11.499852	14.280486	12.176239
H	11.996014	4.218078	17.701805	C	6.393234	5.648165	8.841009
C	5.794055	9.762363	14.070777	C	7.424113	6.220548	8.092063
C	5.534331	9.562062	12.712947	H	7.921716	7.106013	8.464573
H	5.732077	10.356479	12.002688	C	7.796943	5.624319	6.894206
C	4.934709	8.382657	12.254512	H	8.595040	6.050285	6.292682
C	4.588225	7.399329	13.184664	C	7.135002	4.466698	6.480229
H	4.053882	6.513528	12.861549	H	7.398388	3.962933	5.555581
C	4.840435	7.572361	14.551670	C	6.122556	3.966078	7.290489
C	5.438283	8.759880	14.980913	H	5.580612	3.065032	7.010644
H	5.569293	8.946384	16.040411	C	6.966760	4.664314	17.428906
C	6.193071	11.101695	14.590803	C	7.114081	3.393246	16.867851
C	7.400158	11.779832	14.308169	H	6.927863	3.254554	15.810930
C	7.573928	13.078059	14.804994	C	7.508747	2.339404	17.682060
H	8.488670	13.616928	14.584623	H	7.628033	1.341304	17.270316
C	6.609392	13.703305	15.594227	C	7.754152	2.585571	19.034440
H	6.782244	14.711221	15.961129	H	8.071581	1.794228	19.706059
C	5.440418	13.019518	15.915367	C	7.585287	3.882361	19.505562
H	4.680914	13.480015	16.541194	H	7.768265	4.122578	20.550816
C	5.244402	11.736739	15.409913	N	8.528848	9.728249	11.566386
H	4.320747	11.207819	15.630240	N	6.382977	4.999585	12.100465
C	4.462133	8.325097	10.840316	N	8.112018	7.571975	16.314784
C	4.843689	7.372166	9.868305	N	10.162350	12.820699	12.774551
C	4.252333	7.431069	8.600180	N	5.747913	4.542300	8.448355
H	4.529873	6.701857	7.847426	N	7.193642	4.908383	18.725936
C	3.321465	8.413011	8.262904	O	12.650535	7.934311	12.852703
H	2.885976	8.425391	7.267584	O	10.968740	9.412104	12.529229
C	2.971628	9.375953	9.204764	O	10.643614	4.000215	11.087750
H	2.257591	10.158072	8.961776	O	8.558003	4.741509	10.618161
C	3.539780	9.320142	10.475124	O	11.482101	4.624983	15.137135
H	3.253717	10.054222	11.223932	O	9.544527	5.333007	16.075394
C	4.240272	6.612920	15.523362	O	8.749932	9.812935	14.086448
C	4.939434	5.858957	16.493760	O	7.051511	7.004979	10.709658
C	4.205586	5.066386	17.385520	O	6.950415	5.606375	15.223217
H	4.727356	4.491502	18.142411	O	13.640941	5.348169	11.593481
C	2.815502	4.976229	17.324163	C	14.213488	6.200120	10.885763
H	2.283068	4.349098	18.033832	C	12.232634	6.671553	9.547023
C	2.127373	5.681478	16.341327	C	14.359935	7.927188	7.170866
H	1.045516	5.616310	16.264345	N	13.637661	6.882825	9.888468
C	2.842037	6.489541	15.460578	H	15.275561	6.446327	11.027238
H	2.309318	7.065906	14.708576	H	14.400379	7.691401	8.102691
C	8.548317	11.088383	13.537604	H	13.856247	8.891180	9.299707
C	5.951524	6.334393	10.157698	H	15.376124	7.998649	9.563422
C	6.484508	5.827430	16.526624	H	12.110889	6.791538	8.467573
C	8.229802	10.943098	12.058575	H	11.584389	7.390133	10.061649
C	7.702385	11.942467	11.246522	H	11.945017	5.658063	9.831996
H	7.459789	12.909273	11.671472				
C	7.480649	11.665783	9.900414				
H	7.055774	12.423554	9.249288				
C	7.816628	10.408151	9.398542				
H	7.664873	10.159503	8.353871				
C	8.349814	9.462350	10.263002				
H	8.636979	8.465611	9.958463				
C	5.484187	5.269148	11.137087				
C	4.267503	4.596592	11.074419				
H	3.556791	4.842505	10.294629				
C	3.985123	3.629873	12.035393				
H	3.036733	3.101743	12.017473				
C	4.935531	3.345720	13.016236				
H	4.752390	2.594726	13.776925				
C	6.132752	4.047813	13.013283				
H	6.920185	3.892507	13.737490				
C	7.071620	7.130936	17.044007				
C	6.630049	7.823903	18.166994				
H	5.782414	7.451779	18.730037				
C	7.283209	8.998166	18.530245				
H	6.948606	9.565508	19.393287				
C	8.374129	9.432727	17.777022				
H	8.910917	10.338927	18.035626				

Mn(III)Mn(IV)₂SrO₄

146			
Sr	11.317301	5.716862	12.927107
Mn	9.323742	8.448033	12.930300
Mn	8.614397	6.355577	14.814551
Mn	8.144099	6.173770	11.920416
O	7.733996	7.533342	13.086457
O	10.035539	7.477745	14.294854
O	9.670067	7.162031	11.615758
O	8.841473	5.219613	13.330126
C	12.252145	9.084162	12.625737
C	13.260161	10.207769	12.425469
H	13.483481	10.659228	13.398775
H	12.858609	10.992757	11.780848
H	14.193488	9.816838	12.012463
C	9.595063	3.949461	10.459130
C	9.457523	2.919937	9.345072
H	10.135141	3.186618	8.525441
H	8.438619	2.883548	8.955895
H	9.755535	1.931097	9.707865
C	11.009988	4.470802	16.113178

C	11.385080	3.586805	17.304040	H	12.951422	14.092897	14.200646
H	10.601260	2.836681	17.457781	C	11.234596	13.625931	12.987715
H	11.431489	4.189012	18.217745	H	11.458015	14.366080	12.221628
H	12.342024	3.081117	17.151648	C	6.386053	5.642404	8.727908
C	5.798029	9.729903	14.036460	C	7.509571	6.097010	8.032677
C	5.533126	9.523995	12.680922	H	8.087159	6.909658	8.453063
H	5.727290	10.316532	11.967158	C	7.868402	5.470460	6.845958
C	4.939812	8.338838	12.224662	H	8.738509	5.805115	6.287454
C	4.604543	7.356422	13.160679	C	7.102746	4.395943	6.389188
H	4.074186	6.465440	12.844051	H	7.351931	3.869626	5.472895
C	4.869697	7.529809	14.528003	C	6.004946	4.006178	7.148117
C	5.464824	8.721805	14.949377	H	5.381612	3.170636	6.834860
H	5.606901	8.909896	16.007278	C	6.931265	4.693827	17.578383
C	6.165060	11.081095	14.553359	C	7.185853	3.431209	17.036533
C	7.353449	11.792816	14.270286	H	7.079183	3.289744	15.968638
C	7.490016	13.096189	14.764938	C	7.586171	2.403076	17.880552
H	8.391396	13.657629	14.543624	H	7.784555	1.410676	17.484671
C	6.508893	13.696921	15.553699	C	7.740722	2.668411	19.242718
H	6.654146	14.709648	15.920395	H	8.063518	1.899268	19.937692
C	5.358812	12.981613	15.874830	C	7.474650	3.956100	19.693380
H	4.586514	13.421296	16.500459	H	7.585443	4.210114	20.745909
C	5.198887	11.693074	15.369901	N	8.562656	9.786317	11.525132
H	4.289938	11.138961	15.590629	N	6.374259	5.083847	12.042355
C	4.464953	8.300544	10.805586	N	8.132287	7.548036	16.428745
C	4.869277	7.399336	9.790022	N	10.119872	12.894565	12.791999
C	4.300135	7.523876	8.516914	N	5.641606	4.615149	8.292564
H	4.602663	6.839746	7.731825	N	7.068487	4.954793	18.886626
C	3.362961	8.511492	8.212962	O	12.676494	7.927368	12.852842
H	2.948512	8.574298	7.210125	O	11.023889	9.447476	12.552483
C	2.977071	9.412028	9.200807	O	10.656933	3.971828	11.128334
H	2.252735	10.194443	8.989942	O	8.593504	4.735324	10.591936
C	3.527802	9.295196	10.475377	O	11.767083	4.441178	15.090896
H	3.220754	9.986761	11.256083	O	9.958741	5.161436	16.245711
C	4.261318	6.582114	15.510508	O	8.732067	9.856190	14.070644
C	4.927945	5.873058	16.541064	O	7.093310	7.020621	10.554522
C	4.162067	5.106019	17.428490	O	6.970830	5.557484	15.355015
H	4.659722	4.567556	18.227752	O	13.600409	5.338323	11.586324
C	2.777137	4.989203	17.311610	C	14.123321	6.228913	10.892066
H	2.223169	4.379629	18.020696	C	12.131954	6.583188	9.532285
C	2.123883	5.646751	16.273692	C	14.178865	7.976980	9.195067
H	1.047257	5.562739	16.150517	N	13.521216	6.873615	9.882396
C	2.867509	6.433550	15.397515	H	15.164808	6.548122	11.049336
H	2.359274	6.976262	14.604464	H	14.219555	7.780276	8.118482
C	8.524181	11.118671	13.516634	H	13.631088	8.911424	9.360415
C	5.985909	6.356821	10.044973	H	15.195830	8.086340	9.577730
C	6.474059	5.828619	16.625922	H	12.013316	6.685986	8.449766
C	8.224686	10.984366	12.028372	H	11.438506	7.262301	10.042577
C	7.661598	11.974206	11.225967	H	11.899257	5.560040	9.832113
H	7.391494	12.930757	11.658899				
C	7.437492	11.699512	9.879494				
H	6.984878	12.448561	9.236041				
C	7.799779	10.452332	9.369355				
H	7.635466	10.200559	8.326851				
C	8.369485	9.518382	10.225187				
H	8.666664	8.524924	9.917303				
C	5.505531	5.309708	11.043432				
C	4.285912	4.638184	10.977677				
H	3.599782	4.848250	10.166122				
C	3.967802	3.723994	11.978342				
H	3.016235	3.200405	11.959240				
C	4.882460	3.496676	13.007036				
H	4.666141	2.799237	13.809600				
C	6.085728	4.190707	13.001413				
H	6.843101	4.088502	13.767208				
C	7.058292	7.142903	17.132903				
C	6.573257	7.888006	18.204748				
H	5.704176	7.541668	18.752032				
C	7.206217	9.084104	18.532906				
H	6.836338	9.691380	19.353952				
C	8.313370	9.496905	17.789859				
H	8.822010	10.429314	18.010688				
C	8.752265	8.697700	16.743184				
H	9.586020	8.947231	16.098140				
C	9.811840	11.959313	13.700384				
C	10.596480	11.730518	14.834697				
H	10.303849	10.947820	15.522637				
C	11.732466	12.502162	15.037136				
H	12.355206	12.347178	15.914071				
C	12.066640	13.473563	14.089896				

Mn(IV)₃ZnO₄

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Zn	4.983711	6.496483	18.443567
Mn	6.059417	6.495151	15.707162
Mn	3.486416	7.540058	16.146167
Mn	3.926478	4.768695	16.317025
O	4.281538	6.173183	15.060376
O	5.237724	7.781085	16.714796
O	5.626678	5.125714	16.884988
O	3.177424	6.154960	17.300809
C	9.291208	7.201877	18.386390
H	9.938256	6.375775	18.074492
H	9.351810	7.326424	19.468173
H	9.653928	8.105830	17.887497
C	7.868751	6.923163	17.951704
C	3.668586	2.646157	20.006148
H	4.294005	2.696156	20.899240
H	3.796833	1.684959	19.503953
C	2.619253	2.728311	20.313345
H	3.990145	3.785460	19.063377
C	2.497920	9.905267	19.547234
H	2.832216	9.899985	20.585359
H	1.415620	9.745524	19.508317
H	2.698973	10.882395	19.097615
C	3.190832	8.822361	18.749112
C	4.816755	6.725830	12.015718
C	4.955737	5.338613	12.115068
H	5.906675	4.873747	11.882210
C	3.862692	4.517483	12.424202

