

The additional computational details are as follows. Lattice constants and cell shapes were optimized for all VASP calculations. Electronic self-consistent iterations were performed using the Normal (blocked Davidson) algorithm. All oxygen atoms were described using the same PAW potential (O, 08Apr2002). Even with these settings, some calculations did not converge in a single run and occasionally encountered convergence failures. In such cases, we restarted and repeated the calculations until they completed successfully. □

<Section 3.2>

	PAW	U - J	AMIX	Gaussian smearing	Magmomet
Ce ₃₂ O ₆₄	Ce 23Dec2003	6.3000	0.20	0.05	Not set
Ce ₃₂ O ₆₃	Ce 23Dec2003	6.3000	0.18	0.05	#1
Ce ₃₁ MnO ₆₄	Ce 23Dec2003 Mn_pv 02Aug2007	4.0000	0.10	0.10	Not set
Ce ₃₁ MnO ₆₃	Ce 23Dec2003 Mn_pv 02Aug2007	4.0000	Not set	0.10	#2
Ce ₃₁ FeO ₆₄	Ce 23Dec2003 Fe 06Sep2000	4.6000	0.30	0.05	#3
Ce ₃₁ CoO ₆₄	Ce 23Dec2003 Co 02Aug2007	5.0000	0.20	0.05	#4
Ce ₃₁ NiO ₆₄	Ce 23Dec2003 Ni 02Aug2007	5.1000	0.20	0.05	#5

#1< MAGMOM = -0.009 14*0 -0.002 5*0 -0.002 4*0 -0.004 2*0 -0.001 0 -0.001 3*0 -0.002 ¥ 7*0 -0.001 -0.004 2*0 -0.001 -0.009 2*0 -0.002 0 -0.002 -0.007 2*0 -0.004 ¥ -0.001 -0.004 2*-0.001 -0.002 0.972 3*0.002 0.001 2*0.002 0 2*0.002 0 0.002 0 ¥ 0.015 2*0 0.002 0 2*0.002 2*0 0.015 0 3*0.002 0.972 0 2*0.002 0.001>, #2< MAGMOM = 0 0.007 -0.001 0 -0.001 9*0 0.007 4*0 0.007 3*0 -0.001 2*0 0.007 -0.001 ¥ 5*0 0.007 5*0 -0.001 0 -0.001 2*0 0.007 9*0 0.008 0.007 7*0 4.517 7*0 0.007 ¥ 2*0 0.007 0 0.002 0 2*0.007 0 0.007 2*0 0.002 0.007 0 0.007 0.002 2*0.007 0 ¥ 3*0.007>, #3< MAGMOM = 8*0 0.086 -0.003 -0.304 0.065 -0.002 0.084 0.091 -0.232 0 -0.001 -0.006 ¥ 5*-0.001 -0.002 0 -0.001 2*0 -0.003 2*-0.001 0 -0.001 -0.026 0 3*-0.001 -0.012 ¥ 2*0 -0.001 4*0 -0.001 0 -0.001 -0.007 0 2*-0.001 0 -0.002 0 -0.002 -0.001 0 ¥ -0.003 2*0 -0.001 4.156 0 0.001 8*0 0.001 3*0 0.009 0.005 0 0.01 0 0.008 0 ¥ 0.035 0.009 0.001 0 0.008 0.013 0.012 0.01 -0.001 0.001>, #4< MAGMOM = 8*0 0.004 3*0.295 0.24 4*0.001 4*0.004 6*0 0.003 0.002 2*0.001 2*0 ¥ 0.005 2*0.004 0.005 4*0 0.003 2*0 0.002 0 2*0.001 0 3*0.004 0.005 5*0 0.003 0 ¥ 0.002 0.001 0 0.001 3.172 15*0 0.012 0.004 0.012 2*0 0.004 2*0.012 0.002 2*0 ¥ 2*0.012 0.004 2*0.002>, #5< MAGMOM = 8*0.001 2*0.129 2*0.016 2*0.128 2*0.016 2*0.002 2*0.001 2*0.002 2*0.001 ¥ 2*0.003 2*0.001 2*0.003 2*0.001 2*0.002 2*0.001 2*0.002 2*0.001 2*0.003 ¥ 2*0.001 2*0.003 2*0.001 2*0.015 2*0.004 2*0.015 2*0.004 2*0.001 2*0.002 ¥ 2*0.001 2*0.002 0.998 14*0 4*0.003 0 2*0.002 4*0 0.002 0 0.002 2*0 -0.001>

<Section 3.3>

All calculations were performed with ISPIN = 2, Gaussian smearing 0.1. When convergence issues were encountered, initial magnetic moments (MAGMOM) were specified. The MAGMOM settings were as follows: Ce₇MoO₁₅ <MAGMOM = 0.006 0.993 0.994 0.008 0.031 0.986 0.987 -0.012 -0.002 -0.007 -0.002 ¥ -0.007 -0.005 -0.004 -0.002 -0.007 -0.006 -0.008 -0.006 -0.008 -0.001 -0.01 ¥ 0.009>, Ce₆Fe₂O₁₅ <MAGMOM = 2*3 21*0>, Ce₆Cu₂O₁₆ <MAGMOM = 2*1 22*0>

dopant	PAW	U - J	AMIX (Ce ₇ MO ₁₆)	AMIX (Ce ₇ MO ₁₅)
Ce (pure)	Ce 23Dec2003	6.3000	0.20	0.10
Ti	Ti_sv 26Sep2005	4.4000	0.22	Not set
V	V_sv 02Aug2007	2.7000	0.22	0.22
Cr	Cr_pv 02Aug2007	3.5000	0.22	0.22
Mn	Mn_pv 02Aug2007	4.0000	0.22	0.20
Fe	Fe_pv 02Aug2007	4.6000	Not set	Not set
Co	Co 02Aug2007	5.0000	Not set	Not set
Ni	Ni_pv 06Sep2000	5.1000	Not set	Not set
Cu	Cu_pv 06Sep2000	4.0000	Not set	Not set
Zn	Zn 06Sep2000	7.5000	Not set	Not set
Zr	Zr_sv 04Jan2005	Not set	Not set	Not set
Nb	Nb_sv 25May2007	2.1000	Not set	Not set
Mo	Mo_pv 04Feb2005	2.4000	Not set	0.22
Ru	Ru_pv 28Jan2005	3.0000	Not set	Not set
Rh	Rh_pv 25Jan2005	3.3000	Not set	Not set
Pd	Pd 04Jan2005	3.6000	Not set	Not set
Hf	Hf_pv 06Sep2000	Not set	Not set	Not set

dopant	PAW	U - J	AMIX (Ce ₆ M ₂ O ₁₆)	AMIX (Ce ₆ M ₂ O ₁₅)
Ce (pure)	Ce 23Dec2003	6.3000	0.20	0.10
Ti	Ti_sv 26Sep2005	4.4000	0.10	0.10
V	V_sv 02Aug2007	2.7000	0.10	0.10
Cr	Cr_pv 02Aug2007	3.5000	0.10	0.10
Mn	Mn_pv 02Aug2007	4.0000	Not set	0.10
Fe	Fe_pv 02Aug2007	4.6000	0.10	0.10
Co	Co 02Aug2007	5.0000	0.10	0.10
Ni	Ni_pv 06Sep2000	5.1000	0.10	0.05
Cu	Cu_pv 06Sep2000	4.0000	0.10	0.05
Zn	Zn 06Sep2000	7.5000	0.10	0.10
Zr	Zr_sv 04Jan2005	Not set	0.10	0.10
Nb	Nb_sv 25May2007	2.1000	0.10	0.05
Mo	Mo_pv 04Feb2005	2.4000	0.05	0.05
Ru	Ru_pv 28Jan2005	3.0000	0.10	0.10
Rh	Rh_pv 25Jan2005	3.3000	0.10	0.10
Pd	Pd 04Jan2005	3.6000	0.10	0.10
Hf	Hf_pv 06Sep2000	Not set	0.10	0.10

The following thermodynamic functions are obtained from the phonon density of states within the harmonic approximation.

<Section 3.2>

Definitions:

C_v : vibrational heat capacity at constant volume

$E_{\text{vib}}(T) = E(T) - E(0)$: the change in vibrational internal energy from 0 K, where

$E(0) = E_{\text{elec}} + \text{ZPE}$ is the electronic energy of formation E_{elec} plus the zero point energy

$S(T)$: the vibrational entropy at temperature T

$-(A(T) - E(0))$: the change in the vibrational Helmholtz free energy from 0 K

$E(T)$: the electronic energy of formation plus the vibrational internal energy,

so this term is $E_{\text{elec}} + \text{ZPE} + E_{\text{vib}}(T)$

$A(T)$: the electronic plus vibrational Helmholtz free energy, $E(T) - TS(T)$

Note that the electronic energy, which is part of the enthalpy and free energies, is set to zero because the reference energies of the elements in their standard state are unavailable.