C	2.613238	5.110930	12.626414	C	3.842388	-0.892185	17.380881
H	1.740787	4.488982	12.789642	H	3.883980	-1.743635	18.052578
C	2.443210	6.499007	12.533691	C	2.638514	-0.516458	16.795001
C	3.551744	7.292006	12.223793	H	1.724480	-1.070034	16.998621
H	3.426490	8.357574	12.070629	C	0.416325	9.310120	15.592583
C	5.901731	7.584008	11.452019	C	-0.283038	8.603915	16.573859
C	7.175140	7.818022	12.022626	H	-0.172630	7.529461	16.638654
C	8.097305	8.601467	11.318369	C	-1.095594	9.305423	17.456292
H	9.078778	8.779700	11.743780	H	-1.650915	8.780198	18.227936
C	7.789197	9.177893	10.086864	C	-1.179724	10.693795	17.338493
H	8.531227	9.780710	9.571036	H	-1.793403	11.282999	18.012398
C	6.524142	8.984488	9.540183	C	-0.450772	11.312223	16.328930
H	6.255497	9.434180	8.588377	H	-0.487150	12.391609	16.198259
C	5.602662	8.193166	10.221754	N	7.112191	5.204836	14.507622
H	4.621982	8.017850	9.787383	N	2.076567	4.164663	15.663689
C	4.012341	3.038316	12.277626	N	3.627976	9.139297	14.867451
C	3.781406	2.064474	13.277559	N	9.998360	7.356265	13.718989
C	3.902583	0.710326	12.943459	N	2.518770	0.530571	19.547784
H	3.719170	-0.043273	13.701530	N	0.331487	10.640428	15.463855
C	4.269561	0.295012	11.664133	O	6.970538	6.845630	18.833870
H	4.353821	-0.765177	11.442911	O	7.724501	6.791761	16.680394
C	4.538341	1.249573	10.687777	O	4.507961	4.831163	19.547736
H	4.839305	0.951368	9.687373	O	3.673381	3.566028	17.836817
C	4.404619	2.599955	11.001622	O	3.984611	8.044721	19.346738
H	4.588140	3.348808	10.235623	O	2.879290	8.808007	17.501674
C	1.056422	7.054033	12.515872	O	6.486216	7.647093	14.305389
C	0.528689	8.030743	13.392764	O	4.435546	3.424408	15.130458
C	-0.776814	8.491614	13.184882	O	1.833978	7.408887	15.295394
H	-1.186443	9.246291	13.847378	Mn(III)Mn(IV)₂ZnO₄			
C	-1.579818	7.997260	12.157890	¹³⁴			
H	-2.588607	8.378918	12.028500	Zn	4.923641	6.506012	18.418123
C	-1.080617	7.005846	11.318444	Mn	6.026438	6.473178	15.704596
H	-1.691631	6.594791	10.519684	Mn	3.399730	7.651294	16.185890
C	0.222871	6.550909	11.502910	Mn	3.966048	4.750022	16.291156
H	0.626493	5.795519	10.833836	O	4.402613	5.978949	14.986389
C	7.531445	7.302285	13.431626	O	5.206227	7.771654	16.693641
C	3.485863	2.466108	14.736196	O	5.652257	5.107584	16.910555
C	1.327200	8.528801	14.613654	O	3.170587	6.113759	17.250539
C	7.715911	5.794552	13.459163	C	9.288671	7.158705	18.433416
C	8.447233	5.055163	12.535544	H	9.800555	6.192708	18.523740
H	8.914426	5.554774	11.695456	H	9.302180	7.644250	19.411838
C	8.544402	3.677287	12.706356	H	9.837222	7.759966	17.704252
H	9.096697	3.075469	11.991566	C	7.862136	6.919551	17.964958
C	7.929006	3.080702	13.807417	C	3.638705	2.617260	20.028432
H	7.989186	2.011013	13.974178	H	4.242245	2.681057	20.936511
C	7.224121	3.878875	14.696116	H	3.786047	1.648772	19.543696
H	6.715227	3.494605	15.569066	H	2.581672	2.690805	20.312176
C	2.096286	3.058706	14.896938	C	3.973426	3.749652	19.070545
C	0.928594	2.534607	14.352812	C	2.811774	9.817735	20.219907
H	0.975193	1.648136	13.731746	H	2.754376	9.373095	21.217042
C	-0.278000	3.179786	14.607928	H	1.835558	10.214592	19.929307
H	-1.201647	2.799653	14.183064	H	3.515924	10.657948	20.267704
C	-0.286975	4.315476	15.418464	C	3.311900	8.809060	19.189875
H	-1.209537	4.839243	15.642556	C	4.793661	6.709213	12.036952
C	0.912906	4.778276	15.938168	C	4.937866	5.323052	12.127446
H	0.992496	5.652520	16.569140	H	5.890206	4.862704	11.890345
C	2.487127	9.424249	14.212825	C	3.850895	4.495175	12.444249
C	2.421709	10.464394	13.291880	C	2.602862	5.085895	12.658456
H	1.492406	10.665549	12.772568	H	1.732096	4.462848	12.826377
C	3.567877	11.214424	13.045284	C	2.425274	6.476594	12.577974
H	3.547288	12.021928	12.320273	C	3.530475	7.272399	12.265290
C	4.739833	10.919323	13.742717	H	3.406077	8.338830	12.120882
H	5.649669	11.485908	13.578796	C	5.865335	7.574916	11.457653
C	4.732384	9.875376	14.655886	C	7.140463	7.829910	12.016119
H	5.598389	9.579447	15.231307	C	8.039177	8.632384	11.303027
C	8.829490	7.967003	13.953573	H	9.020713	8.829872	11.719875
C	8.739424	9.176332	14.645969	C	7.709109	9.204846	10.074730
H	7.768638	9.623085	14.815464	H	8.434478	9.824166	9.553913
C	9.905037	9.770849	15.114608	C	6.444438	8.984870	9.537218
H	9.862849	10.712014	15.655085	H	6.158686	9.428259	8.587072
C	11.126608	9.135822	14.885509	C	5.545218	8.175684	10.228225
H	12.060247	9.559000	15.242048	H	4.563095	7.982308	9.804278
C	11.120685	7.935014	14.184355	C	4.025734	3.016993	12.284965
H	12.048824	7.405181	13.981195	C	3.847617	2.016462	13.273368
C	3.615869	1.248982	15.685242	C	4.043425	0.676938	12.915730
C	4.867483	0.943002	16.224051	H	3.908743	-0.096166	13.664166
H	5.720388	1.561420	15.977200	C	4.423627	0.296788	11.628928
C	4.982785	-0.145186	17.080691				
H	5.944578	-0.404280	17.513604				

H	4.567807	-0.754724	11.395373	O	7.731140	6.812543	16.695528
C	4.623394	1.275783	10.660890	O	4.502651	4.790444	19.550572
H	4.926036	1.008621	9.651908	O	3.657650	3.526382	17.850984
C	4.421630	2.612343	10.997837	O	4.107795	7.910722	19.634938
H	4.558997	3.380445	10.241038	O	2.921442	8.956642	18.001837
C	1.027081	7.009904	12.555037	O	6.462891	7.658171	14.294848
C	0.465552	8.017348	13.381844	O	4.493185	3.300680	15.177391
C	-0.868195	8.388092	13.167719	O	1.694053	7.542017	15.364468
H	-1.311014	9.153571	13.793905				
C	-1.662622	7.797212	12.185841				
H	-2.693797	8.116487	12.060010				
C	-1.123029	6.795575	11.385832				
H	-1.719363	6.312965	10.616075				
C	0.203988	6.420907	11.577694				
H	0.637522	5.652588	10.942895				
C	7.505646	7.324680	13.429842				
C	3.541280	2.381648	14.746033				
C	1.237245	8.604474	14.588661				
C	7.719840	5.816011	13.447259				
C	8.443410	5.092425	12.502609				
H	8.895524	5.605717	11.662097				
C	8.548652	3.712306	12.651535				
H	9.093540	3.123052	11.919869				
C	7.943104	3.097002	13.747700				
H	7.997703	2.023335	13.892587				
C	7.248193	3.881977	14.657880				
H	6.735109	3.482194	15.522161				
C	2.149260	2.986468	14.870713				
C	0.991150	2.458169	14.304681				
H	1.045257	1.545769	13.723294				
C	-0.211154	3.137477	14.478924				
H	-1.124382	2.756908	14.030983				
C	-0.224804	4.315800	15.225638				
H	-1.139757	4.879795	15.371793				
C	0.963402	4.776094	15.776843				
H	1.040454	5.690875	16.348636				
C	2.417899	9.472548	14.163364				
C	2.395289	10.440354	13.162565				
H	1.486308	10.607447	12.597215				
C	3.559013	11.156528	12.894575				
H	3.571215	11.904322	12.107157				
C	4.709722	10.895033	13.639641				
H	5.636694	11.424567	13.447875				
C	4.659026	9.925133	14.630597				
H	5.509387	9.640711	15.237230				
C	8.803735	8.002488	13.938488				
C	8.699714	9.155231	14.720044				
H	7.716526	9.532978	14.967546				
C	9.860760	9.766490	15.177892				
H	9.806438	10.664869	15.786525				
C	11.095478	9.201464	14.853184				
H	12.027501	9.638274	15.198149				
C	11.104326	8.050311	14.073036				
H	12.042884	7.573728	13.796802				
C	3.615432	1.131714	15.660990				
C	4.798840	0.879002	16.358637				
H	5.625071	1.570209	16.255170				
C	4.870196	-0.237810	17.183429				
H	5.780186	-0.456884	17.735183				
C	3.752154	-1.065435	17.299703				
H	3.758947	-1.941668	17.940500				
C	2.614534	-0.735477	16.570610				
H	1.718509	-1.350184	16.631044				
C	0.326893	9.505916	15.466310				
C	-0.129684	9.020921	16.692296				
H	0.168988	8.029380	17.005698				
C	-0.930175	9.839880	17.483465				
H	-1.299192	9.486190	18.442282				
C	-1.241863	11.121936	17.032827				
H	-1.855448	11.797203	17.621064				
C	-0.735609	11.525166	15.799878				
H	-0.948970	12.518729	15.410340				
N	7.139033	5.210490	14.497252				
N	2.122295	4.122137	15.589839				
N	3.533326	9.233699	14.882116				
N	9.985913	7.458227	13.614414				
N	2.539970	0.335969	15.760009				
N	0.031627	10.740424	15.024557				
O	6.960446	6.830345	18.842775				

Mn(IV)₃GdO₄

158			
Gd	-5.693369	8.142569	16.245748
Mn	-5.883704	9.072510	13.150897
Mn	-8.012974	7.456181	14.075659
Mn	-5.509683	6.308461	13.504212
O	-6.762160	7.459709	12.635918
O	-7.087003	9.024512	14.560570
O	-4.732829	7.892506	14.045888
O	-6.741449	6.418304	14.915676
C	-6.373868	6.387483	9.659164
C	-7.467816	5.648865	10.117165
H	-7.397791	4.569890	10.190341
C	-8.693951	6.264588	10.397696
C	-8.814954	7.643602	10.204970
H	-9.776087	8.126114	10.341487
C	-7.734376	8.408824	9.746975
C	-6.523269	7.767295	9.473110
H	-5.701986	8.327637	9.041868
O	-4.515056	6.104715	11.948617
C	-4.353757	4.810265	11.412922
C	-4.246481	4.925479	9.878918
C	-3.191847	4.292387	9.209472
H	-2.498944	3.673557	9.768731
C	-2.991615	4.444768	7.838326
H	-2.161950	3.937637	7.354161
C	-3.851244	5.260382	7.108246
H	-3.706117	5.406309	6.041530
C	-4.916213	5.879655	7.757664
H	-5.608614	6.494004	7.188168
C	-5.150615	5.715379	9.132909
C	-5.534706	3.961424	11.849607
C	-5.882929	2.727970	11.310563
H	-5.315987	2.325067	10.479852
C	-6.969031	2.043749	11.848046
H	-7.269273	1.085564	11.436302
C	-7.658771	2.597014	12.927391
H	-8.500124	2.084282	13.379866
C	-7.254228	3.828006	13.421618
H	-7.732677	4.322051	14.255415
N	-6.227663	4.497492	12.871467
C	-3.055847	4.203377	11.999855
C	-1.971171	5.045859	12.253903
H	-2.056958	6.105567	12.052165
C	-0.803918	4.500136	12.773110
H	0.053955	5.133120	12.980034
C	-0.755136	3.128318	13.027504
H	0.132655	2.660498	13.440820
C	-1.880708	2.366132	12.736163
H	-1.887588	1.292916	12.914171
N	-3.013980	2.885381	12.227281
O	-8.982924	6.055168	13.342713
C	-10.343755	6.261981	13.034853
C	-10.702741	5.409435	11.799444
C	-11.829500	4.578291	11.835172
H	-12.470730	4.583534	12.709396
C	-12.150982	3.726070	10.779979
H	-13.033578	3.096180	10.844542
C	-11.325905	3.683091	9.660068
H	-11.548447	3.017129	8.831086
C	-10.212046	4.516997	9.604151
H	-9.578027	4.507576	8.721546
C	-9.886099	5.401482	10.645948
C	-10.556829	7.742565	12.776761
C	-11.685352	8.300699	12.185521
H	-12.489219	7.657192	11.849203
C	-11.744751	9.681247	12.022490
H	-12.608484	10.139894	11.552200
C	-10.682568	10.467555	12.470384