Thermodynamic Properties for empirical formula **CeO₂** unit

Zero-point energy = 16.17 kJ/mol

T K	C_v J K ⁻¹ mol ⁻¹	$E(T) - E(0)$ kJ mol ⁻¹	$S(T)$ J K ⁻¹ mol ⁻¹	$-(A(T) - E(0))$ kJ mol ⁻¹	$E(T)$ kJ mol ⁻¹	$A(T)$ kJ mol ⁻¹
0	0.0000	0.0000	0.0000	0.0000	16.1678	16.1678
1	0.0000	0.0000	0.0000	0.0000	16.1678	16.1678
2	0.0001	0.0000	0.0000	0.0000	16.1678	16.1678
3	0.0012	0.0000	0.0002	0.0000	16.1678	16.1678
4	0.0039	0.0000	0.0009	0.0000	16.1678	16.1678
5	0.0083	0.0000	0.0022	0.0000	16.1679	16.1678
10	0.0527	0.0001	0.0194	0.0001	16.1680	16.1678
15	0.1746	0.0007	0.0593	0.0002	16.1685	16.1676
20	0.5233	0.0023	0.1498	0.0007	16.1701	16.1671
25	1.2282	0.0065	0.3353	0.0019	16.1743	16.1659
30	2.2881	0.0151	0.6480	0.0043	16.1830	16.1635
35	3.6244	0.0298	1.0981	0.0086	16.1977	16.1592
40	5.1511	0.0517	1.6800	0.0155	16.2195	16.1523
45	6.8010	0.0815	2.3811	0.0256	16.2494	16.1422
50	8.5279	0.1198	3.1865	0.0395	16.2877	16.1284

55	10.3013	0.1669	4.0822	0.0576	16.3347	16.1102
60	12.1007	0.2229	5.0555	0.0804	16.3907	16.0874
65	13.9121	0.2879	6.0956	0.1083	16.4558	16.0596
70	15.7251	0.3620	7.1929	0.1415	16.5299	16.0264
75	17.5317	0.4452	8.3395	0.1803	16.6130	15.9875
80	19.3252	0.5373	9.5283	0.2249	16.7052	15.9429
85	21.1000	0.6384	10.7533	0.2756	16.8062	15.8922
90	22.8507	0.7483	12.0090	0.3325	16.9161	15.8353
95	24.5728	0.8668	13.2907	0.3958	17.0347	15.7721
100	26.2622	0.9939	14.5943	0.4655	17.1618	15.7024
105	27.9152	1.1294	15.9157	0.5417	17.2972	15.6261
110	29.5287	1.2730	17.2517	0.6247	17.4409	15.5432
115	31.1002	1.4246	18.5992	0.7143	17.5925	15.4536
120	32.6277	1.5840	19.9552	0.8107	17.7518	15.3572
125	34.1094	1.7508	21.3174	0.9138	17.9187	15.2540
130	35.5443	1.9250	22.6833	1.0238	18.0928	15.1440
135	36.9318	2.1062	24.0509	1.1407	18.2740	15.0272
140	38.2715	2.2942	25.4184	1.2643	18.4620	14.9035
145	39.5634	2.4888	26.7840	1.3948	18.6567	14.7730
150	40.8080	2.6898	28.1464	1.5322	18.8576	14.6357
155	42.0057	2.8968	29.5041	1.6763	19.0647	14.4915
160	43.1575	3.1097	30.8561	1.8272	19.2776	14.3406
165	44.2642	3.3283	32.2012	1.9848	19.4961	14.1830
170	45.3270	3.5523	33.5385	2.1492	19.7201	14.0186
175	46.3471	3.7815	34.8672	2.3202	19.9493	13.8476
180	47.3258	4.0157	36.1867	2.4979	20.1835	13.6700
185	48.2645	4.2547	37.4962	2.6821	20.4225	13.4858
190	49.1646	4.4983	38.7954	2.8728	20.6661	13.2950
195	50.0275	4.7463	40.0837	3.0700	20.9141	13.0978
200	50.8546	4.9985	41.3608	3.2736	21.1663	12.8942
205	51.6474	5.2548	42.6263	3.4836	21.4226	12.6843
210	52.4073	5.5149	43.8801	3.6999	21.6827	12.4680
215	53.1357	5.7788	45.1219	3.9224	21.9466	12.2455
220	53.8338	6.0462	46.3515	4.1510	22.2141	12.0168
225	54.5030	6.3171	47.5688	4.3859	22.4849	11.7820
230	55.1447	6.5912	48.7738	4.6267	22.7590	11.5411
235	55.7599	6.8685	49.9664	4.8736	23.0363	11.2943
240	56.3500	7.1488	51.1466	5.1264	23.3166	11.0415
245	56.9160	7.4319	52.3143	5.3850	23.5998	10.7828
250	57.4590	7.7179	53.4697	5.6495	23.8857	10.5184
255	57.9802	8.0065	54.6127	5.9197	24.1743	10.2482
260	58.4804	8.2976	55.7434	6.1956	24.4655	9.9723
265	58.9607	8.5912	56.8620	6.4771	24.7591	9.6907
270	59.4220	8.8872	57.9684	6.7642	25.0550	9.4037
273	59.7033	9.0748	58.6593	6.9479	25.2427	9.2200
275	59.8652	9.1854	59.0628	7.0568	25.3533	9.1111
277	60.0504	9.3143	59.5298	7.1842	25.4822	8.9836
280	60.2911	9.4858	60.1454	7.3548	25.6537	8.8131
285	60.7004	9.7883	61.2161	7.6582	25.9561	8.5097
290	61.0941	10.0928	62.2752	7.9669	26.2606	8.2009
294	61.3681	10.3132	63.0307	8.1925	26.4811	7.9754
295	61.4727	10.3992	63.3228	8.2809	26.5671	7.8869
296	61.5466	10.4607	63.5310	8.3443	26.6286	7.8235
298	61.7038	10.5932	63.9770	8.4814	26.7611	7.6864
300	61.8369	10.7075	64.3591	8.6001	26.8753	7.5677

310	62.5250	11.3293	66.3981	9.2539	27.4972	6.9139
320	63.1632	11.9578	68.3934	9.9279	28.1257	6.2399
330	63.7558	12.5924	70.3462	10.6217	28.7603	5.5462
340	64.3067	13.2328	72.2578	11.3347	29.4006	4.8331
350	64.8197	13.8784	74.1294	12.0667	30.0463	4.1012
360	65.2978	14.5291	75.9622	12.8172	30.6969	3.3507
370	65.7440	15.1843	77.7574	13.5858	31.3521	2.5821
373	65.8784	15.3916	78.3153	13.8316	31.5594	2.3362
380	66.1610	15.8438	79.5163	14.3722	32.0117	1.7957
390	66.5510	16.5074	81.2400	15.1760	32.6753	0.9919
400	66.9164	17.1748	82.9295	15.9969	33.3426	0.1710
425	67.7339	18.8582	87.0115	18.1215	35.0260	-1.9537
450	68.4347	20.5605	90.9034	20.3458	36.7283	-4.1780
475	69.0392	22.2791	94.6201	22.6652	38.4469	-6.4974
500	69.5640	24.0117	98.1749	25.0754	40.1796	-8.9076
525	70.0220	25.7567	101.5803	27.5727	41.9245	-11.4048
550	70.4240	27.5124	104.8472	30.1533	43.6802	-13.9854
575	70.7784	29.2775	107.9857	32.8139	45.4453	-16.6461
600	71.0925	31.0509	111.0048	35.5515	47.2188	-19.3837
650	71.6217	34.6192	116.7169	41.2463	50.7871	-25.0784
700	72.0472	38.2113	122.0407	47.2167	54.3792	-31.0488
750	72.3942	41.8226	127.0237	53.4446	57.9905	-37.2767
800	72.6807	45.4497	131.7054	59.9140	61.6175	-43.7461
850	72.9199	49.0899	136.1190	66.6106	65.2577	-50.4427
900	73.1216	52.7410	140.2928	73.5218	68.9089	-57.3539
950	73.2931	56.4015	144.2510	80.6362	72.5693	-64.4683
1000	73.4402	60.0699	148.0144	87.9435	76.2377	-71.7757
1050	73.5673	63.7451	151.6007	95.4346	79.9130	-79.2667
1100	73.6778	67.4263	155.0257	103.1008	83.5941	-86.9330
1150	73.7745	71.1127	158.3029	110.9346	87.2805	-94.7667
1200	73.8595	74.8035	161.4445	118.9287	90.9714	-102.7609
1250	73.9347	78.4984	164.4612	127.0768	94.6662	-110.9090
1300	74.0015	82.1968	167.3623	135.3728	98.3647	-119.2050
1350	74.0612	85.8984	170.1563	143.8112	102.0662	-127.6434
1400	74.1146	89.6027	172.8507	152.3867	105.7706	-136.2188
1450	74.1627	93.3097	175.4523	161.0946	109.4775	-144.9267
1500	74.2061	97.0190	177.9673	169.9304	113.1868	-153.7626
1550	74.2454	100.7302	180.4011	178.8898	116.8980	-162.7220
1600	74.2812	104.4433	182.7590	187.9691	120.6112	-171.8013
1650	74.3137	108.1582	185.0452	197.1644	124.3260	-180.9966
1700	74.3435	111.8746	187.2641	206.4724	128.0425	-190.3045
1750	74.3707	115.5925	189.4195	215.8896	131.7603	-199.7218
1800	74.3958	119.3116	191.5151	225.4132	135.4795	-209.2454
1850	74.4188	123.0320	193.5537	235.0401	139.1998	-218.8723
1900	74.4401	126.7534	195.5386	244.7676	142.9213	-228.5998
1950	74.4598	130.4759	197.4725	254.5930	146.6438	-238.4251
2000	74.4780	134.1994	199.3579	264.5139	150.3672	-248.3460
2050	74.4949	137.9236	201.1971	274.5279	154.0915	-258.3601
2100	74.5106	141.6487	202.9924	284.6328	157.8166	-268.4650
2150	74.5253	145.3747	204.7459	294.8264	161.5426	-278.6585
2200	74.5389	149.1013	206.4594	305.1065	165.2691	-288.9387
2250	74.5517	152.8285	208.1346	315.4714	168.9963	-299.3036
2300	74.5636	156.5564	209.7733	325.9193	172.7242	-309.7514
2350	74.5748	160.2848	211.3770	336.4480	176.4526	-320.2802
2400	74.5853	164.0138	212.9472	347.0563	180.1817	-330.8885