H	-10.696186	11.546227	12.359378	O	-4.996385	8.195087	18.520356
C	-9.592040	9.846388	13.059388	C	-5.164002	7.407049	19.480796
H	-8.723434	10.380419	13.417227	H	-4.548018	6.505531	19.593331
N	-9.533621	8.511080	13.193291	N	-6.069805	7.577316	20.438115
C	-11.192801	5.823177	14.250873	C	-6.978531	8.722618	20.423188
C	-10.763340	4.738987	15.019755	H	-6.938540	9.187726	19.439143
H	-9.830741	4.246879	14.776986	H	-6.683763	9.441003	21.196495
C	-11.547358	4.319681	16.087275	H	-7.992463	8.373988	20.635543
H	-11.237478	3.477626	16.699126	C	-6.170137	6.643556	21.555772
C	-12.735881	4.999309	16.359439	H	-5.426943	5.853690	21.434250
H	-13.376665	4.710078	17.186072	H	-7.170683	6.200629	21.579978
C	-13.082759	6.069256	15.541957	H	-5.989744	7.169740	22.498417
H	-13.997851	6.630210	15.717849	Mn(III)Mn(IV)₂GdO₄			
N	-12.332621	6.478388	14.501369	158			
O	-6.948171	10.105205	12.036912	Gd	-5.692085	8.240582	16.171728
C	-6.326618	10.864496	11.023351	Mn	-5.723612	9.135551	13.057961
C	-7.293773	10.960782	9.826947	Mn	-8.028369	7.662773	14.084507
C	-7.569223	12.211132	9.260086	Mn	-5.424060	6.427014	13.472780
H	-7.046541	13.089084	9.623676	O	-6.470552	7.562150	12.471778
C	-8.512875	12.368572	8.246150	O	-6.939130	9.190692	14.442629
H	-8.699858	13.354542	7.830603	O	-4.594472	7.984451	14.026576
C	-9.217251	11.258332	7.789708	O	-6.672196	6.559927	14.840296
H	-9.968751	11.359070	7.011679	C	-6.357255	6.346047	9.701403
C	-8.937714	10.005516	8.330014	C	-7.475682	5.667634	10.194757
H	-9.462517	9.130404	7.955948	H	-7.449463	4.589390	10.303447
C	-7.969864	9.822267	9.331349	C	-8.672676	6.343003	10.476697
C	-5.015035	10.192303	10.659282	C	-8.736558	7.719929	10.245339
C	-4.251183	10.475227	9.532796	H	-9.673811	8.247137	10.383951
H	-4.607490	11.199311	8.809911	C	-7.636369	8.424223	9.738988
C	-3.044973	9.804352	9.354175	C	-6.457062	7.725186	9.470820
H	-2.436856	9.997961	8.476422	H	-5.618087	8.238677	9.015249
C	-2.622506	8.890167	10.319658	O	-4.340240	6.082427	11.959130
H	-1.682294	8.359708	10.219398	C	-4.277708	4.783981	11.448789
C	-3.428669	8.660233	11.424483	C	-4.216306	4.867805	9.905838
H	-3.172152	7.971148	12.216530	C	-3.168539	4.243806	9.217748
N	-4.608095	9.287347	11.569431	H	-2.446627	3.653892	9.771823
C	-6.029821	12.271441	11.596947	C	-3.008127	4.366609	7.837943
C	-6.937838	12.836789	12.495436	H	-2.179211	3.868018	7.342971
H	-7.826878	12.284945	12.771775	C	-3.910214	5.139137	7.113322
C	-6.673178	14.096594	13.016185	H	-3.803403	5.258714	6.038568
H	-7.362503	14.560994	13.715058	C	-4.965938	5.754766	7.781968
C	-5.505978	14.755760	12.625724	H	-5.685182	6.343477	7.218403
H	-5.253850	15.737350	13.013727	C	-5.155713	5.630344	9.169196
C	-4.666459	14.121416	11.716845	C	-5.504095	4.004235	11.898813
H	-3.749387	14.599402	11.379912	C	-5.902361	2.770744	11.390305
N	-4.918167	12.902658	11.203349	H	-5.328109	2.304945	10.598711
O	-4.268217	5.202100	14.510490	C	-7.049888	2.172539	11.902657
C	-3.863404	5.371012	15.716323	H	-7.390020	1.218067	11.512437
C	-2.842036	4.371173	16.203375	C	-7.755723	2.813508	12.921180
H	-1.847210	4.825639	16.129703	H	-8.654082	2.376818	13.343849
H	-2.854056	3.465810	15.596132	C	-7.296554	4.036867	13.389324
H	-3.022806	4.129890	17.253486	H	-7.789073	4.603781	14.167301
O	-4.233295	6.296004	16.484607	N	-6.201871	4.616741	12.870985
O	-9.175387	7.529102	15.640374	C	-3.011376	4.094407	12.017179
C	-8.850762	7.415952	16.880623	H	-1.918155	4.887611	12.375003
C	-10.000306	7.282750	17.849901	C	-1.986798	5.961803	12.262794
H	-9.990631	8.139063	18.532500	C	-0.780225	4.276486	12.886542
H	-9.864198	6.380223	18.453465	H	0.082673	4.871676	13.172011
H	-10.957843	7.239336	17.332465	C	-0.767645	2.888366	13.035864
O	-7.676891	7.427391	17.325561	H	0.095229	2.369349	13.441313
O	-4.967414	10.650621	13.827673	C	-1.899296	2.178149	12.651314
C	-4.247463	10.776200	14.888486	H	-1.935152	1.094928	12.748485
C	-3.388350	12.016117	14.927278	N	-3.002462	2.760568	12.144857
H	-3.059148	12.228625	15.945419	O	-9.089505	6.259674	13.424214
H	-3.934136	12.868320	14.516181	C	-10.418074	6.529418	13.077620
H	-2.506382	11.853871	14.296345	C	-10.783422	5.665891	11.847722
O	-4.222854	9.962679	15.844125	C	-11.959531	4.905558	11.863160
O	-6.751834	10.169003	17.207789	H	-12.640049	4.998412	12.702791
C	-7.486591	11.001666	16.636661	C	-12.280849	4.012853	10.841372
H	-7.776540	10.862761	15.588199	H	-13.202502	3.439688	10.892855
N	-7.975076	12.100381	17.217176	C	-11.403035	3.856674	9.772819
C	-8.844868	13.011461	16.481695	H	-11.621598	3.157126	8.970550
H	-8.990955	12.632637	15.468505	C	-10.241438	4.623994	9.731443
H	-8.393885	14.007736	16.437467	H	-9.568968	4.530957	8.882582
H	-9.818405	13.083181	16.976448	C	-9.911406	5.548291	10.738063
C	-7.678286	12.430209	18.607746	C	-10.571838	8.015929	12.785635
H	-6.971666	11.698879	18.998047	C	-11.649207	8.605919	12.130793
H	-8.598809	12.410134	19.200719				
H	-7.242292	13.432333	18.661601				

H	-12.472738	7.990508	11.788216	C	-8.937301	11.475889	18.809479
C	-11.630859	9.979561	11.906397	H	-7.967126	11.140925	19.174164
H	-12.453918	10.597774	11.386224	H	-9.732769	10.912482	19.311257
C	-10.537652	10.728794	12.344627	H	-9.067589	12.540249	19.029429
H	-10.482033	11.797826	12.169948	O	-4.756649	8.491786	18.413646
C	-9.503699	10.078966	13.001803	C	-4.771990	7.636732	19.324184
H	-8.604597	10.576728	13.342407	H	-4.082962	6.780951	19.318591
N	-9.529880	8.752279	13.219660	N	-5.595456	7.669907	20.371964
C	-11.312398	6.159674	14.284978	C	-6.607346	8.716283	20.489186
C	-10.916173	5.104874	15.111587	H	-6.711434	9.201405	19.518948
H	-9.986512	4.591039	14.903348	H	-6.312187	9.445493	21.253075
C	-11.720928	4.753895	16.187687	H	-7.555729	8.260902	20.786094
H	-11.437757	3.935022	16.842913	C	-5.517311	6.669033	21.428777
C	-12.892497	5.477536	16.419197	H	-4.714926	5.964843	21.200154
H	-13.546026	5.245548	17.254327	H	-6.465631	6.126456	21.502123
C	-13.203295	6.517634	15.550988	H	-5.309102	7.151459	22.389456
H	-14.103071	7.112169	15.695748				
N	-12.438171	6.855249	14.495569				
O	-6.780372	10.194034	11.922260				
C	-6.149909	10.897104	10.888240				
C	-7.125759	10.969113	9.693808				
C	-7.389173	12.198914	9.078226				
H	-6.843918	13.080925	9.396045				
C	-8.348472	12.333505	8.075045				
H	-8.525523	13.305494	7.622826				
C	-9.080312	11.218796	7.676377				
H	-9.843170	11.300741	6.906901				
C	-8.814599	9.985325	8.266553				
H	-9.363353	9.105420	7.940756				
C	-7.835288	9.824684	9.261239				
C	-4.852757	10.189085	10.522439				
C	-4.117474	10.403710	9.360389				
H	-4.476348	11.107952	8.619101				
C	-2.938564	9.688112	9.170042				
H	-2.354288	9.827309	8.265550				
C	-2.517216	8.793679	10.154254				
H	-1.603884	8.219986	10.040471				
C	-3.294749	8.635008	11.293233				
H	-3.043694	7.954140	12.094799				
N	-4.441203	9.313414	11.456663				
C	-5.813244	12.322052	11.394723				
C	-6.633095	12.902553	12.365593				
H	-7.465532	12.335452	12.760393				
C	-6.342437	14.183904	12.815466				
H	-6.964301	14.657036	13.570254				
C	-5.232515	14.848686	12.289290				
H	-4.960941	15.846745	12.618492				
C	-4.472638	14.194452	11.326370				
H	-3.598736	14.672811	10.888894				
N	-4.753409	12.956588	10.876562				
O	-4.224910	5.266502	14.569277				
C	-3.825947	5.467647	15.764175				
C	-2.818962	4.470307	16.302172				
H	-1.836017	4.952530	16.356721				
H	-2.742933	3.594790	15.656053				
H	-3.094047	4.167943	17.316821				
O	-4.182331	6.419273	16.512297				
O	-9.043442	7.883525	16.096401				
C	-8.635167	7.422021	17.203807				
C	-9.674586	7.054985	18.249816				
H	-9.570358	7.723790	19.111897				
H	-9.505631	6.034806	18.610064				
H	-10.684551	7.140510	17.847532				
O	-7.412465	7.268572	17.523321				
O	-4.748502	10.744655	13.703486				
C	-4.223985	10.937017	14.854513				
C	-3.388097	12.194956	14.982307				
H	-3.420442	12.577680	16.005042				
H	-3.726715	12.959374	14.280226				
H	-2.345142	11.952210	14.744322				
O	-4.334067	10.176376	15.851043				
O	-7.016887	10.111372	17.249629				
C	-8.042392	10.580276	16.716587				
H	-8.215340	10.461839	15.641808				
N	-8.996307	11.258427	17.370023				
C	-10.185939	11.723798	16.668570				
H	-10.101659	11.470840	15.610209				
H	-10.288392	12.809257	16.772105				
H	-11.081148	11.242807	17.078218				

Mn(IV)₃YO₄

158			
Y	6.139165	9.405074	15.564380
Mn	4.296725	6.755905	16.081570
Mn	7.011875	6.559945	16.766958
Mn	6.235132	6.590470	14.048746
O	5.784165	5.638931	15.641101
O	5.575529	7.670435	17.100543
O	4.813530	7.689246	14.579050
O	7.395788	7.494133	15.179745
O	2.886995	8.017840	16.518576
O	8.211433	7.647963	17.859283
O	6.678562	7.722403	12.531674
O	3.976905	9.962603	16.160929
O	7.376244	9.718267	17.523628
O	6.061211	9.768634	13.263615
C	8.114220	8.900599	18.130733
C	8.970007	9.387899	19.274259
H	9.307799	10.410203	19.089578
H	9.820519	8.726066	19.440400
H	8.359741	9.395268	20.184324
C	2.952327	9.298644	16.462426
C	6.583373	9.457659	10.941609
H	6.444672	10.537472	10.879318
H	5.852302	8.955202	10.299629
H	7.577352	9.186633	10.574393
C	6.417362	8.973368	12.361328
C	1.664546	10.025703	16.764781
H	0.989969	9.404725	17.355104
H	1.170450	10.265100	15.815855
H	1.873596	10.964924	17.281506
O	3.099726	5.613810	15.237059
O	6.737925	5.375956	18.172135
O	7.437400	5.286214	13.497390
N	3.584030	5.740975	17.711097
N	5.058560	5.598088	12.706655
N	8.650555	5.366491	16.528659
C	6.497525	2.714568	14.601248
C	6.043355	2.766084	16.993989
C	4.200988	2.881509	15.403000
C	6.944575	2.694031	15.927993
H	8.000751	2.545186	16.123010
C	6.481655	2.487672	18.392164
C	2.387262	1.535474	14.454338
H	3.173793	0.829162	14.202032
C	5.124843	2.805363	14.353820
H	4.755855	2.741847	13.336728
C	4.673528	2.856048	16.717937
H	3.971882	2.831742	17.543733
C	2.748585	2.730840	15.097488
C	7.751358	2.818645	20.427638
H	8.439083	3.408389	21.023437
C	7.725876	3.184999	12.373891
C	8.547729	2.670760	11.363149
H	8.751174	3.271129	10.482926
C	1.061879	1.223537	14.161398
H	0.820309	0.286081	13.668386
C	7.361221	3.278950	19.163470
C	7.448413	2.381403	13.502176
C	5.982998	1.300872	18.954659
H	5.298911	0.699239	18.362069

C	1.729744	3.656077	15.417166	H	11.910562	7.809972	15.534860
C	8.072474	1.126584	13.597959	C	5.484157	14.412997	16.398363
H	7.865626	0.514500	14.471865	C	4.751662	13.628544	16.212794
C	0.057507	2.117546	14.520990	H	5.376800	15.207474	15.653105
H	-0.985471	1.892382	14.317420	H	5.332955	14.837272	17.395524
C	7.269373	1.622807	20.957328	C	10.202818	8.531181	13.436543
H	7.595099	1.298110	21.941379	H	9.144647	8.296803	13.326867
C	8.910713	0.638783	12.598339	H	10.804521	7.626020	13.343408
H	9.370737	-0.339666	12.704317	H	10.514081	9.239302	12.660684
C	0.399759	3.321453	15.134904	C	7.954594	14.714662	16.590904
H	-0.391579	4.018723	15.387149	H	8.883261	14.148951	16.496287
C	6.361525	0.865926	20.222198	H	7.874891	15.113905	17.606637
H	5.959889	-0.061202	20.621349	H	7.964106	15.545729	15.878876
C	9.131823	1.408722	11.459834	O	6.088905	11.756297	15.725848
H	9.764066	1.042864	10.655909	O	8.379728	10.087386	14.862866
C	7.203415	4.630322	12.267095	N	7.379417	5.621184	9.993510
C	7.846428	4.658088	18.669992	N	9.779997	5.441245	20.015076
C	2.060315	5.043457	16.000519	N	0.032897	6.090451	16.979304
C	3.750862	5.826235	12.497647	N	10.431024	9.091555	14.767419
H	3.311567	6.593058	13.119991	N	6.822825	13.835416	16.314128
C	2.515527	4.966506	17.447268	Mn(III)Mn(IV)₂YO₄ 158			
C	5.718333	4.690528	11.964490				
C	9.969012	3.673776	17.566964	Y	6.122362	9.370929	15.461768
H	10.121679	3.003467	18.404283	Mn	4.309194	6.761978	16.051080
C	10.602625	4.570022	15.426453	Mn	6.959490	6.598861	16.781601
H	11.264019	4.608083	14.567860	Mn	6.258741	6.611225	13.896164
C	9.495843	5.402926	15.484741	O	5.727985	5.609575	15.848463
H	9.233578	6.106632	14.707559	O	5.533299	7.740491	17.083054
C	10.839910	3.688142	16.481846	O	4.812046	7.658383	14.525928
H	11.695747	3.021321	16.459206	O	7.386039	7.476907	15.196111
C	8.874595	4.531900	17.559841	O	2.846584	8.058279	16.424752
C	1.901763	4.219404	18.446394	O	8.209880	7.738520	17.860683
H	1.050333	3.594526	18.204543	O	6.732795	8.088008	12.287704
C	4.061542	5.837281	18.963253	O	3.952233	9.992946	16.050277
H	4.904781	6.502531	19.086091	O	7.386804	9.795505	17.426940
C	5.064480	3.938102	10.995752	O	5.912028	9.964188	13.232296
H	5.617589	3.205234	10.419974	C	8.120482	8.995140	18.068816
C	3.702472	4.139502	10.796259	C	8.976129	9.544705	19.192270
H	3.166496	3.556586	10.054132	H	9.348098	10.541031	18.938815
C	2.410611	4.283827	19.740015	H	9.806411	8.875032	19.420694
H	1.957688	3.700288	20.535108	H	8.356694	9.639904	20.091454
C	3.500637	5.113609	20.004851	C	2.918435	9.330138	16.333120
H	3.912662	5.198668	21.004174	C	6.349855	9.984056	10.888836
C	3.037788	5.106879	11.550864	H	5.401515	10.500087	10.707223
H	1.980341	5.301070	11.410631	H	6.548245	9.276308	10.081532
C	8.452411	5.453000	19.849569	H	7.139612	10.744856	10.892878
C	7.589744	6.117353	20.724991	C	6.325293	9.284355	12.238768
H	6.522925	6.096595	20.543182	C	1.624892	10.082200	16.573888
C	9.348649	6.797954	9.257858	H	0.868998	9.437718	17.024334
H	9.852517	7.353089	8.473167	H	1.244690	10.449185	15.613416
C	0.580983	6.650721	14.711738	H	1.808407	10.952815	17.209870
H	1.256783	6.522380	13.876284	O	3.097632	5.604201	15.195927
C	7.973864	5.402192	11.170690	O	6.738233	5.481663	18.293389
C	0.828075	5.975714	15.909413	O	7.492135	5.293252	13.353604
C	8.126685	6.791423	21.814398	N	3.533882	5.789924	17.696572
H	7.478158	7.311446	22.513319	N	5.094250	5.595913	12.551796
C	-0.527044	7.484004	14.626436	N	8.606128	5.389642	16.580572
H	-0.741526	8.020909	13.707043	C	6.550503	2.767774	14.640555
C	10.292193	6.105743	21.068555	C	6.095194	2.833867	17.036444
H	11.375278	6.079918	21.165722	C	4.251583	2.918905	15.442262
C	9.271822	5.835490	11.452038	C	6.996261	2.755986	15.970107
H	9.710495	5.610356	12.415875	H	8.053646	2.614607	16.165553
C	9.511448	6.789820	21.993040	C	6.519561	2.567602	18.445404
H	9.975027	7.307491	22.826600	C	2.477312	1.506298	14.518966
C	-1.355070	7.621712	15.742013	H	3.283623	0.811421	14.298371
H	-2.226481	8.268336	15.723752	C	5.177248	2.852545	14.394085
C	9.970151	6.541972	10.481908	H	4.808482	2.784774	13.377056
H	10.982609	6.886693	10.670259	C	4.723725	2.908490	16.757078
C	8.060927	6.313024	9.061021	H	4.021905	2.891224	17.583431
H	7.542876	6.478985	8.118909	C	2.803532	2.727939	15.131410
C	-1.035690	6.904748	16.889348	C	7.702050	2.927150	20.529452
H	-1.653646	6.978208	17.781577	H	8.354398	3.533440	21.148651
C	9.486947	9.808533	15.369527	C	7.730842	3.129190	12.353192
H	9.768456	10.159279	16.372125	C	8.519820	2.547149	11.352582
C	7.012343	12.558915	15.991584	H	8.690906	3.091753	10.429431
H	8.061111	12.244229	15.964573	C	1.164074	1.156221	14.212570
C	11.733960	8.880455	15.390464	H	0.951442	0.199881	13.742492
H	11.757805	9.384641	16.358242				
H	12.524206	9.290369	14.754165				

C	7.358489	3.376280	19.248190	H	8.092825	12.067216	16.125245
C	7.489727	2.397365	13.540476	C	11.628038	8.629854	15.231654
C	6.026150	1.371900	18.994983	H	11.693854	9.132044	16.198917
H	5.376192	0.755545	18.379198	H	12.451863	8.971940	14.596580
C	1.759028	3.637815	15.410912	H	11.719164	7.548792	15.379444
C	8.127967	1.154372	13.694718	C	5.662252	14.330422	16.834379
H	7.949543	0.597110	14.610796	H	4.885802	13.638402	16.509571
C	0.135003	2.038764	14.528098	H	5.630468	15.238291	16.222587
H	-0.899433	1.786237	14.311777	H	5.502840	14.603844	17.882454
C	7.219644	1.726053	21.048386	C	10.075242	8.397690	13.281440
H	7.508485	1.413756	22.048223	H	8.998439	8.298085	13.147141
C	8.940217	0.605097	12.705326	H	10.555112	7.420365	13.214698
H	9.410928	-0.361553	12.862806	H	10.495606	9.045390	12.502737
C	0.441942	3.265884	15.115345	C	8.136560	14.404334	17.145175
H	-0.367722	3.953438	15.335137	H	9.024305	13.788775	16.986296
C	6.360870	0.947021	20.278902	H	8.045529	14.638490	18.211072
H	5.961646	0.012677	20.664140	H	8.243679	15.338787	16.584424
C	9.117220	1.297179	11.510566	O	6.106411	11.778380	15.744493
H	9.724519	0.881496	10.711237	O	8.378322	10.097143	14.722099
C	7.229116	4.577519	12.173953	N	7.383232	5.545848	9.880683
C	7.841818	4.763386	18.764327	N	9.798732	5.493826	20.122821
C	2.060984	5.048502	15.957457	N	-0.034876	6.042093	16.860144
C	3.775251	5.784318	12.373781	N	10.349157	8.945576	14.608003
H	3.344115	6.572080	12.978295	N	6.958249	13.675967	16.690573
C	2.482753	4.999899	17.419425	Mn(IV)₃ScO₄			
C	5.740749	4.635141	11.865242				
C	9.955805	3.750893	17.666039	146			
H	10.132492	3.125076	18.532655	Sc	4.480277	3.370488	8.812989
C	10.518613	4.523708	15.459965	Mn	6.000230	1.935051	6.584101
H	11.147674	4.507221	14.576329	Mn	6.703086	1.323618	9.243715
C	9.415183	5.363991	15.508840	Mn	7.427619	3.807061	8.129952
H	9.123969	6.021183	14.701351	O	7.567455	1.962922	7.669180
C	10.793367	3.704147	16.555612	O	5.159055	1.410458	8.156275
H	11.648439	3.035183	16.542475	O	5.852685	3.727773	7.152632
C	8.859125	4.608520	17.644348	O	6.487030	3.131649	9.620459
C	1.865805	4.243404	18.411664	O	4.328514	2.011097	5.602799
H	1.025826	3.606683	18.159605	O	5.695137	0.779590	10.808120
C	4.003785	5.880225	18.950490	O	3.116927	3.090844	7.166897
H	4.850261	6.541353	19.077864	O	4.013819	2.265381	10.595726
C	5.068892	3.815543	10.963809	O	7.115404	5.653071	8.647866
H	5.611310	3.044734	10.427488	O	4.919769	5.455707	9.112957
C	3.700691	3.994604	10.783054	O	6.380798	0.246075	5.944621
H	3.151855	3.359457	10.094384	O	8.311631	1.089394	10.117826
C	2.359603	4.311157	19.711311	O	8.539290	4.316256	6.747111
H	1.904913	3.720818	20.501044	O	2.563344	4.200901	9.530609
C	3.441966	5.147521	19.986923	C	5.978547	6.132946	8.985040
H	3.850347	5.226628	20.988616	C	3.244257	2.530971	6.043284
C	3.042922	4.998084	11.496733	C	4.600240	1.322625	11.193245
H	1.976991	5.162252	11.381849	C	2.044647	2.425099	5.138325
C	8.474120	5.552812	19.934954	H	1.405912	1.612229	5.502938
H	7.630382	6.288339	20.772563	H	2.343233	2.200635	4.114161
C	6.567915	6.308350	20.565843	H	1.463221	3.349229	5.175017
C	9.378150	6.650583	9.099837	C	5.925521	7.619635	9.218395
H	9.881070	7.195287	8.306828	H	6.925698	8.034325	9.343281
C	0.606178	6.642679	14.627948	H	5.306811	7.841378	10.091151
H	1.331890	6.541909	13.831671	H	5.455787	8.090799	8.347172
C	8.001447	5.287457	11.038590	C	3.988057	0.763101	12.450899
C	0.812376	5.954797	15.826526	H	3.721546	1.581493	13.125414
C	8.180117	6.983614	21.841426	H	4.670255	0.073923	12.948212
H	7.545138	7.558605	22.509550	H	3.064506	0.234103	12.191093
C	-0.514041	7.453087	14.499692	N	6.936715	-0.680341	8.969490
H	-0.696757	7.998538	13.578071	N	9.163764	4.038589	9.171476
C	10.324551	6.183570	21.153598	N	6.817787	2.440402	4.788047
H	11.405042	6.120327	21.265773	C	6.547951	0.072334	4.551347
C	9.325221	5.666058	11.283857	C	9.719685	1.194490	5.443038
H	9.775141	5.418674	12.237426	H	9.544273	1.448559	4.404163
C	9.562216	6.937198	22.038003	C	10.742508	1.727146	7.557572
H	10.036854	7.473092	22.853961	H	11.356624	2.378100	8.168917
C	-1.395842	7.561436	15.577353	C	10.361132	0.481370	8.071388
H	-2.278474	8.191218	15.526387	C	9.325708	-0.054622	5.930511
C	10.024742	6.352804	10.302398	C	8.789109	-1.109650	5.022087
H	11.055294	6.655212	10.465689	C	8.652781	-0.205760	10.571850
C	8.066473	6.223514	8.937419	C	10.185179	-0.354687	10.517085
H	7.527891	6.424836	8.013384	C	11.922636	3.064303	4.566845
C	-1.113245	6.838646	16.730370	H	12.092174	2.034108	4.265352
H	-1.772063	6.891555	17.594804	C	10.424818	2.098007	6.248120
C	9.458415	9.724735	15.219360	C	12.327666	-0.009850	9.446692
H	9.770534	10.038976	16.226351	H	12.895467	0.300382	8.573597
C	7.067824	12.450727	16.166910				