2450	74.5952	167.7433	214.4852	357.7421	183.9111	-341.5743
2500	74.6045	171.4732	215.9922	368.5041	187.6411	-352.3363
2550	74.6132	175.2036	217.4698	379.3408	191.3715	-363.1729
2600	74.6215	178.9345	218.9187	390.2505	195.1024	-374.0826
2650	74.6293	182.6658	220.3401	401.2319	198.8336	-385.0641
2700	74.6366	186.3974	221.7352	412.2839	202.5652	-396.1161
2750	74.6436	190.1294	223.1048	423.4050	206.2973	-407.2372
2800	74.6502	193.8617	224.4498	434.5939	210.0295	-418.4260
2850	74.6565	197.5944	225.7711	445.8494	213.7622	-429.6816
2900	74.6624	201.3273	227.0696	457.1704	217.4952	-441.0026
2950	74.6680	205.0605	228.3459	468.5559	221.2284	-452.3881
3000	74.6734	208.7940	229.6010	480.0046	224.9619	-463.8367

Thermodynamic Properties for empirical formula $\text{Ce}_{32}\text{O}_{63}$ unit

Zero-point energy = 507.73 kJ/mol

T K	Cv J K ⁻¹ mol ⁻¹	E(T) - E(0) kJ mol ⁻¹	S(T) J K ⁻¹ mol ⁻¹	-(A(T) - E(0)) kJ mol ⁻¹	E(T) kJ mol ⁻¹	A(T) kJ mol ⁻¹
0	0.0000	0.0000	0.0000	0.0000	507.7268	507.7268
1	0.0000	0.0000	0.0000	0.0000	507.7268	507.7268
2	0.0001	0.0000	0.0000	0.0000	507.7268	507.7268
3	0.0069	0.0000	0.0008	0.0000	507.7268	507.7268
4	0.0553	0.0000	0.0077	0.0000	507.7268	507.7268
5	0.2022	0.0002	0.0335	0.0001	507.7270	507.7267
10	3.5728	0.0076	0.9405	0.0017	507.7345	507.7251
15	11.7149	0.0436	3.7496	0.0126	507.7704	507.7142
20	27.1864	0.1370	9.0156	0.0433	507.8638	507.6835
25	52.9816	0.3330	17.6535	0.1084	508.0598	507.6184
30	88.8004	0.6836	30.3420	0.2266	508.4104	507.5002
35	132.4012	1.2340	47.2211	0.4188	508.9608	507.3080
40	181.4085	2.0166	68.0513	0.7055	509.7435	507.0213
45	233.9681	3.0539	92.4252	1.1052	510.7807	506.6216
50	288.7758	4.3600	119.8975	1.6349	512.0868	506.0919
55	344.9404	5.9438	150.0467	2.3087	513.6706	505.4181
60	401.8491	7.8106	182.4967	3.1391	515.5374	504.5877
65	459.0682	9.9628	216.9204	4.1370	517.6896	503.5898
70	516.2767	12.4013	253.0354	5.3112	520.1281	502.4156
75	573.2237	15.1250	290.5988	6.6697	522.8519	501.0571
80	629.7027	18.1327	329.3998	8.2192	525.8595	499.5076
85	685.5361	21.4210	369.2543	9.9654	529.1478	497.7614
90	740.5673	24.9866	410.0004	11.9131	532.7134	495.8137
95	794.6573	28.8251	451.4943	14.0666	536.5519	493.6602
100	847.6836	32.9314	493.6080	16.4291	540.6582	491.2977
105	899.5379	37.3000	536.2262	19.0036	545.0268	488.7233
110	950.1300	41.9247	579.2456	21.7921	549.6515	485.9348
115	999.3844	46.7989	622.5722	24.7964	554.5258	482.9304
120	1047.2386	51.9161	666.1218	28.0181	559.6430	479.7088
125	1093.6493	57.2689	709.8181	31.4578	564.9957	476.2690
130	1138.5851	62.8500	753.5919	35.1163	570.5769	472.6105
135	1182.0251	68.6522	797.3819	38.9938	576.3790	468.7331
140	1223.9643	74.6678	841.1318	43.0900	582.3946	464.6368

145	1264.4045	80.8892	884.7921	47.4050	588.6161	460.3219
150	1303.3588	87.3092	928.3178	51.9378	595.0360	455.7891
155	1340.8456	93.9203	971.6705	56.6877	601.6472	451.0391
160	1376.8923	100.7151	1014.8136	61.6539	608.4420	446.0729
165	1411.5298	107.6868	1057.7165	66.8354	615.4136	440.8915
170	1444.7928	114.8281	1100.3517	72.2306	622.5550	435.4962
175	1476.7205	122.1325	1142.6966	77.8384	629.8593	429.8885
180	1507.3545	129.5931	1184.7298	83.6570	637.3199	424.0698
185	1536.7372	137.2038	1226.4329	89.6850	644.9306	418.0418
190	1564.9125	144.9584	1267.7918	95.9207	652.6852	411.8062
195	1591.9264	152.8508	1308.7932	102.3622	660.5776	405.3646
200	1617.8219	160.8757	1349.4262	109.0079	668.6026	398.7189
205	1642.6433	169.0272	1389.6817	115.8558	676.7540	391.8710
210	1666.4361	177.3002	1429.5523	122.9040	685.0271	384.8228
215	1689.2428	185.6898	1469.0346	130.1506	693.4167	377.5763
220	1711.1049	194.1910	1508.1211	137.5936	701.9178	370.1333
225	1732.0633	202.7993	1546.8110	145.2310	710.5261	362.4958
230	1752.1595	211.5101	1585.1010	153.0609	719.2369	354.6659
235	1771.4301	220.3193	1622.9911	161.0814	728.0461	346.6455
240	1789.9132	229.2229	1660.4812	169.2900	736.9498	338.4368
245	1807.6439	238.2171	1697.5714	177.6853	745.9439	330.0415
250	1824.6571	247.2981	1734.2634	186.2650	755.0250	321.4618
255	1840.9843	256.4624	1770.5587	195.0272	764.1892	312.6996
260	1856.6588	265.7068	1806.4599	203.9698	773.4337	303.7570
265	1871.7097	275.0280	1841.9695	213.0910	782.7548	294.6358
270	1886.1662	284.4228	1877.0909	222.3888	792.1496	285.3380
273	1894.9795	290.3780	1899.0204	228.3362	798.1049	279.3907
275	1900.0539	293.8886	1911.8289	231.8611	801.6154	275.8657
277	1905.8583	297.9797	1926.6487	235.9875	805.7066	271.7393
280	1913.4020	303.4223	1946.1853	241.5063	811.1491	266.2205
285	1926.2321	313.0216	1980.1659	251.3222	820.7484	256.4046
290	1938.5700	322.6836	2013.7740	261.3072	830.4105	246.4196
294	1947.1614	329.6781	2037.7439	268.6001	837.4050	239.1268
295	1950.4382	332.4064	2047.0146	271.4593	840.1332	236.2675
296	1952.7571	334.3579	2053.6188	273.5096	842.0847	234.2172
298	1957.6826	338.5617	2067.7701	277.9400	846.2886	229.7868
300	1961.8565	342.1873	2079.8926	281.7767	849.9141	225.9502
310	1983.4285	361.9150	2144.5770	302.9001	869.6418	204.8267
320	2003.4374	381.8504	2207.8688	324.6633	889.5772	183.0635
330	2022.0195	401.9786	2269.8061	347.0525	909.7055	160.6743
340	2039.2979	422.2861	2330.4280	370.0547	930.0129	137.6721
350	2055.3856	442.7605	2389.7778	393.6566	950.4873	114.0702
360	2070.3825	463.3901	2447.8921	417.8458	971.1169	89.8810
370	2084.3783	484.1643	2504.8116	442.6102	991.8912	65.1167
373	2088.5938	490.7369	2522.4999	450.5282	998.4638	57.1987
380	2097.4579	505.0746	2560.5737	467.9379	1012.8015	39.7889
390	2109.6952	526.1104	2615.2158	493.8176	1033.8372	13.9093
400	2121.1567	547.2657	2668.7754	520.2383	1054.9926	-12.5115
425	2146.8087	600.6231	2798.1592	588.5876	1108.3499	-80.8608
450	2168.8005	654.5748	2921.5058	660.0951	1162.3016	-152.3683
475	2187.7751	709.0378	3039.2875	734.6157	1216.7647	-226.8889
500	2204.2461	763.9418	3151.9350	812.0156	1271.6687	-304.2888
525	2218.6244	819.2318	3259.8358	892.1719	1326.9586	-384.4450
550	2231.2434	874.8575	3363.3440	974.9699	1382.5843	-467.2430
575	2242.3723	930.7804	3462.7764	1060.3040	1438.5072	-552.5772

600	2252.2333	986.9647	3558.4241	1148.0761	1494.6916	-640.3493
650	2268.8499	1100.0069	3739.3794	1330.5749	1607.7338	-822.8480
700	2282.2130	1213.7949	3908.0268	1521.8067	1721.5218	-1014.0799
750	2293.1116	1328.1860	4065.8670	1721.1946	1835.9128	-1213.4678
800	2302.1113	1443.0730	4214.1572	1928.2318	1950.7998	-1420.5050
850	2309.6234	1558.3720	4353.9532	2142.4668	2066.0988	-1634.7400
900	2315.9583	1674.0144	4486.1523	2363.4973	2181.7413	-1855.7705
950	2321.3461	1789.9502	4611.5177	2590.9653	2297.6770	-2083.2384
1000	2325.9664	1906.1349	4730.7079	2824.5437	2413.8618	-2316.8168
1050	2329.9582	2022.5348	4844.2916	3063.9401	2530.2616	-2556.2133
1100	2333.4295	2139.1209	4952.7627	3308.8845	2646.8477	-2801.1577
1150	2336.4660	2255.8691	5056.5561	3559.1355	2763.5959	-3051.4087
1200	2339.1383	2372.7601	5156.0534	3814.4656	2880.4869	-3306.7388
1250	2341.5004	2489.7765	5251.5904	4074.6710	2997.5033	-3566.9442
1300	2343.6007	2606.9039	5343.4666	4339.5608	3114.6307	-3831.8340
1350	2345.4748	2724.1316	5431.9513	4608.9575	3231.8584	-4101.2306
1400	2347.1535	2841.4471	5517.2823	4882.6998	3349.1740	-4374.9730
1450	2348.6642	2958.8427	5599.6733	5160.6334	3466.5696	-4652.9066
1500	2350.0278	3076.3097	5679.3205	5442.6176	3584.0366	-4934.8907
1550	2351.2633	3193.8424	5756.3977	5728.5199	3701.5692	-5220.7931
1600	2352.3858	3311.4319	5831.0637	6018.2132	3819.1587	-5510.4864
1650	2353.4093	3429.0774	5903.4673	6311.5845	3936.8042	-5803.8577
1700	2354.3439	3546.7711	5973.7382	6608.5210	4054.4980	-6100.7941
1750	2355.2003	3664.5093	6041.9979	6908.9212	4172.2361	-6401.1944
1800	2355.9868	3782.2879	6108.3560	7212.6859	4290.0148	-6704.9591
1850	2356.7110	3900.1052	6172.9174	7519.7224	4407.8320	-7011.9956
1900	2357.3787	4017.9572	6235.7767	7829.9449	4525.6840	-7322.2181
1950	2357.9973	4135.8410	6297.0189	8143.2694	4643.5678	-7635.5425
2000	2358.5693	4253.7547	6356.7254	8459.6177	4761.4815	-7951.8908
2050	2359.1006	4371.6955	6414.9711	8778.9136	4879.4223	-8271.1868
2100	2359.5945	4489.6632	6471.8257	9101.0877	4997.3900	-8593.3609
2150	2360.0551	4607.6532	6527.3525	9426.0695	5115.3800	-8918.3427
2200	2360.4841	4725.6663	6581.6139	9753.7964	5233.3931	-9246.0695
2250	2360.8849	4843.6997	6634.6663	10084.2084	5351.4265	-9576.4815
2300	2361.2607	4961.7533	6686.5605	10417.2409	5469.4801	-9909.5141
2350	2361.6124	5079.8233	6737.3463	10752.8361	5587.5502	-10245.1093
2400	2361.9425	5197.9127	6787.0688	11090.9496	5705.6395	-10583.2228
2450	2362.2518	5316.0165	6835.7744	11431.5235	5823.7433	-10923.7966
2500	2362.5436	5434.1357	6883.5013	11774.5094	5941.8626	-11266.7826
2550	2362.8188	5552.2685	6930.2879	12119.8593	6059.9953	-11612.1325
2600	2363.0783	5670.4157	6976.1716	12467.5152	6178.1425	-11959.7883
2650	2363.3235	5788.5764	7021.1855	12817.4577	6296.3033	-12309.7309
2700	2363.5547	5906.7459	7065.3638	13169.6195	6414.4727	-12661.8926
2750	2363.7742	6024.9288	7108.7365	13523.9714	6532.6556	-13016.2446
2800	2363.9812	6143.1223	7151.3300	13880.4750	6650.8492	-13372.7482
2850	2364.1774	6261.3255	7193.1737	14239.0916	6769.0523	-13731.3648
2900	2364.3637	6379.5403	7234.2914	14599.7730	6887.2671	-14092.0462
2950	2364.5408	6497.7599	7274.7108	14962.4999	7005.4867	-14454.7730
3000	2364.7087	6615.9910	7314.4533	15327.2336	7123.7179	-14819.5068

Thermodynamic Properties for empirical formula $\text{Ce}_{31}\text{MnO}_{64}$ unit

Zero-point energy = 513.84 kJ/mol

T	Cv	E(T) - E(0)	S(T)	-(A(T) - E(0))	E(T)	A(T)
K	J K ⁻¹ mol ⁻¹	kJ mol ⁻¹	J K ⁻¹ mol ⁻¹	kJ mol ⁻¹	kJ mol ⁻¹	kJ mol ⁻¹
0	0.0000	0.0000	0.0000	0.0000	513.8438	513.8438
1	0.0000	0.0000	0.0000	0.0000	513.8438	513.8438
2	0.0001	0.0000	0.0000	0.0000	513.8438	513.8438
3	0.0086	0.0000	0.0009	0.0000	513.8438	513.8438
4	0.0776	0.0000	0.0103	0.0000	513.8438	513.8438
5	0.2916	0.0002	0.0473	0.0001	513.8440	513.8437
10	4.1789	0.0096	1.1955	0.0024	513.8534	513.8414
15	12.0581	0.0482	4.2256	0.0151	513.8920	513.8287
20	26.8766	0.1417	9.5030	0.0483	513.9855	513.7955
25	52.0937	0.3345	18.0061	0.1156	514.1783	513.7282
30	87.5630	0.6798	30.4980	0.2351	514.5236	513.6087
35	131.0479	1.2235	47.1749	0.4275	515.0673	513.4163
40	180.1291	1.9996	67.8274	0.7135	515.8434	513.1303
45	232.9044	3.0310	92.0619	1.1118	516.8748	512.7320
50	288.0317	4.3325	119.4378	1.6394	518.1763	512.2044
55	344.5954	5.9136	149.5343	2.3107	519.7574	511.5331
60	401.9676	7.7798	181.9737	3.1386	521.6236	510.7052
65	459.7050	9.9338	216.4270	4.1338	523.7776	509.7100
70	517.4797	12.3768	252.6098	5.3057	526.2207	508.5381
75	575.0341	15.1082	290.2767	6.6623	528.9521	507.1815
80	632.1543	18.1264	329.2148	8.2106	531.9702	505.6332
85	688.6553	21.4287	369.2378	9.9563	535.2725	503.8875
90	744.3731	25.0117	410.1816	11.9045	538.8555	501.9394
95	799.1610	28.8709	451.9000	14.0594	542.7147	499.7844
100	852.8893	33.0014	494.2626	16.4245	546.8453	497.4193
105	905.4445	37.3978	537.1518	19.0029	551.2416	494.8409
110	956.7293	42.0537	580.4619	21.7967	555.8975	492.0471
115	1006.6646	46.9628	624.0969	24.8079	560.8066	489.0359
120	1055.1856	52.1180	667.9705	28.0381	565.9618	485.8058
125	1102.2440	57.5121	712.0043	31.4879	571.3559	482.3559
130	1147.8067	63.1379	756.1277	35.1582	576.9817	478.6856
135	1191.8537	68.9876	800.2770	39.0491	582.8314	474.7947
140	1234.3766	75.0538	844.3952	43.1609	588.8976	470.6829
145	1275.3780	81.3287	888.4305	47.4929	595.1725	466.3509
150	1314.8694	87.8049	932.3378	52.0449	601.6487	461.7990
155	1352.8717	94.4748	976.0755	56.8160	608.3187	457.0279
160	1389.4107	101.3312	1019.6086	61.8052	615.1750	452.0386
165	1424.5179	108.3665	1062.9039	67.0116	622.2103	446.8323
170	1458.2307	115.5740	1105.9340	72.4337	629.4178	441.4101
175	1490.5866	122.9465	1148.6748	78.0704	636.7903	435.7734
180	1521.6297	130.4775	1191.1037	83.9199	644.3213	429.9239
185	1551.4023	138.1606	1233.2043	89.9808	652.0044	423.8631
190	1579.9502	145.9894	1274.9589	96.2513	659.8332	417.5925
195	1607.3182	153.9580	1316.3552	102.7296	667.8018	411.1142
200	1633.5513	162.0606	1357.3823	109.4141	675.9044	404.4297
205	1658.6961	170.2917	1398.0303	116.3028	684.1355	397.5410
210	1682.7965	178.6457	1438.2917	123.3937	692.4895	390.4501
215	1705.8967	187.1178	1478.1614	130.6850	700.9616	383.1588
220	1728.0383	195.7030	1517.6346	138.1746	709.5468	375.6692
225	1749.2652	204.3966	1556.7078	145.8605	718.2404	367.9833
230	1769.6167	213.1940	1595.3794	153.7409	727.0378	360.1030
235	1789.1308	222.0912	1633.6478	161.8136	735.9350	352.0302