C	10.795713	4.649700	6.006067	C	3.669540	-0.150990	2.209110
C	11.026099	3.309978	5.619819	H	3.461157	0.240938	1.216100
C	10.925387	0.037397	9.379025	N	7.691232	-1.546285	12.423475
C	9.730148	5.012603	7.057584	N	4.873318	0.161197	2.724362
C	9.657256	-0.400272	7.246586	N	10.039709	7.327158	7.894387
H	9.423965	-1.398492	7.598371	C	2.020701	5.277815	9.184885
C	9.612125	-2.234844	4.850804	H	2.591718	6.069465	8.688281
H	10.550452	-2.273716	5.397587	C	0.186005	6.852835	8.991195
C	11.511267	5.670653	5.368694	H	-0.640944	6.698512	8.291437
H	11.351981	6.701246	5.666053	H	0.964470	7.444521	8.506982
C	7.244711	-2.105169	3.442240	H	-0.184442	7.388812	9.870559
H	6.311952	-2.072846	2.890165	C	-0.161845	4.618157	10.046546
C	8.087955	-3.200809	3.264542	H	-1.008072	4.405913	9.386196
H	7.807970	-3.991459	2.574477	H	-0.537844	5.052631	10.978156
C	7.563490	-1.061932	4.319937	H	0.383392	3.699905	10.259559
C	12.419273	5.404453	4.345105	N	0.739686	5.562830	9.392376
H	12.956975	6.222210	3.874084	Mn(III)Mn(IV)₂ScO₄			
C	9.274624	-3.274650	3.988007				
H	9.940245	-4.125955	3.876976	146			
C	12.999659	-0.465877	10.577986	Sc	4.541321	3.368474	8.846810
H	14.085523	-0.494049	10.590355	Mn	5.991598	1.897873	6.642553
C	12.613372	4.090927	3.927811	Mn	6.710707	1.299896	9.245060
H	13.304030	3.861149	3.121417	Mn	7.483764	3.914082	8.220308
C	10.872677	-0.829369	11.640898	O	7.515975	1.735471	7.653180
H	10.314441	-1.144943	12.515299	O	5.124377	1.385419	8.211887
C	12.264419	-0.896445	11.678515	O	5.877400	3.681870	7.187131
H	12.763053	-1.270942	12.567805	O	6.523680	3.102910	9.653037
C	7.009667	1.393145	3.963467	O	4.287289	2.055409	5.625640
C	7.938878	-1.215901	9.692677	O	5.710765	0.768508	10.869340
C	10.147297	4.628712	8.465474	O	3.108616	3.141129	7.211581
C	7.543959	1.566111	2.692171	O	4.075606	2.312903	10.700550
H	7.699213	0.705230	2.053076	O	6.966132	5.978584	8.881179
C	9.355191	3.706666	10.459802	O	4.785802	5.465625	9.109169
H	8.503585	3.264257	10.956901	O	6.255878	0.183548	5.921082
C	7.651395	3.928931	3.130202	O	8.338638	1.065340	10.130488
H	7.889560	4.943688	2.832290	O	8.600476	4.437684	6.806420
C	6.161921	-1.460684	8.196680	O	2.488223	4.097370	9.609592
H	5.364475	-0.951551	7.674361	O	5.760919	6.295724	9.033727
C	10.575845	3.918027	11.082305	C	3.230637	2.609565	6.070891
H	10.709096	3.628775	12.118530	C	4.671155	1.373437	11.296548
C	7.107276	3.688674	4.382585	C	2.027062	2.599780	5.155099
H	6.895294	4.470300	5.098188	H	1.284705	1.897445	5.551247
C	6.398232	-2.822343	8.085682	H	2.301407	2.289430	4.146168
H	5.767648	-3.427606	7.444448	H	1.564472	3.590564	5.133262
C	11.392048	4.875696	9.032164	C	5.396726	7.765031	9.134415
H	12.169819	5.340995	8.438620	H	6.289285	8.392229	9.114403
C	11.613027	4.502137	10.354373	H	4.831809	7.951783	10.053514
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C	7.882610	2.850153	2.276047	C	4.139380	0.920638	12.638017
H	8.314135	3.009803	1.293319	H	4.373987	1.686393	13.386472
C	8.223385	-2.574884	9.632947	H	4.595902	-0.020571	12.946224
H	9.042667	-2.978252	10.215819	H	3.051340	0.819766	12.598575
C	7.451061	-3.386105	8.807058	N	6.933146	-0.724756	9.005468
H	7.661799	-4.447957	8.732752	N	9.245756	4.130854	9.243635
C	8.146068	-0.352531	12.026407	N	6.819199	2.404157	4.837718
C	5.170794	-0.292714	3.947101	C	6.459417	0.051358	4.542137
C	9.420851	6.528430	7.017861	C	9.673819	1.215964	5.428673
C	7.259193	-0.617762	14.603360	H	9.495416	1.485227	4.394025
H	6.891181	-0.766984	15.613280	C	10.699444	1.722371	7.547877
C	8.519876	7.009082	6.064919	H	11.312910	2.365552	8.168016
H	8.047957	6.320926	5.375650	C	10.325335	0.467349	8.044056
C	8.196774	0.755757	12.874771	C	9.274416	-0.037614	5.901235
H	8.575999	1.699468	12.504697	C	8.731342	-1.093467	4.991637
C	4.294041	-1.085037	4.691357	C	8.671127	-0.223814	10.578657
H	4.583974	-1.429594	5.675479	C	10.202540	-0.389188	10.490520
C	2.728492	-0.922870	2.881270	C	11.864017	3.051762	4.542867
H	1.769287	-1.140883	2.422966	H	11.976159	2.019756	4.220699
C	8.871765	9.210180	6.950669	C	10.381331	2.111375	6.243971
H	8.678783	10.277976	6.965718	C	12.318766	-0.059110	9.364915
C	7.254171	-1.667070	13.691069	H	12.865212	0.249889	8.477574
H	6.885816	-2.650182	13.975336	C	10.855408	4.662795	6.042667
C	3.055125	-1.404738	4.149973	C	11.007621	3.318255	5.625382
H	2.353386	-2.017255	4.708286	C	10.915365	0.002764	9.334659
C	8.242162	8.369824	6.030802	C	9.814676	5.067538	7.110998
H	7.544594	8.769937	5.300987	C	9.615238	-0.401243	7.211470
C	9.761673	8.643873	7.856342	H	9.375413	-1.401532	7.553838
H	10.278922	9.260373	8.588070	C	9.567472	-2.209504	4.816691
C	7.747626	0.620494	14.182451	H	10.517085	-2.225544	5.345238
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C	11.606097	5.655077	5.399502	H	-0.810639	6.210397	7.965421
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C	7.172408	-2.141582	3.459609	C	-0.332110	7.243529	9.336302
H	6.227644	-2.132961	2.927135	H	-0.232156	4.584644	10.133439
C	8.025698	-3.230532	3.284779	H	-1.089494	4.202635	9.569681
H	7.740671	-4.039795	2.618190	H	-0.598537	5.210715	10.953846
C	7.491312	-1.074442	4.307950	H	0.347607	3.753770	10.533833
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H	13.032764	6.166109	3.870543				
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C	13.018192	-0.523197	10.476555				
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H	13.241368	3.802640	3.068395				
C	10.916880	-0.871067	11.594241				
H	10.378303	-1.184120	12.482139				
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C	7.801712	0.623415	14.192884				
H	7.810930	1.481330	14.859161				
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O	-21.395146	-30.782481	204.076998	H	-27.669364	-37.502082	210.204114
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C	-22.931398	-33.712825	202.308840	H	-22.953590	-45.390862	202.208724
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C	-24.183030	-29.633648	202.973097	H	-24.301770	-40.645848	203.246112
C	-24.763943	-30.182739	201.672726	H	-26.349289	-29.880680	209.643211
C	-25.659004	-31.401555	201.804048	H	-26.066965	-33.032798	207.963722
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O	-26.037812	-31.910726	200.700324	H	-23.649825	-33.538441	201.515068
H	-24.918541	-28.925972	209.193186	H	-22.158900	-34.957540	205.201577
C	-25.289739	-29.704836	209.874338	H	-19.710428	-30.712843	201.273265
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C	-24.472941	-31.007886	209.717235	H	-29.872053	-34.533104	197.431616
C	-24.435384	-31.527752	208.308834	H	-32.788830	-34.311341	197.974079
C	-25.226632	-32.434217	207.633578	H	-32.953123	-31.269176	196.727886
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C	-23.719281	-31.698458	206.181891	H	-30.650385	-28.091405	201.507670
N	-24.764280	-32.512202	206.332813	H	-19.865216	-33.254806	201.116348
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C	-25.333665	-37.110846	209.273415	H	-25.931620	-36.237963	209.574887
C	-26.279470	-38.250186	208.897121	H	-30.072188	-39.225860	205.731185
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C	-24.375132	-36.729952	208.144029	H	-32.109823	-37.824992	205.437171
C	-24.967163	-36.055766	206.907052	H	-32.100488	-38.594108	207.044018
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C	-29.322363	-39.441703	208.231310	H	-23.850497	-37.625184	207.781315
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H	-31.843803	-31.521736	208.767318	H	-33.118284	-34.984005	205.733648
C	-30.252639	-32.111299	207.409157	H	-37.628552	-33.124305	206.165742
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C	-20.112713	-31.328697	202.090235	H	-27.620412	-44.016230	202.514937
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238				H	-22.557559	-28.453986	203.752878
Mn	-25.099398	-35.557453	203.701220	C	-24.168290	-29.657495	202.984147
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Mn	-27.302639	-33.395253	203.193601	C	-25.660349	-31.432101	201.823497
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H	-22.367373	-34.988567	205.172701				
H	-19.713189	-30.742827	201.251272				
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H	-29.890223	-34.499709	197.426939	Mn	-27.332961	-35.229432	205.265724
H	-32.795263	-34.324768	197.998552	Mn	-27.238815	-33.417581	203.188337
H	-32.947712	-31.275677	196.724055	Mn	-27.500863	-33.241040	200.332511
H	-32.272482	-34.518431	195.600753	Sc	-27.934894	-36.334490	202.430944
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H	-19.931780	-33.297913	201.182636	O	-28.393175	-34.734505	203.843039
H	-21.307481	-32.365361	200.597512	O	-25.979169	-34.129231	204.567092
H	-25.947034	-36.251890	209.584843	O	-28.352357	-32.748299	201.954157
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H	-32.181282	-38.643217	207.558016	O	-27.093597	-36.953030	200.581200
H	-31.834835	-36.890651	207.503828	O	-27.580076	-38.564151	202.489329
H	-29.045806	-39.297437	210.371429	H	-30.546698	-26.886750	200.189207
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C	-30.214563	-40.124643	197.603745	C	-29.661193	-37.163627	205.387294
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C	-29.401895	-39.982859	198.738652	O	-28.688962	-36.499592	205.946788
C	-28.886152	-41.125357	199.378316	O	-26.315297	-38.608121	197.149462
O	-28.091184	-40.950263	200.489782	O	-27.507524	-35.989711	197.682919
H	-33.785375	-32.318034	197.913159	O	-26.649220	-29.825593	197.627420
C	-32.844739	-31.791422	197.688620	O			