240	1807.8476	231.0840	1671.5121	170.0766	744.9278	343.7672
245	1825.8011	240.1683	1708.9748	178.5279	754.0121	335.3159
250	1843.0272	249.3406	1746.0350	187.1656	763.1844	326.6782
255	1859.5589	258.5973	1782.6962	195.9875	772.4411	317.8563
260	1875.4288	267.9350	1818.9600	204.9917	781.7788	308.8521
265	1890.6668	277.3505	1854.8296	214.1764	791.1943	299.6675
270	1905.3020	286.8406	1890.3076	223.5393	800.6844	290.3045
273	1914.2252	292.8564	1912.4591	229.5286	806.7002	284.3152
275	1919.3627	296.4024	1925.3974	233.0786	810.2462	280.7652
277	1925.2386	300.5353	1940.3676	237.2343	814.3791	276.6095
280	1932.8746	306.0332	1960.1038	242.7924	819.8770	271.0514
285	1945.8635	315.7301	1994.4303	252.6789	829.5739	261.1649
290	1958.3528	325.4909	2028.3809	262.7361	839.3347	251.1077
294	1967.0489	332.5566	2052.5953	270.0818	846.4004	243.7620
295	1970.3664	335.3128	2061.9607	272.9620	849.1566	240.8818
296	1972.7136	337.2843	2068.6331	275.0272	851.1281	238.8166
298	1977.6998	341.5310	2082.9283	279.4902	855.3748	234.3537
300	1981.9252	345.1937	2095.1747	283.3549	859.0375	230.4889
310	2003.7608	365.1234	2160.5218	304.6344	878.9672	209.2094
320	2024.0125	385.2633	2224.4629	326.5604	899.1071	187.2834
330	2042.8207	405.5986	2287.0362	349.1189	919.4424	164.7249
340	2060.3086	426.1151	2348.2834	372.2964	939.9589	141.5474
350	2076.5901	446.8004	2408.2444	396.0799	960.6442	117.7639
360	2091.7674	467.6434	2466.9589	420.4568	981.4872	93.3870
370	2105.9329	488.6318	2524.4663	445.4148	1002.4756	68.4290
373	2110.1990	495.2729	2542.3375	453.3950	1009.1167	60.4488
380	2119.1696	509.7582	2580.8062	470.9419	1023.6020	42.9019
390	2131.5532	531.0120	2636.0146	497.0268	1044.8558	16.8170
400	2143.1528	552.3864	2690.1279	523.6582	1066.2302	-9.8144
425	2169.1115	606.2976	2820.8553	592.5583	1120.1414	-78.7145
450	2191.3653	660.8108	2945.4849	664.6493	1174.6546	-150.8055
475	2210.5660	715.8402	3064.4922	739.7848	1229.6840	-225.9410
500	2227.2324	771.3174	3178.3137	817.8297	1285.1612	-303.9859
525	2241.7820	827.1833	3287.3402	898.6595	1341.0271	-384.8157
550	2254.5506	883.3908	3391.9293	982.1588	1397.2346	-468.3150
575	2265.8118	939.8975	3492.4010	1068.2206	1453.7413	-554.3768
600	2275.7892	996.6704	3589.0489	1156.7459	1510.5142	-642.9021
650	2292.6020	1110.8945	3771.8983	1340.8237	1624.7383	-826.9799
700	2306.1230	1225.8741	3942.3101	1533.7263	1739.7179	-1019.8825
750	2317.1506	1341.4645	4101.8048	1734.8702	1855.3083	-1221.0264
800	2326.2558	1457.5556	4251.6506	1943.7436	1971.3994	-1429.8997
850	2333.8569	1574.0636	4392.9134	2159.8899	2087.9074	-1646.0461
900	2340.2657	1690.9208	4526.4993	2382.9042	2204.7646	-1869.0604
950	2345.7176	1808.0732	4653.1809	2612.4215	2321.9171	-2098.5777
1000	2350.3928	1925.4775	4773.6224	2848.1148	2439.3213	-2334.2710
1050	2354.4312	2043.0999	4888.3984	3089.6870	2556.9437	-2575.8432
1100	2357.9432	2160.9104	4998.0095	3336.8660	2674.7542	-2823.0222
1150	2361.0154	2278.8859	5102.8937	3589.4057	2792.7297	-3075.5619
1200	2363.7193	2397.0051	5203.4361	3847.0794	2910.8489	-3333.2355
1250	2366.1097	2515.2507	5299.9767	4109.6796	3029.0946	-3595.8358
1300	2368.2341	2633.6102	5392.8199	4377.0124	3147.4540	-3863.1686
1350	2370.1298	2752.0691	5482.2342	4648.9012	3265.9129	-4135.0574
1400	2371.8285	2870.6177	5568.4615	4925.1792	3384.4615	-4411.3354
1450	2373.3575	2989.2474	5651.7188	5205.6938	3503.0912	-4691.8500
1500	2374.7369	3107.9504	5732.2033	5490.3014	3621.7942	-4976.4576

1550	2375.9865	3226.7180	5810.0912	5778.8677	3740.5618	-5265.0239
1600	2377.1223	3345.5454	5885.5437	6071.2664	3859.3892	-5557.4226
1650	2378.1575	3464.4269	5958.7081	6367.3799	3978.2707	-5853.5360
1700	2379.1037	3583.3586	6029.7173	6667.0970	4097.2024	-6153.2532
1750	2379.9700	3702.3346	6098.6945	6970.3137	4216.1784	-6456.4699
1800	2380.7657	3821.3531	6165.7511	7276.9305	4335.1969	-6763.0867
1850	2381.4991	3940.4092	6230.9917	7586.8548	4454.2530	-7073.0110
1900	2382.1750	4059.5001	6294.5113	7899.9979	4573.3439	-7386.1541
1950	2382.8003	4178.6237	6356.3979	8216.2748	4692.4675	-7702.4310
2000	2383.3790	4297.7783	6416.7321	8535.6074	4811.6221	-8021.7636
2050	2383.9161	4416.9598	6475.5914	8857.9195	4930.8036	-8344.0756
2100	2384.4166	4536.1674	6533.0438	9183.1386	5050.0112	-8669.2948
2150	2384.8814	4655.3991	6589.1560	9511.1974	5169.2429	-8997.3536
2200	2385.3163	4774.6540	6643.9877	9842.0291	5288.4978	-9328.1853
2250	2385.7220	4893.9291	6697.5972	10175.5740	5407.7729	-9661.7302
2300	2386.1020	5013.2245	6750.0368	10511.7674	5527.0684	-9997.9236
2350	2386.4578	5132.5373	6801.3573	10850.5563	5646.3811	-10336.7125
2400	2386.7912	5251.8684	6851.6035	11191.8827	5765.7122	-10678.0389
2450	2387.1055	5371.2150	6900.8205	11535.6888	5885.0588	-11021.8450
2500	2387.4007	5490.5769	6949.0496	11881.9360	6004.4207	-11368.0922
2550	2387.6784	5609.9534	6996.3293	12230.5760	6123.7972	-11716.7322
2600	2387.9411	5729.3433	7042.6960	12581.5510	6243.1871	-12067.7072
2650	2388.1889	5848.7458	7088.1847	12934.8223	6362.5896	-12420.9785
2700	2388.4226	5968.1599	7132.8269	13290.3514	6482.0037	-12776.5075
2750	2388.6446	6087.5865	7176.6544	13648.0899	6601.4303	-13134.2461
2800	2388.8541	6207.0228	7219.6961	14007.9994	6720.8666	-13494.1556
2850	2389.0528	6326.4707	7261.9796	14370.0413	6840.3145	-13856.1975
2900	2389.2415	6445.9272	7303.5313	14734.1865	6959.7710	-14220.3427
2950	2389.4203	6565.3924	7344.3756	15100.3772	7079.2362	-14586.5334
3000	2389.5907	6684.8673	7384.5363	15468.6037	7198.7111	-14954.7599

Thermodynamic Properties for empirical formula $\text{Ce}_{31}\text{MnO}_{63}$ unit