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O	-24.640473	-31.574412	198.397733	H	-24.963978	-31.799405	210.373878
O	-29.435409	-30.294685	202.570834	H	-23.477092	-30.899528	210.069882
O	-25.798468	-39.623796	199.650542	H	-25.303000	-33.228383	205.610239
O	-26.378367	-39.070988	204.960705	H	-37.548238	-31.526089	205.357493
H	-30.349140	-30.582549	208.992052	H	-35.236918	-31.767669	204.718056
C	-30.997751	-31.051074	208.236197	H	-35.172444	-34.238254	206.544136
H	-31.843803	-31.521736	208.767318	H	-32.934651	-34.721510	205.905341
C	-30.239051	-32.117780	207.441779	H	-37.611328	-33.147293	206.125553
C	-28.925806	-31.585127	206.847696	H	-35.993359	-33.295781	204.272674
C	-28.281566	-32.597698	205.919895	H	-34.235720	-32.760134	206.741519
O	-28.079227	-33.772753	206.395555	H	-32.654582	-32.203294	204.786866
O	-27.999129	-32.202018	204.748693	H	-33.958237	-34.806752	204.455209
H	-36.704300	-31.820528	206.892411	H	-31.118294	-31.659767	203.051295
C	-36.971479	-32.276075	205.926511	H	-31.712828	-35.551838	203.984932
C	-35.703724	-32.674014	205.135417	H	-30.138741	-32.935293	202.451834
C	-34.666904	-33.436128	205.983857	H	-30.913427	-35.098548	202.548814
C	-33.534598	-34.119708	205.202631	H	-23.923017	-30.484176	203.634586
N	-32.659725	-33.172424	204.495821	H	-25.379604	-29.398559	201.174512
C	-31.757237	-33.553575	203.561577	H	-24.910244	-29.027423	203.529459
N	-31.628392	-34.852380	203.255483	H	-23.998696	-30.466635	200.983246
N	-31.052936	-32.656833	202.865942	H	-20.398198	-33.737648	204.054078
O	-27.621410	-29.235188	204.329773	H	-25.932924	-33.338866	198.675079
H	-32.895024	-42.741365	197.136111	H	-29.064335	-31.969009	198.597270
H	-33.263127	-41.009854	197.113473	H	-28.465577	-30.811453	199.517950
H	-33.700323	-42.030393	195.723193	H	-29.304441	-29.843715	201.685304
H	-31.534238	-40.646082	195.322590	H	-28.966920	-31.164353	202.418590
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H	-28.773417	-43.291603	199.349603	H	-32.938301	-35.824937	193.653968
H	-29.154520	-38.997724	199.141860	H	-31.692451	-37.033891	194.115007
H	-30.596721	-39.222401	197.120832	H	-26.584616	-40.143187	199.949837
H	-27.668175	-41.851727	200.794255	H	-25.492646	-39.152334	200.485269
H	-25.376747	-42.602992	199.539187	H	-27.617845	-39.234767	203.558104
H	-27.585168	-44.294834	202.707371	H	-27.787194	-36.788831	199.234606
H	-28.751642	-37.600942	207.625331	H	-26.832367	-36.654872	197.431895
H	-27.704041	-37.459050	210.117221	H	-27.029310	-35.234582	198.158218
H	-21.609958	-29.485327	201.185453	H	-27.252525	-38.848323	197.039709
H	-21.799508	-43.048057	200.802889	H	-26.091030	-38.946956	198.059292
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H	-23.464746	-44.672579	199.259981	H	-25.036084	-31.674600	199.297549
H	-22.406706	-38.836349	201.718382	H	-25.244372	-30.883096	198.012242
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H	-23.239095	-31.606188	205.281393	Y-S ₁ 238			
H	-23.709534	-33.489985	201.439514				
H	-22.371942	-34.936746	205.166305				
H	-19.708254	-30.729337	201.262024				
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H	-32.183480	-34.466888	195.563398	Y	-27.927113	-36.432387	202.421554
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H	-30.217161	-39.193853	205.763656	O	-26.478354	-34.665355	202.121121
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H	-32.315159	-37.853839	205.721030	O	-26.507665	-33.919578	198.906292
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H	-27.858742	-40.306732	209.536504	C	-30.241434	-27.113395	201.222163
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H	-30.013299	-32.983340	208.081163	C	-32.924381	-41.850903	196.489835
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H	-30.875525	-32.496981	206.626794	C	-30.534163	-41.261223	197.114145
H	-29.084023	-30.660909	206.276981	C	-30.097727	-42.320011	197.938270
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C	-29.154994	-39.743366	198.472734	O	-29.414060	-37.331470	204.062030
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C	-22.775853	-42.907282	202.604071	C	-33.770835	-34.380453	204.932018
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N	-23.344034	-34.486729	203.421998	H	-22.212474	-38.957420	201.574473
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C	-22.896307	-28.815019	202.759171	H	-21.990042	-41.301972	203.744000
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H	-28.232023	-26.250644	201.035584	C	-30.174871	-40.135150	197.557729
H	-28.400033	-27.420570	202.353663	C	-29.165410	-42.388336	198.881866
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H	-23.399367	-30.774874	210.054203	C	-28.830333	-41.099121	199.338154
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H	-37.548238	-31.526089	205.357493	H	-33.785375	-32.318034	197.913159
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H	-35.364240	-34.469836	206.328921	C	-31.628739	-32.690198	197.619443
H	-33.205542	-35.099116	205.545581	O	-30.491928	-32.228500	197.405069
H	-37.636975	-33.107562	206.198254	H	-32.670500	-31.019712	198.450242
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H	-34.290574	-34.941188	204.138820	O	-30.548712	-37.078684	196.312733
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H	-23.884607	-30.567548	201.013207	H	-21.516057	-41.187718	202.032943
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238							
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C	-25.002722	-44.401543	200.622751	H	-30.297782	-43.506321	197.539199
C	-25.544549	-43.185399	200.257277	H	-28.795203	-43.167580	199.479276
N	-25.825355	-44.858755	201.640951	H	-28.975844	-38.897411	198.883148
C	-26.801316	-43.943498	201.861625	H	-30.489609	-39.228501	196.944763
N	-26.658542	-42.916689	201.032567	H	-27.504243	-41.687382	200.708265
H	-19.262626	-31.517297	202.779917	H	-25.205619	-42.495438	199.491226
C	-20.112713	-31.328697	202.090235	H	-27.578883	-44.062430	202.607580
C	-21.156351	-30.545820	202.869139	H	-28.786932	-37.532135	207.691772
O	-21.412716	-30.792378	204.065786	H	-27.649401	-37.525877	210.241518
C	-20.715592	-32.637573	201.502148	H	-21.545700	-29.416054	201.211766
C	-21.607756	-33.385962	202.442930	H	-21.712711	-43.076550	200.852668
C	-22.946254	-33.721384	202.377422	H	-22.959262	-45.394397	202.205095
N	-21.176381	-33.875789	203.666288	H	-23.938550	-46.173722	200.030472
C	-22.203046	-34.471291	204.301343	H	-23.420585	-44.675659	199.241655
N	-23.298028	-34.393376	203.540018	H	-22.415465	-38.837187	201.641193
N	-21.826554	-29.607500	202.165479	H	-24.000556	-40.713755	201.496992
C	-22.896307	-28.815019	202.759171	H	-21.982855	-41.304656	203.742185
H	-22.557559	-28.453986	203.752878	H	-22.409824	-38.892728	203.406604
C	-24.186744	-29.630279	202.983021	H	-24.310428	-40.667965	203.238487
C	-24.783589	-30.172304	201.685403	H	-26.350803	-29.860193	209.635915
C	-25.697987	-31.374076	201.824614	H	-26.073915	-33.022025	207.922520
O	-26.021239	-31.831063	202.964489	H	-23.068807	-31.511034	205.309882
O	-26.076763	-31.871168	200.705945	H	-23.662723	-33.561085	201.579408
H	-24.899163	-28.932233	209.196889	H	-22.140382	-34.960577	205.265072
C	-25.289739	-29.704836	209.874338	H	-19.716157	-30.733642	201.256502

H	-23.075293	-27.950415	202.109983	Mn	-24.969458	-35.628138	203.838935
H	-29.890340	-34.510209	197.399232	Mn	-27.337832	-35.267825	205.191991
H	-32.803509	-34.331102	197.960409	Mn	-27.289122	-33.343514	203.197726
H	-32.940311	-31.292656	196.714207	Mn	-27.449302	-33.287727	200.408529
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H	-30.701229	-28.080310	201.466169	O	-26.562548	-36.556570	204.111147
H	-19.893021	-33.283635	201.161564	O	-28.345082	-34.765740	203.745472
H	-21.310935	-32.389429	200.613626	O	-25.990978	-34.132239	204.486144
H	-25.931520	-36.241821	209.587854	O	-28.432485	-32.669632	201.971995
H	-30.065637	-39.244866	205.727714	O	-26.623948	-34.244761	201.733212
C	-31.592150	-37.866731	206.403602	O	-28.404493	-31.579074	199.031073
H	-32.112271	-37.861275	205.436439	O	-26.504190	-33.846650	198.959895
H	-32.078661	-38.602805	207.055055	O	-27.106425	-37.033293	200.982429
H	-31.670114	-36.874711	206.869766	O	-28.355239	-38.769668	202.639029
H	-29.085435	-39.297590	210.340316	H	-30.535913	-26.874230	200.188702
H	-27.858742	-40.306732	209.536504	C	-30.241434	-27.113395	201.222163
H	-23.649250	-35.994765	208.488461	H	-30.724377	-26.361921	201.871645
H	-23.837994	-37.589466	207.771557	C	-28.714076	-27.220319	201.318269
H	-30.117141	-36.801754	198.614592	C	-28.167840	-28.349781	200.423957
H	-31.588594	-36.157397	199.349808	O	-28.901939	-29.405601	200.342581
H	-31.376161	-30.222124	207.622072	O	-27.058121	-28.196706	199.840988
H	-30.075629	-33.006282	207.988415	C	-32.924381	-41.850903	196.489835
H	-28.256740	-31.383247	207.579717	C	-31.524765	-41.499307	195.946661
H	-30.959679	-32.443708	206.569113	C	-30.524457	-41.249506	197.070006
H	-29.116199	-30.684120	206.191943	C	-30.051267	-42.307949	197.873715
H	-28.222314	-26.273988	201.034536	C	-30.059649	-39.953083	197.372369
H	-28.399518	-27.447455	202.347684	C	-29.156651	-42.090606	198.932260
H	-24.949050	-31.806057	210.343421	C	-29.156303	-39.717651	198.422372
H	-23.467032	-30.884655	210.080203	C	-28.698075	-40.786479	199.212982
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H	-37.548238	-31.526089	205.357493	H	-33.785375	-32.318034	197.913159
H	-35.242228	-31.897668	204.674794	C	-32.844739	-31.791422	197.688620
H	-35.367669	-34.439357	206.406043	C	-31.636766	-32.701013	197.618583
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H	-37.639529	-33.106358	206.196332	H	-32.665697	-31.022924	198.452190
H	-36.153400	-33.337249	204.217876	N	-31.865774	-34.035181	197.763885
H	-34.301968	-33.059267	206.663665	C	-30.825021	-35.049751	197.618281
H	-32.944357	-32.451470	204.524370	C	-31.005949	-35.920647	196.354744
H	-34.245972	-34.982776	204.261280	O	-30.329212	-36.945507	196.200132
H	-31.197915	-31.933447	203.042419	C	-30.630374	-35.905495	198.891928
H	-32.115641	-35.842289	203.835910	C	-29.736057	-35.350896	200.017034
H	-30.226519	-33.201387	202.435384	O	-29.763976	-35.945196	201.143540
H	-30.940893	-35.431633	202.624998	O	-28.995473	-34.355042	199.718159
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H	-25.362851	-29.407028	201.142647	C	-31.935591	-35.967611	194.072817
H	-24.919647	-28.999659	203.505006	H	-31.190723	-35.442656	193.449429
H	-23.979042	-30.484018	200.999662	H	-21.516057	-41.187718	202.032943
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H	-29.167256	-31.884574	198.565320	O	-23.555188	-43.424052	203.420940
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H	-29.580849	-29.912633	201.780693	C	-22.876977	-39.032498	202.406579
H	-29.169910	-31.207529	202.479207	C	-23.903403	-37.924635	202.278453
H	-27.277637	-30.020622	204.430284	O	-24.588370	-37.785974	201.239074
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H	-31.699815	-37.035657	194.105762	C	-22.629343	-44.962153	201.252063
H	-26.471257	-39.946543	199.857330	H	-21.726399	-45.520632	200.924621
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H	-26.886752	-35.221858	198.114359	C	-26.782801	-43.739211	201.745960
H	-25.755442	-38.590452	196.530018	N	-26.555687	-42.714259	200.933419
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H	-25.253421	-31.061050	198.003547	C	-20.729917	-32.637533	201.505320
H	-27.203792	-30.602260	198.019427	C	-21.633337	-33.405390	202.426007
H	-26.624972	-29.284626	198.564016	C	-22.961028	-33.779319	202.319807
H	-26.615278	-39.288805	205.799530	N	-21.214353	-33.930477	203.639485
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H	-25.696352	-45.713757	202.169034	N	-23.317163	-34.510158	203.447220
H	-22.758074	-30.423158	207.578096	N	-21.823287	-29.604605	202.167079
				C	-22.896307	-28.815019	202.759171
				H	-22.557559	-28.453986	203.752878
				C	-24.187911	-29.630424	202.972923
				C	-24.778968	-30.163401	201.668398