Zero-point energy = 502.71 kJ/mol

T	Cv	E(T) - E(0)	S(T)	-(A(T) - E(0))	E(T)	A(T)
K	J K ⁻¹ mol ⁻¹	kJ mol ⁻¹	J K ⁻¹ mol ⁻¹	kJ mol ⁻¹	kJ mol ⁻¹	kJ mol ⁻¹
0	0.0000	0.0000	0.0000	0.0000	502.7091	502.7091
1	0.0000	0.0000	0.0000	0.0000	502.7091	502.7091
2	0.0001	0.0000	0.0000	0.0000	502.7091	502.7091
3	0.0058	0.0000	0.0006	0.0000	502.7091	502.7091
4	0.0436	0.0000	0.0063	0.0001	502.7091	502.7090
5	0.1538	0.0001	0.0261	0.0001	502.7092	502.7090
10	2.9731	0.0060	0.7448	0.0014	502.7151	502.7077
15	11.3018	0.0389	3.2960	0.0106	502.7480	502.6985
20	28.5174	0.1339	8.6481	0.0391	502.8430	502.6700
25	57.0446	0.3431	17.8662	0.1035	503.0522	502.6056
30	95.8189	0.7215	31.5574	0.2252	503.4306	502.4839
35	142.1647	1.3139	49.7288	0.4267	504.0230	502.2825
40	193.5422	2.1515	72.0220	0.7293	504.8606	501.9798
45	248.0656	3.2545	97.9424	1.1529	505.9637	501.5562
50	304.4522	4.6352	126.9849	1.7140	507.3443	500.9951

55	361.8506	6.3007	158.6887	2.4271	509.0098	500.2820
60	419.6927	8.2545	192.6521	3.3047	510.9636	499.4044
65	477.5871	10.4977	228.5323	4.3568	513.2068	498.3523
70	535.2516	13.0300	266.0376	5.5926	515.7391	497.1165
75	592.4694	15.8494	304.9204	7.0195	518.5586	495.6896
80	649.0635	18.9536	344.9679	8.6437	521.6627	494.0654
85	704.8814	22.3388	385.9962	10.4708	525.0479	492.2383
90	759.7890	26.0009	427.8451	12.5050	528.7100	490.2041
95	813.6661	29.9349	470.3731	14.7503	532.6440	487.9588
100	866.4062	34.1356	513.4548	17.2096	536.8447	485.4995
105	917.9163	38.5968	556.9783	19.8855	541.3059	482.8236
110	968.1177	43.3124	600.8437	22.7800	546.0216	479.9291
115	1016.9446	48.2757	644.9606	25.8943	550.9849	476.8148
120	1064.3465	53.4795	689.2481	29.2298	556.1886	473.4793
125	1110.2842	58.9166	733.6330	32.7870	561.6257	469.9221
130	1154.7352	64.5797	778.0501	36.5662	567.2889	466.1429
135	1197.6847	70.4615	822.4403	40.5673	573.1706	462.1418
140	1239.1300	76.5541	866.7505	44.7903	579.2633	457.9188
145	1279.0796	82.8501	910.9346	49.2346	585.5592	453.4745
150	1317.5475	89.3423	954.9500	53.8993	592.0514	448.8098
155	1354.5562	96.0231	998.7600	58.7838	598.7323	443.9253
160	1390.1340	102.8854	1042.3305	63.8865	605.5945	438.8226
165	1424.3133	109.9220	1085.6341	69.2065	612.6312	433.5026
170	1457.1315	117.1262	1128.6451	74.7423	619.8353	427.9668
175	1488.6277	124.4911	1171.3410	80.4924	627.2002	422.2167
180	1518.8435	132.0102	1213.7034	86.4551	634.7193	416.2540
185	1547.8221	139.6772	1255.7158	92.6287	642.3864	410.0804
190	1575.6083	147.4865	1297.3649	99.0115	650.1956	403.6976
195	1602.2464	155.4315	1338.6389	105.6017	658.1406	397.1074
200	1627.7811	163.5070	1379.5289	112.3972	666.2161	390.3119
205	1652.2565	171.7074	1420.0264	119.3962	674.4165	383.3129
210	1675.7159	180.0277	1460.1248	126.5967	682.7368	376.1124
215	1698.2025	188.4628	1499.8207	133.9967	691.1719	368.7124
220	1719.7579	197.0081	1539.1101	141.5941	699.7173	361.1150
225	1740.4227	205.6587	1577.9913	149.3870	708.3678	353.3222
230	1760.2371	214.4109	1616.4617	157.3732	717.1200	345.3359
235	1779.2382	223.2597	1654.5230	165.5508	725.9688	337.1583
240	1797.4620	232.2017	1692.1745	173.9177	734.9109	328.7914
245	1814.9449	241.2331	1729.4185	182.4718	743.9422	320.2373
250	1831.7202	250.3499	1766.2543	191.2111	753.0590	311.4980
255	1847.8213	259.5490	1802.6876	200.1336	762.2581	302.5755
260	1863.2780	268.8271	1838.7194	209.2372	771.5362	293.4719
265	1878.1194	278.1807	1874.3529	218.5200	780.8898	284.1891
270	1892.3754	287.6071	1909.5931	227.9799	790.3162	274.7292
275	1901.0683	293.5818	1931.5933	234.0298	796.2909	268.6793
275	1906.0728	297.1032	1944.4426	237.6151	799.8123	265.0940
277	1911.7965	301.2076	1959.3089	241.8117	803.9167	260.8974
280	1919.2363	306.6668	1978.9062	247.4236	809.3759	255.2855
285	1931.8902	316.2948	2012.9882	257.4034	819.0039	245.3057
290	1944.0593	325.9849	2046.6928	267.5528	828.6940	235.1563
294	1952.5326	332.9987	2070.7309	274.9641	835.7078	227.7450
295	1955.7645	335.7343	2080.0265	277.8696	838.4434	224.8395
296	1958.0518	337.6914	2086.6490	279.9529	840.4006	222.7562
298	1962.9108	341.9063	2100.8377	284.4545	844.6154	218.2546
300	1967.0281	345.5416	2112.9919	288.3523	848.2507	214.3568

310	1988.3066	365.3192	2177.8417	309.8075	868.0284	192.9016
320	2008.0453	385.3024	2241.2840	331.9042	888.0115	170.8050
330	2026.3771	405.4754	2303.3584	354.6283	908.1845	148.0808
340	2043.4244	425.8254	2364.1084	377.9666	928.5345	124.7425
350	2059.2976	446.3398	2423.5738	401.9059	949.0489	100.8032
360	2074.0958	467.0078	2481.7962	426.4337	969.7169	76.2754
370	2087.9078	487.8178	2538.8146	451.5375	990.5269	51.1716
373	2092.0676	494.4019	2556.5320	459.5627	997.1110	43.1464
380	2100.8153	508.7628	2594.6690	477.2057	1011.4719	25.5034
390	2112.8921	529.8313	2649.3960	503.4268	1032.5404	-0.7177
400	2124.2048	551.0176	2703.0345	530.1897	1053.7267	-27.4806
425	2149.5258	604.4473	2832.5929	599.3977	1107.1564	-96.6886
450	2171.2359	658.4626	2956.0867	671.7679	1161.1718	-169.0588
475	2189.9693	712.9836	3073.9931	747.1546	1215.6927	-244.4455
500	2206.2333	767.9407	3186.7471	825.4236	1270.6498	-322.7145
525	2220.4312	823.2769	3294.7409	906.4513	1325.9860	-403.7422
550	2232.8938	878.9470	3398.3298	990.1230	1381.6561	-487.4139
575	2243.8847	934.9095	3497.8329	1076.3327	1437.6186	-573.6236
600	2253.6244	991.1305	3593.5421	1164.9820	1493.8396	-662.2729
650	2270.0380	1104.2364	3774.6005	1349.2392	1606.9455	-846.5301
700	2283.2390	1218.0794	3943.3286	1542.2341	1720.7885	-1039.5250
750	2294.0063	1332.5187	4101.2353	1743.3896	1835.2278	-1240.6805
800	2302.8970	1447.4471	4249.5803	1952.1963	1950.1563	-1449.4872
850	2310.3194	1562.7818	4389.4213	2168.2028	2065.4909	-1665.4937
900	2316.5794	1678.4581	4521.6586	2391.0086	2181.1672	-1888.2995
950	2321.9040	1794.4228	4647.0556	2620.2519	2297.1319	-2117.5428
1000	2326.4695	1910.6345	4766.2724	2855.6086	2413.3436	-2352.8995
1050	2330.4139	2027.0585	4879.8785	3096.7832	2529.7676	-2594.0741
1100	2333.8444	2143.6658	4988.3705	3343.5078	2646.3750	-2840.7986
1150	2336.8451	2260.4343	5092.1821	3595.5390	2763.1434	-3092.8299
1200	2339.4858	2377.3427	5191.6935	3852.6511	2880.0518	-3349.9420
1250	2341.8205	2494.3764	5287.2447	4114.6386	2997.0856	-3611.9295
1300	2343.8958	2611.5193	5379.1342	4381.3115	3114.2284	-3878.6024
1350	2345.7483	2728.7605	5467.6289	4652.4921	3231.4696	-4149.7830
1400	2347.4071	2846.0895	5552.9682	4928.0185	3348.7986	-4425.3094
1450	2348.9004	2963.4977	5635.3692	5207.7371	3466.2068	-4705.0280
1500	2350.2481	3080.9762	5715.0239	5491.5062	3583.6854	-4988.7971
1550	2351.4695	3198.5185	5792.1069	5779.1926	3701.2276	-5276.4835
1600	2352.5787	3316.1196	5866.7812	6070.6728	3818.8287	-5567.9636
1650	2353.5897	3433.7738	5939.1906	6365.8290	3936.4829	-5863.1199
1700	2354.5135	3551.4762	6009.4657	6664.5524	4054.1854	-6161.8433
1750	2355.3607	3669.2231	6077.7295	6966.7396	4171.9322	-6464.0304
1800	2356.1381	3787.0085	6144.0926	7272.2892	4289.7176	-6769.5801
1850	2356.8540	3904.8334	6208.6589	7581.1146	4407.5425	-7078.4055
1900	2357.5142	4022.6922	6271.5208	7893.1240	4525.4013	-7390.4148
1950	2358.1253	4140.5827	6332.7663	8208.2363	4643.2919	-7705.5272
2000	2358.6907	4258.5032	6392.4753	8526.3706	4761.2123	-8023.6614
2050	2359.2162	4376.4498	6450.7252	8847.4544	4879.1589	-8344.7453
2100	2359.7042	4494.4214	6507.5823	9171.4163	4997.1305	-8668.7072
2150	2360.1590	4612.4181	6563.1124	9498.1860	5115.1272	-8995.4769
2200	2360.5831	4730.4360	6617.3762	9827.7027	5233.1452	-9324.9936
2250	2360.9788	4848.4752	6670.4295	10159.8948	5351.1843	-9657.1857
2300	2361.3505	4966.5327	6722.3262	10494.7182	5469.2418	-9992.0090
2350	2361.6981	5084.6076	6773.1137	10832.1080	5587.3167	-10329.3989
2400	2362.0248	5202.7017	6822.8386	11172.0064	5705.4108	-10669.2973