Zn-S₂
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C	-25.719364	-31.345382	201.801727	H	-26.084974	-33.078672	207.923784
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C	-24.411376	-36.713425	208.107119	H	-32.177903	-37.794325	205.517611
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C	-29.305494	-39.426312	208.214655	H	-23.822797	-37.580265	207.777713
O	-29.908215	-40.474845	207.940813	H	-30.124766	-36.831212	198.577925
N	-29.412997	-38.288654	207.495643	H	-31.595532	-36.199375	199.327561
C	-30.167017	-38.200898	206.244908	H	-31.374615	-30.220320	207.623793
C	-29.476587	-37.194408	205.315308	H	-30.093046	-33.015295	207.980980
O	-29.762693	-37.151421	204.103507	H	-28.253128	-31.412845	207.588147
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O	-25.942979	-38.178858	197.056500	H	-29.100390	-30.691316	206.205168
O	-27.361989	-36.367225	198.502168	H	-28.218451	-26.282077	201.034799
O	-26.558423	-29.948603	197.778254	H	-28.401682	-27.453412	202.349690
O	-24.697995	-31.851380	198.210476	H	-25.029850	-31.820753	210.333671
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O	-26.753536	-39.146879	204.883738	H	-37.548238	-31.526089	205.357493
H	-30.313881	-30.639381	208.993011	H	-35.258113	-31.911314	204.649875
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C	-28.310639	-32.628602	205.846725	H	-34.300997	-33.120627	206.607195
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N	-31.767522	-35.133683	203.102642	H	-23.972226	-30.495890	200.994688
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O	-27.870035	-29.211723	204.341158	H	-25.871355	-33.174788	198.574574
H	-32.871511	-42.756208	197.113662	H	-29.211612	-31.872561	198.538934
H	-33.289498	-41.037226	197.135319	H	-28.627525	-30.731758	199.566302
H	-33.700323	-42.030393	195.723193	H	-29.609427	-29.902857	201.796807
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H	-31.163521	-42.320168	195.306390	H	-27.326472	-30.009773	204.458965
H	-30.383612	-43.329480	197.672197	H	-28.601667	-29.558139	203.759998
H	-28.807830	-42.929287	199.534789	H	-32.938579	-35.809166	193.662857
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H	-30.390744	-39.099697	196.777959	H	-26.223956	-39.869210	199.622252
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H	-28.823578	-37.494927	207.732323	H	-26.817187	-36.958253	197.911756
H	-27.637984	-37.543855	210.274206	H	-26.976692	-35.453758	198.459307
H	-21.536180	-29.406915	201.216511	H	-26.589593	-38.707064	196.557252
H	-21.672135	-43.090657	200.889312	H	-25.691032	-38.754765	197.840666
H	-22.978605	-45.405504	202.192894	H	-27.972430	-39.187128	201.836714
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H	-23.371144	-44.651101	199.227687	H	-24.697990	-31.760325	199.181255
H	-22.211062	-38.967293	201.532480	H	-25.318317	-31.096780	197.956602
H	-23.997591	-40.672860	201.514828	H	-27.255924	-30.612402	198.007624
H	-21.976839	-41.318206	203.742063	H	-26.653588	-29.302198	198.539714
H	-22.279342	-38.847406	203.307998	H	-26.768045	-39.248690	205.854969
H	-24.244162	-40.513660	203.262805	H	-26.519123	-38.195508	204.729037
H	-26.352789	-29.822398	209.623187	H	-25.786915	-45.569743	202.079637

H	-22.812193	-30.425087	207.577971	N	-21.823279	-29.604348	202.166884
Mg-S₂				C	-22.896307	-28.815019	202.759171
				H	-22.557559	-28.453986	203.752878
238				C	-24.188503	-29.627387	202.971236
Mn	-24.998209	-35.635315	203.819427	C	-24.777988	-30.156903	201.665268
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Mn	-27.298771	-33.319990	203.205705	O	-26.027925	-31.799368	202.943128
Mn	-27.455304	-33.267119	200.410138	O	-26.138520	-31.799774	200.680059
Mg	-28.233564	-36.601407	202.550199	H	-24.867887	-28.943957	209.202118
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C	-30.241434	-27.113395	201.222163	C	-26.299298	-38.231870	208.886585
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C	-28.712239	-27.203858	201.303808	C	-24.416827	-36.714200	208.100594
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C	-24.420828	-31.518066	208.310499	H	-32.809742	-34.333588	197.932141
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				O	-27.775783	-29.200945	204.307546

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H	-26.711032	-35.082298	198.139920	C	-26.802077	-44.110805	201.942794
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H	-27.970220	-40.026389	201.938372	C	-20.112713	-31.328697	202.090235
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H	-23.853502	-31.714712	198.737487	O	-21.471131	-30.857422	204.042081
H	-25.189775	-31.183881	198.111781	C	-20.658021	-32.641490	201.468572
H	-27.171288	-30.819132	198.225251	C	-21.510579	-33.420399	202.413290
H	-26.646182	-29.460160	198.714177	C	-22.850541	-33.741057	202.384396
H	-26.565952	-39.287128	205.962918	N	-21.049930	-33.896736	203.630860
H	-26.386730	-38.226077	204.840919	C	-22.060786	-34.470990	204.303296
H	-25.574573	-45.893412	202.232512	N	-23.176278	-34.390707	203.567460
H	-22.736233	-30.403869	207.582110	N	-21.820198	-29.606008	202.170708

Gd-S₂Yz⁺

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Mn	-24.784507	-35.523296	203.936637	C	-24.730128	-30.246576	201.660960
Mn	-27.261321	-35.226953	205.246993	O	-25.708028	-31.395380	201.815145
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Gd	-27.819078	-36.550041	202.279146	H	-24.913731	-28.926907	209.195017
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O	-25.948920	-34.077239	204.502339	C	-24.473132	-31.008550	209.725532
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O	-28.398976	-31.732830	199.422983	C	-23.455097	-31.051572	207.400541
O	-26.528045	-33.776183	199.061605	C	-23.629949	-31.624117	206.198883
O	-27.540186	-37.182295	200.052552	H	-24.684862	-32.438031	206.306367
O	-27.856774	-38.947963	202.377354	N	-24.708982	-37.374838	210.156821
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C	-30.241434	-27.113395	201.222163	C	-26.306360	-38.221005	208.873023
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O	-28.949290	-29.580694	200.563715	O	-26.201788	-35.758522	206.852008
O	-27.097445	-28.406230	200.008860	N	-24.126640	-35.854680	205.966022
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C	-28.895353	-41.022427	199.360972	C	-29.324034	-37.351845	204.006416
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C	-31.620430	-32.682579	197.750918	O	-26.536847	-30.121484	197.970624
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H	-36.587209	-31.785060	206.833094	H	-31.220703	-31.994055	203.153274
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H	-29.126295	-38.879348	199.035858	H	-31.708274	-37.037387	194.100818
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H	-22.956432	-45.397268	202.205237	H	-28.000610	-39.655748	201.705397
H	-23.915175	-46.195342	200.023157	H	-26.907368	-37.933551	199.892756
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C	-21.622155	-33.397376	202.433996	H	-21.549011	-43.141757	200.970392
C	-22.953849	-33.758278	202.344837	H	-22.991423	-45.408971	202.186355
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C	-24.182929	-29.638027	202.969286	H	-24.230328	-40.506734	203.294198
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N	-24.668487	-32.483873	206.330691	H	-19.903793	-23.285375	201.161281
H	-24.708982	-37.374838	210.156821	H	-21.316302	-32.384219	200.615590
C	-25.333665	-37.110846	209.273415	H	-25.922094	-36.233923	209.583071
C	-26.302876	-38.225102	208.878775	H	-30.270959	-39.090466	205.874750
O	-26.053531	-39.052955	207.986349	C	-31.673225	-37.604390	206.592366
C	-24.385594	-36.725544	208.128630	H	-32.223094	-37.561711	205.643017
C	-25.002551	-36.109724	206.874788	H	-32.190515	-38.303667	207.260488
O	-26.245194	-35.777576	206.890801	H	-31.666322	-36.609646	207.059053
O	-24.234122	-35.948090	205.882164	H	-29.084911	-39.303096	210.341741
N	-27.485485	-38.237035	209.555761	H	-27.858742	-40.306732	209.536504
C	-28.420988	-39.357108	209.469748	H	-23.640534	-36.003681	208.496243
C	-29.308406	-39.407057	208.223998	H	-23.820535	-37.604193	207.788785
O	-29.867627	-40.462932	207.892967	H	-30.146003	-36.840224	198.561641
N	-29.476913	-38.229963	207.586070	H	-31.629744	-36.214424	199.292234
C	-30.234774	-38.100486	206.348166	H	-31.380684	-30.239893	207.601513
C	-29.486740	-37.159132	205.397681	H	-30.055552	-33.002070	208.025327
O	-29.753029	-37.175404	204.181919	H	-28.227827	-31.383978	207.716705
O	-28.628500	-36.394725	206.000342	H	-30.877139	-32.439120	206.569501
O	-25.314826	-37.927825	197.154796	H	-29.034845	-30.640843	206.317027
O	-27.241011	-36.369175	198.318562	H	-28.199677	-26.321206	201.078016
O	-26.373593	-30.097888	198.022219	H	-28.438034	-27.469391	202.402148
O	-24.672164	-32.152628	198.038689	H	-24.839677	-31.780949	210.358247
O	-29.774968	-30.392978	202.725473	H	-23.408903	-30.791197	210.062895
O	-25.204486	-39.626399	199.288776	H	-25.091417	-33.087409	205.581829
O	-26.522714	-39.118074	204.949859	H	-37.548238	-31.526089	205.357493
H	-30.338075	-30.607060	208.996467	H	-35.244894	-31.901784	204.669576
C	-30.997751	-31.051074	208.236197	H	-35.380306	-34.455461	206.381730
H	-31.843803	-31.521736	208.767318	H	-33.205474	-35.091050	205.638220

H	-37.640133	-33.104216	206.201201	H	-32.669168	-31.017894	198.447764
H	-36.169432	-33.330895	204.207341	N	-31.865275	-34.035146	197.761739
H	-34.305985	-33.084211	206.646950	C	-30.825021	-35.049751	197.612821
H	-32.877233	-32.475476	204.602567	C	-31.010344	-35.924081	196.357914
H	-34.273323	-34.973333	204.216876	O	-30.346072	-36.960685	196.212607
H	-31.222117	-31.929547	203.023628	C	-30.635980	-35.908171	198.892455
H	-32.186967	-35.844889	203.719412	C	-29.727553	-35.354653	200.006460
H	-30.247507	-33.191672	202.421441	O	-29.761696	-35.943647	201.142356
H	-31.095457	-35.425993	202.442716	O	-28.976586	-34.379810	199.696225
H	-23.949952	-30.463533	203.650952	N	-31.871607	-35.445380	195.435295
H	-25.319039	-29.446456	201.098694	C	-31.935591	-35.967611	194.072817
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H	-23.952172	-30.553743	201.005466	H	-21.516057	-41.187718	202.032943
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H	-25.749727	-33.272516	198.744958	C	-22.840146	-42.879507	202.542970
H	-29.177845	-31.927838	198.633910	O	-23.726634	-43.359970	203.269471
H	-28.605025	-30.778051	199.657750	C	-23.471384	-40.417668	202.508492
H	-29.639066	-29.924114	201.849896	C	-22.848093	-39.007820	202.496542
H	-29.202380	-31.191939	202.576897	C	-23.876139	-37.903739	202.354259
H	-27.377135	-29.973182	204.542235	O	-24.578482	-37.800104	201.319284
H	-28.642786	-29.535203	203.818344	O	-23.948091	-37.105789	203.366966
H	-32.938829	-35.810785	193.663052	N	-22.248031	-43.592580	201.548933
H	-31.701697	-37.036453	194.096635	C	-22.629343	-44.962153	201.252063
H	-26.144219	-39.742124	199.559114	H	-21.726399	-45.520632	200.924621
H	-24.825844	-39.031090	199.985662	C	-23.719851	-45.060123	200.155131
H	-27.580637	-39.193750	203.528720	C	-24.937942	-44.273176	200.509892
H	-27.139026	-36.885844	199.789415	C	-25.354009	-43.022797	200.111507
H	-26.532962	-36.846374	197.806906	N	-25.852385	-44.673652	201.475792
H	-26.922335	-35.433088	198.443951	C	-26.773830	-43.721928	201.669112
H	-25.608253	-38.398412	196.356291	N	-26.484137	-42.712220	200.845158
H	-25.258252	-38.623955	197.869411	H	-19.262626	-31.517297	202.779917
H	-27.636056	-39.215197	201.933457	C	-20.112713	-31.328697	202.090235
H	-26.055799	-37.268061	200.930544	C	-21.159662	-30.549848	202.867600
H	-23.893782	-32.003926	198.599869	O	-21.427679	-30.810963	204.058682
H	-25.206343	-31.295788	198.098610	C	-20.722083	-32.637506	201.501998
H	-27.112404	-30.728659	198.210953	C	-21.623153	-33.399085	202.427412
H	-26.509613	-29.422605	198.750832	C	-22.956638	-33.753248	202.336894
H	-26.584467	-39.242899	205.918316	N	-21.199435	-33.917338	203.641826
H	-26.378500	-38.144022	204.827353	C	-22.223138	-34.547128	204.247573
H	-25.813056	-45.573266	201.990165	N	-23.311739	-34.466059	203.475621
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Zn-S₂Yz[•]