2450	2362.3316	5320.8094	6871.5451	11514.3749	5823.5185	-11011.6658
2500	2362.6193	5438.9315	6919.2729	11859.1459	5941.6406	-11356.4368
2550	2362.8912	5557.0681	6966.0628	12206.2807	6059.7773	-11703.5716
2600	2363.1481	5675.2192	7011.9481	12555.7312	6177.9283	-12053.0221
2650	2363.3892	5793.3829	7056.9620	12907.4588	6296.0920	-12404.7496
2700	2363.6179	5911.5571	7101.1420	13261.4055	6414.2662	-12758.6964
2750	2363.8349	6029.7420	7144.5163	13617.5520	6532.4511	-13114.8429
2800	2364.0394	6147.9384	7187.1082	13975.8406	6650.6475	-13473.1315
2850	2364.2340	6266.1454	7228.9527	14336.2422	6768.8545	-13833.5331
2900	2364.4177	6384.3602	7270.0729	14698.7278	6887.0693	-14196.0187
2950	2364.5932	6502.5846	7310.4923	15063.2300	7005.2937	-14560.5209
3000	2364.7595	6620.8187	7350.2365	15429.7584	7123.5278	-14927.0493

Thermodynamic Properties for empirical formula $\text{Ce}_{31}\text{FeO}_{64}$ unit

Zero-point energy = 512.59 kJ/mol

T K	Cv J K ⁻¹ mol ⁻¹	E(T) - E(0) kJ mol ⁻¹	S(T) J K ⁻¹ mol ⁻¹	-(A(T) - E(0)) kJ mol ⁻¹	E(T) kJ mol ⁻¹	A(T) kJ mol ⁻¹
0	0.0000	0.0000	0.0000	0.0000	512.5876	512.5876
1	0.0000	0.0000	0.0000	0.0000	512.5876	512.5876
2	0.0003	0.0000	0.0000	0.0000	512.5876	512.5876
3	0.0184	0.0001	0.0021	0.0000	512.5877	512.5876
4	0.1297	0.0001	0.0193	0.0000	512.5877	512.5876
5	0.4124	0.0004	0.0750	0.0000	512.5880	512.5876
10	4.6512	0.0112	1.4132	0.0030	512.5988	512.5846
15	13.2186	0.0537	4.7475	0.0175	512.6413	512.5701
20	29.1147	0.1556	10.5014	0.0543	512.7432	512.5332
25	55.4135	0.3625	19.6231	0.1281	512.9501	512.4594
30	91.7280	0.7265	32.7993	0.2574	513.3141	512.3301
35	135.7841	1.2927	50.1645	0.4631	513.8803	512.1244
40	185.2123	2.0932	71.4742	0.7656	514.6808	511.8220
45	238.1733	3.1506	96.3194	1.1838	515.7382	511.4038
50	293.3765	4.4788	124.2551	1.7339	517.0663	510.8536
55	349.9425	6.0867	154.8617	2.4308	518.6742	510.1568
60	407.2679	7.9794	187.7646	3.2864	520.5670	509.3012
65	464.9252	10.1598	222.6392	4.3116	522.7474	508.2759
70	522.5968	12.6286	259.2050	5.5157	525.2161	507.0719
75	580.0312	15.3853	297.2210	6.9061	527.9728	505.6814
80	637.0199	18.4282	336.4775	8.4899	531.0158	504.0976
85	693.3812	21.7544	376.7913	10.2727	534.3420	502.3149
90	748.9539	25.3606	418.0010	12.2592	537.9482	500.3283
95	803.5935	29.2424	459.9632	14.4540	541.8299	498.1336
100	857.1721	33.3947	502.5494	16.8599	545.9823	495.7276
105	909.5777	37.8121	545.6440	19.4802	550.3997	493.1074
110	960.7161	42.4883	589.1428	22.3171	555.0758	490.2705
115	1010.5059	47.4169	632.9520	25.3722	560.0045	487.2154
120	1058.8855	52.5910	676.9859	28.6469	565.1785	483.9407
125	1105.8068	58.0033	721.1679	32.1422	570.5909	480.4453
130	1151.2373	63.6465	765.4285	35.8587	576.2341	476.7289
135	1195.1554	69.5130	809.7049	39.7964	582.1006	472.7911
140	1237.5561	75.5955	853.9411	43.9556	588.1830	468.6319

145	1278.4394	81.8860	898.0862	48.3357	594.4736	464.2519
150	1317.8186	88.3772	942.0949	52.9361	600.9647	459.6515
155	1355.7128	95.0617	985.9282	57.7563	607.6492	454.8313
160	1392.1486	101.9319	1029.5494	62.7951	614.5195	449.7925
165	1427.1585	108.9806	1072.9271	68.0513	621.5682	444.5363
170	1460.7766	116.2010	1116.0353	73.5236	628.7886	439.0639
175	1493.0436	123.5862	1158.8484	79.2111	636.1738	433.3765
180	1524.0018	131.1292	1201.3455	85.1116	643.7168	427.4759
185	1553.6929	138.8239	1243.5093	91.2240	651.4115	421.3636
190	1582.1635	146.6639	1285.3238	97.5461	659.2515	415.0415
195	1609.4567	154.6437	1326.7774	104.0764	667.2312	408.5112
200	1635.6200	162.7566	1367.8570	110.8132	675.3442	401.7744
205	1660.6974	170.9978	1408.5548	117.7543	683.5854	394.8332
210	1684.7330	179.3618	1448.8644	124.8979	691.9493	387.6896
215	1707.7717	187.8435	1488.7791	132.2422	700.4311	380.3454
220	1729.8550	196.4377	1528.2946	139.7850	709.0253	372.8025
225	1751.0246	205.1404	1567.4077	147.5244	717.7280	365.0632
230	1771.3220	213.9465	1606.1176	155.4583	726.5341	357.1293
235	1790.7854	222.8519	1644.4217	163.5848	735.4395	349.0028
240	1809.4515	231.8529	1682.3209	171.9017	744.4405	340.6859
245	1827.3585	240.9451	1719.8161	180.4072	753.5327	332.1804
250	1844.5387	250.1251	1756.9079	189.0991	762.7127	323.4884
255	1861.0272	259.3893	1793.5982	197.9755	771.9768	314.6121
260	1876.8547	268.7343	1829.8902	207.0343	781.3218	305.5532
265	1892.0528	278.1567	1865.7865	216.2736	790.7443	296.3140
270	1906.6490	287.6538	1901.2894	225.6914	800.2413	286.8962
273	1915.5497	293.6737	1923.4568	231.7154	806.2613	280.8722
275	1920.6722	297.2220	1936.4041	235.2857	809.8096	277.3019
277	1926.5323	301.3578	1951.3844	239.4651	813.9453	273.1225
280	1934.1484	306.8594	1971.1330	245.0546	819.4469	267.5329
285	1947.1032	316.5626	2005.4819	254.9963	829.1502	257.5913
290	1959.5592	326.3294	2039.4542	265.1087	838.9170	247.4788
294	1968.2329	333.3996	2063.6835	272.4944	845.9872	240.0932
295	1971.5412	336.1572	2073.0548	275.3901	848.7448	237.1975
296	1973.8826	338.1299	2079.7305	277.4665	850.7174	235.1211
298	1978.8555	342.3792	2094.0340	281.9532	854.9668	230.6343
300	1983.0693	346.0439	2106.2879	285.8385	858.6315	226.7491
310	2004.8458	365.9848	2171.6715	307.2294	878.5724	205.3582
320	2025.0451	386.1354	2235.6459	329.2670	898.7229	183.3205
330	2043.8018	406.4806	2298.2508	351.9374	919.0682	160.6502
340	2061.2432	427.0067	2359.5263	375.2273	939.5943	137.3603
350	2077.4814	447.7011	2419.5138	399.1234	960.2887	113.4642
360	2092.6180	468.5523	2478.2525	423.6131	981.1398	88.9745
370	2106.7452	489.5503	2535.7831	448.6841	1002.1379	63.9034
373	2110.9997	496.1934	2553.6610	456.7000	1008.7809	55.8876
380	2119.9453	510.6835	2592.1439	474.3245	1023.2711	38.2630
390	2132.2957	531.9460	2647.3714	500.5229	1044.5336	12.0647
400	2143.8637	553.3271	2701.5038	527.2680	1065.9147	-14.6805
425	2169.7517	607.2557	2832.2728	596.4530	1119.8432	-83.8654
450	2191.9448	661.7834	2956.9365	668.8298	1174.3709	-156.2422
475	2211.0923	716.8273	3075.9745	744.2520	1229.4149	-231.6644
500	2227.7122	772.3160	3189.8210	822.5844	1284.9036	-309.9968
525	2242.2210	828.1945	3298.8708	903.7021	1340.7821	-391.1145
550	2254.9530	884.4117	3403.4781	987.4898	1396.9992	-474.9022
575	2266.1826	940.9289	3503.9682	1073.8407	1453.5165	-561.2531