238				C	-22.896307	-28.815019	202.759171
Mn	-24.957577	-35.582369	203.869215	H	-22.557559	-28.453986	203.752878
Mn	-27.331562	-35.250096	205.220237	C	-24.186952	-29.630670	202.969402
Mn	-27.282017	-33.318056	203.223673	C	-24.778149	-30.163211	201.664478
Mn	-27.403870	-33.262033	200.437612	C	-25.720582	-31.338917	201.809734
Zn	-28.255238	-36.443942	202.562893	O	-26.019224	-31.801744	202.957195
O	-26.541430	-36.523045	204.133263	O	-26.148139	-31.807214	200.695574
O	-28.345134	-34.741404	203.772852	H	-24.894475	-28.933840	209.197785
O	-25.989835	-34.102845	204.516498	C	-25.289739	-29.704836	209.874338
O	-28.423612	-32.660349	201.992375	H	-25.215628	-29.314217	210.902923
O	-26.603013	-34.232184	201.771777	C	-24.502006	-31.026544	209.722701
O	-28.391067	-31.585865	199.058057	C	-24.442027	-31.531604	208.309361
O	-26.455533	-33.838943	199.010610	C	-25.211242	-32.441370	207.613837
O	-27.082443	-37.040776	201.010041	N	-23.507110	-31.076830	207.384812
O	-28.329788	-38.635422	202.699546	C	-23.682574	-31.670810	206.192953
H	-30.523934	-26.869251	200.186713	N	-24.722166	-32.500709	206.319090
C	-30.241434	-27.113395	201.222163	H	-24.708982	-37.374838	210.156821
H	-30.724377	-26.361921	201.871645	C	-25.333665	-37.110846	209.273415
C	-28.715612	-27.224517	201.337346	O	-26.303647	-38.225580	208.879097
C	-28.151574	-28.365439	200.469975	O	-26.058257	-39.049520	207.982488
O	-28.896401	-29.411557	200.360308	C	-24.406588	-36.710248	208.114147
O	-27.013556	-28.232009	199.938339	C	-25.032814	-36.110294	206.850821
C	-32.924381	-41.850903	196.489835	O	-26.278400	-35.789804	206.844159
C	-31.548870	-41.491216	195.882776	O	-24.256514	-35.948688	205.863783
C	-30.532390	-41.223779	196.962924	N	-27.485208	-38.238391	209.558481
C	-30.158334	-42.269182	197.865281	C	-28.420988	-39.357108	209.469748
C	-29.959192	-39.929732	197.140296	C	-29.302980	-39.411798	208.213918
C	-29.269766	-42.040448	198.893853	O	-29.887261	-40.462723	207.910452
C	-29.053929	-39.677893	198.155763	N	-29.435024	-38.254591	207.530588
C	-28.670955	-40.730416	199.075020	C	-30.206880	-38.140949	206.294632
O	-27.815525	-40.515671	200.011217	C	-29.516574	-37.143268	205.354032
H	-33.785375	-32.318034	197.913159	O	-29.842476	-37.072557	204.155875
C	-32.844739	-31.791422	197.688620	O	-28.616159	-36.421654	205.948704
C	-31.634425	-32.699083	197.626876	O	-25.368000	-37.933012	197.240364
O	-30.493377	-32.245760	197.420608	O	-27.215466	-36.383047	198.514497
				O	-26.372010	-30.043199	197.977626
				O	-24.656485	-32.006950	198.006950
				O	-29.753822	-30.371410	202.690031

O	-25.239425	-39.614012	199.363450	H	-25.136066	-33.100207	205.562343
O	-26.732084	-39.096206	204.886890	H	-37.548238	-31.526089	205.357493
H	-30.318007	-30.635019	208.994376	H	-35.260036	-31.901257	204.649773
C	-30.997751	-31.051074	208.236197	H	-35.366217	-34.468069	206.344245
H	-31.843803	-31.521736	208.767318	H	-33.201828	-35.092125	205.567111
C	-30.286734	-32.114577	207.382246	H	-37.639801	-33.102258	206.207359
C	-28.952684	-31.607348	206.796880	H	-36.191931	-33.327496	204.194864
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O	-28.067105	-33.788727	206.317626	H	-32.894714	-32.462816	204.548970
O	-28.006008	-32.217495	204.693467	H	-34.283202	-34.960139	204.157589
H	-36.611289	-31.795169	206.848210	H	-31.237286	-31.900135	202.979455
C	-36.971479	-32.276075	205.926511	H	-32.141959	-35.822064	203.679596
C	-35.796104	-32.772216	205.060856	H	-30.254041	-33.152517	202.369361
C	-34.809580	-33.673697	205.824110	H	-31.055224	-35.392655	202.417761
C	-33.773471	-34.384942	204.945481	H	-23.953039	-30.471129	203.632472
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C	-31.915688	-33.808113	203.397481	H	-24.923086	-29.002278	203.489908
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O	-27.873924	-29.193782	204.362877	H	-25.746000	-33.204698	198.674763
H	-32.854832	-42.757945	197.106437	H	-29.195176	-31.878954	198.561613
H	-33.278463	-41.034159	197.134859	H	-28.616265	-30.734750	199.589206
H	-33.700323	-42.030393	195.723193	H	-29.615283	-29.902548	201.814736
H	-31.635971	-40.612397	195.230466	H	-29.193383	-31.178121	202.539155
H	-31.198253	-42.332665	195.262386	H	-27.329548	-29.991096	204.480816
H	-30.588139	-43.263490	197.735310	H	-28.604641	-29.539040	203.780885
H	-28.999274	-42.839485	199.583470	H	-32.939118	-35.806813	193.665411
H	-28.608170	-38.690405	198.282864	H	-31.704656	-37.037324	194.090792
H	-30.241849	-39.115677	196.471556	H	-26.183929	-39.749974	199.608377
H	-27.067342	-41.853585	200.684614	H	-24.893349	-38.996199	200.060111
H	-24.941658	-42.330370	199.387817	H	-27.851262	-38.955470	203.513635
H	-27.603156	-43.769769	202.363295	H	-27.158531	-36.737612	200.029951
H	-28.854439	-37.460509	207.786489	H	-26.537261	-36.894535	197.993097
H	-27.622551	-37.561514	210.299908	H	-26.904252	-35.437017	198.527645
H	-21.527458	-29.398576	201.220868	H	-25.705467	-38.389367	196.451084
H	-21.549429	-43.141439	200.971002	H	-25.282888	-38.639384	197.943807
H	-22.992518	-45.410864	202.185015	H	-27.768428	-38.856468	201.930779
H	-23.974227	-46.119192	200.003576	H	-26.107671	-37.125202	201.198342
H	-23.325798	-44.676273	199.205486	H	-23.910245	-31.941546	198.612488
H	-22.156625	-38.926269	201.643551	H	-25.201792	-31.229564	198.064306
H	-23.979207	-40.601602	201.550914	H	-27.116974	-30.672534	198.147048
H	-21.964414	-41.368968	203.743313	H	-26.510561	-29.381189	198.718555
H	-22.277179	-38.837251	203.417564	H	-26.781066	-39.212949	205.856129
H	-24.223064	-40.502634	203.305870	H	-26.490658	-38.141034	204.757127
H	-26.351018	-29.855535	209.633965	H	-25.810481	-45.539064	202.003240
H	-26.048426	-33.052286	207.928269	H	-22.773946	-30.402003	207.578982
H	-23.064691	-31.499714	205.312937	Mg-S₂Yz[•]			
H	-23.669701	-33.577138	201.538964				
H	-22.164240	-35.057118	205.200848	238			
H	-19.717186	-30.736288	201.254441	Mn	-24.984298	-35.588951	203.851348
H	-23.071443	-27.948362	202.111527	Mn	-27.342524	-35.218092	205.218089
H	-29.892825	-34.490083	197.441883	Mn	-27.293234	-33.298294	203.227141
H	-32.807644	-34.340743	197.981263	Mn	-27.419764	-33.250079	200.434125
H	-32.941112	-31.285271	196.718371	Mg	-28.237136	-36.523752	202.591929
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H	-30.711155	-28.077157	201.457136	O	-28.359336	-34.702717	203.791969
H	-19.901170	-33.285021	201.159925	O	-25.988957	-34.097217	204.509101
H	-21.312080	-32.383149	200.611573	O	-28.434543	-32.635052	201.999541
H	-25.926354	-36.239087	209.591301	O	-26.632893	-34.225569	201.774774
H	-30.193782	-39.121573	205.799236	O	-28.395480	-31.571834	199.044831
C	-31.669171	-37.730332	206.554930	O	-26.471295	-33.833065	199.010579
H	-32.223101	-37.690803	205.607803	O	-27.052764	-37.003603	200.995210
H	-32.145100	-38.474273	207.205153	O	-28.204258	-38.726417	202.679860
H	-31.713864	-36.749377	207.047947	H	-30.531081	-26.873810	200.187619
H	-29.091194	-39.302984	210.336522	C	-30.241434	-27.113395	201.222163
H	-27.858742	-40.306732	209.536504	H	-30.724377	-26.361921	201.871645
H	-23.671268	-35.973278	208.471328	C	-28.714589	-27.218005	201.327815
H	-23.827937	-37.579509	207.773076	C	-28.152771	-28.357774	200.457279
H	-30.148346	-36.843404	198.578114	O	-28.903337	-29.398963	200.341415
H	-31.603513	-36.185956	199.333305	O	-27.012505	-28.228326	199.929759
H	-31.375637	-30.222447	207.621564	C	-32.924381	-41.850903	196.489835
H	-30.088590	-33.012859	207.984622	C	-31.548988	-41.486497	195.885375
H	-28.249472	-31.408146	207.621695	C	-30.532435	-41.219166	196.965926
H	-30.946604	-32.429823	206.558173	C	-30.157428	-42.264011	197.868725
H	-29.084272	-30.672834	206.236951	C	-29.957621	-39.925495	197.141504
H	-28.214057	-26.290690	201.049518	C	-29.264841	-42.035322	198.893922
H	-28.415994	-27.443245	202.375761	C	-29.048964	-39.673406	198.153978
H	-24.960550	-31.808434	210.342515	C	-28.663043	-40.726150	199.071544
H	-23.473409	-30.892783	210.088381				

O	-27.801176	-40.512980	200.002948	O	-25.394294	-37.936300	197.185840
H	-33.785375	-32.318034	197.913159	O	-27.247945	-36.376639	198.462352
C	-32.844739	-31.791422	197.688620	O	-26.378097	-30.039503	197.961094
C	-31.634951	-32.699425	197.620501	O	-24.647478	-32.068757	198.034300
O	-30.495615	-32.246532	197.404440	O	-29.755469	-30.346781	202.680957
H	-32.666946	-31.021222	198.450723	O	-25.221127	-39.625604	199.311711
N	-31.864586	-34.034925	197.763054	O	-26.690200	-39.085113	204.957455
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H	-21.510057	-29.378900	201.228855	H	-25.958433	-38.532846	196.367419
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Na-S₂Yz[•]

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C	-25.333665	-37.110846	209.273415	H	-25.939254	-36.244054	209.576534
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O	-26.542443	-33.779169	199.054682	C	-23.461319	-31.056946	207.400224
O	-27.514619	-37.135762	200.122083	C	-23.635301	-31.628267	206.197903
O	-27.632993	-38.852129	202.391023	N	-24.691848	-32.440520	206.303201
				H	-24.708982	-37.374838	210.156821
				C	-25.333665	-37.110846	209.273415

C	-26.303270	-38.224501	208.875935	H	-29.844289	-39.323277	205.650086
O	-26.053222	-39.049314	207.980004	C	-31.472083	-37.988125	206.159047
C	-24.383858	-36.715322	208.142037	H	-31.907972	-38.018872	205.151881
C	-24.971352	-36.063647	206.897047	H	-31.980678	-38.732539	206.782955
O	-26.226165	-35.780303	206.841279	H	-31.625064	-36.992705	206.596983
O	-24.149247	-35.832983	205.962611	H	-29.112332	-39.295926	210.317594
N	-27.486509	-38.236797	209.552645	H	-27.858742	-40.306732	209.536504
C	-28.420988	-39.357108	209.469748	H	-23.622907	-36.018461	208.523457
C	-29.244810	-39.462179	208.172295	H	-23.835034	-37.596471	207.780509
O	-29.791330	-40.533950	207.874559	H	-30.107524	-36.782728	198.658640
N	-29.341005	-38.343655	207.419742	H	-31.577181	-36.129239	199.379709
C	-29.969093	-38.327686	206.096976	H	-31.374512	-30.219332	207.625360
C	-29.222438	-37.323815	205.214855	H	-30.091091	-33.015181	207.976979
O	-29.299963	-37.372178	203.965200	H	-28.256743	-31.401805	207.574858
O	-28.549194	-36.454221	205.893368	H	-30.969657	-32.437128	206.559904
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O	-27.349528	-35.986069	197.868693	H	-28.148300	-26.456440	201.201627
O	-26.533169	-30.128734	197.971058	H	-28.533861	-27.600819	202.494704
O	-24.714793	-32.082638	198.008714	H	-24.930283	-31.804031	210.341118
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O	-26.585071	-39.133043	204.916344	H	-37.548238	-31.526089	205.357493
H	-30.311985	-30.642294	208.992494	H	-35.253197	-31.974658	204.648271
C	-30.997751	-31.051074	208.236197	H	-35.462063	-34.528555	206.360432
H	-31.843803	-31.521736	208.767318	H	-33.250528	-35.157230	205.622210
C	-30.295807	-32.120210	207.371874	H	-37.653061	-33.080970	206.236707
C	-28.966616	-31.621315	206.760706	H	-36.231306	-33.375696	204.207476
O	-28.295486	-32.626960	205.844489	H	-34.361213	-33.180231	206.648538
C	-28.039612	-33.798501	206.309269	H	-33.118609	-32.532760	204.419281
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C	-36.971479	-32.276075	205.926511	H	-32.334102	-35.891377	203.626190
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H	-28.816659	-37.517369	207.692884	H	-26.589062	-36.520512	197.517022
H	-27.624093	-37.559220	210.293659	H	-26.975207	-35.102676	198.168828
H	-21.498820	-29.375607	201.237248	H	-25.443646	-38.324739	196.498873
H	-21.582279	-43.127572	200.935178	H	-25.451740	-38.435184	198.050304
H	-22.962254	-45.400210	202.201890	H	-27.974501	-39.547740	201.785925
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H	-22.238783	-38.852762	203.237964	H	-26.596673	-39.277137	205.883959
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