600	2276.1326	997.7095	3600.6302	1162.6552	1510.2971	-650.0677
650	2292.8971	1111.9501	3783.5045	1347.3128	1624.5376	-834.7252
700	2306.3808	1226.9432	3953.9379	1540.7958	1739.5308	-1028.2082
750	2317.3759	1342.5461	4113.4493	1742.5215	1855.1337	-1229.9339
800	2326.4545	1458.6478	4263.3084	1951.9776	1971.2354	-1439.3900
850	2334.0340	1575.1654	4404.5828	2168.7068	2087.7530	-1656.1192
900	2340.4245	1692.0304	4538.1779	2392.3047	2204.6179	-1879.7172
950	2345.8606	1809.1905	4664.8678	2622.4077	2321.7781	-2109.8201
1000	2350.5217	1926.6016	4785.3168	2858.6848	2439.1892	-2346.0972
1050	2354.5492	2044.2307	4900.0978	3100.8417	2556.8183	-2588.2541
1100	2358.0505	2162.0470	5009.7146	3348.6054	2674.6345	-2836.0178
1150	2361.1144	2280.0273	5114.6030	3601.7307	2792.6148	-3089.1432
1200	2363.8099	2398.1504	5215.1496	3859.9901	2910.7380	-3347.4025
1250	2366.1929	2516.4009	5311.6944	4123.1759	3028.9884	-3610.5884
1300	2368.3114	2634.7642	5404.5400	4391.0954	3147.3518	-3878.5078
1350	2370.2013	2753.2269	5493.9568	4663.5699	3265.8145	-4150.9823
1400	2371.8958	2871.7794	5580.1866	4940.4345	3384.3670	-4427.8469
1450	2373.4190	2990.4129	5663.4473	5221.5357	3503.0005	-4708.9482
1500	2374.7951	3109.1178	5743.9334	5506.7290	3621.7054	-4994.1414
1550	2376.0414	3227.8874	5821.8238	5795.8819	3740.4750	-5283.2944
1600	2377.1739	3346.7177	5897.2772	6088.8683	3859.3053	-5576.2807
1650	2378.2057	3465.6031	5970.4432	6385.5673	3978.1906	-5872.9798
1700	2379.1485	3584.5357	6041.4533	6685.8711	4097.1233	-6173.2835
1750	2380.0124	3703.5146	6110.4321	6989.6763	4216.1022	-6477.0888
1800	2380.8065	3822.5350	6177.4903	7296.8778	4335.1226	-6784.2903
1850	2381.5373	3941.5931	6242.7327	7607.3888	4454.1806	-7094.8012
1900	2382.2108	4060.6868	6306.2522	7921.1195	4573.2744	-7408.5319
1950	2382.8344	4179.8115	6368.1396	8237.9849	4692.3990	-7725.3974
2000	2383.4114	4298.9679	6428.4755	8557.9032	4811.5555	-8045.3156
2050	2383.9477	4418.1504	6487.3348	8880.8038	4930.7380	-8368.2163
2100	2384.4457	4537.3609	6544.7872	9206.6106	5049.9485	-8694.0230
2150	2384.9105	4656.5936	6600.9010	9535.2550	5169.1812	-9022.6674
2200	2385.3429	4775.8485	6655.7336	9866.6743	5288.4361	-9354.0868
2250	2385.7469	4895.1256	6709.3439	10200.8030	5407.7131	-9688.2154
2300	2386.1261	5014.4229	6761.7835	10537.5849	5527.0105	-10024.9974
2350	2386.4811	5133.7366	6813.1048	10876.9624	5646.3242	-10364.3748
2400	2386.8137	5253.0677	6863.3511	11218.8774	5765.6553	-10706.2898
2450	2387.1272	5372.4162	6912.5680	11563.2720	5885.0038	-11050.6845
2500	2387.4215	5491.7801	6960.7980	11910.1078	6004.3677	-11397.5202
2550	2387.6984	5611.1566	7008.0785	12259.3363	6123.7441	-11746.7488
2600	2387.9603	5730.5475	7054.4460	12610.8999	6243.1350	-12098.3123
2650	2388.2072	5849.9519	7099.9347	12964.7597	6362.5395	-12452.1722
2700	2388.4408	5969.3660	7144.5778	13320.8677	6481.9536	-12808.2802
2750	2388.6612	6088.7936	7188.4053	13679.1949	6601.3811	-13166.6073
2800	2388.8707	6208.2318	7231.4470	14039.6929	6720.8193	-13527.1054
2850	2389.0686	6327.6796	7273.7305	14402.3233	6840.2672	-13889.7358
2900	2389.2573	6447.1371	7315.2822	14767.0474	6959.7247	-14254.4599
2950	2389.4361	6566.6033	7356.1273	15133.8363	7079.1909	-14621.2488
3000	2389.6057	6686.0801	7396.2880	15502.6514	7198.6677	-14990.0639

Thermodynamic Properties for empirical formula $\text{Ce}_{31}\text{CoO}_{64}$ unit

Zero-point energy = 514.10 kJ/mol

T K	Cv J K ⁻¹ mol ⁻¹	E(T) - E(0) kJ mol ⁻¹	S(T) J K ⁻¹ mol ⁻¹	-(A(T) - E(0)) kJ mol ⁻¹	E(T) kJ mol ⁻¹	A(T) kJ mol ⁻¹
0	0.0000	0.0000	0.0000	0.0000	514.1030	514.1030
1	0.0000	0.0000	0.0000	0.0000	514.1030	514.1030
2	0.0002	0.0000	0.0000	0.0000	514.1030	514.1030
3	0.0117	0.0000	0.0012	0.0000	514.1030	514.1030
4	0.1004	0.0001	0.0137	0.0000	514.1031	514.1030
5	0.3653	0.0003	0.0605	0.0001	514.1033	514.1029
10	4.9588	0.0115	1.4420	0.0029	514.1144	514.1001
15	14.0629	0.0569	5.0016	0.0181	514.1599	514.0848
20	30.6010	0.1645	11.0826	0.0571	514.2675	514.0458
25	57.6782	0.3807	20.6179	0.1347	514.4837	513.9683
30	94.8086	0.7582	34.2791	0.2702	514.8611	513.8328
35	139.6384	1.3416	52.1781	0.4845	515.4446	513.6184
40	189.7550	2.1634	74.0487	0.7986	516.2664	513.3044
45	243.2933	3.2449	99.4634	1.2311	517.3479	512.8719
50	298.9461	4.5997	127.9631	1.7983	518.7027	512.3047
55	355.8259	6.2363	159.1162	2.5151	520.3393	511.5879
60	413.3284	8.1591	192.5397	3.3933	522.2621	510.7097
65	471.0317	10.3700	227.9019	4.4436	524.4729	509.6593
70	528.6291	12.8692	264.9183	5.6751	526.9722	508.4279
75	585.8836	15.6556	303.3450	7.0950	529.7586	507.0079
80	642.6016	18.7270	342.9709	8.7105	532.8300	505.3925
85	698.6181	22.0804	383.6131	10.5265	536.1833	503.5764
90	753.7873	25.7118	425.1109	12.5481	539.8148	501.5549
95	807.9801	29.6166	467.3226	14.7788	543.7195	499.3242
100	861.0816	33.7897	510.1218	17.2222	547.8927	496.8807
105	912.9933	38.2254	553.3952	19.8808	552.3283	494.2222
110	963.6295	42.9175	597.0416	22.7567	557.0205	491.3462
115	1012.9204	47.8594	640.9690	25.8516	561.9624	488.2514
120	1060.8095	53.0442	685.0953	29.1666	567.1472	484.9363
125	1107.2552	58.4650	729.3462	32.7027	572.5680	481.4002
130	1152.2284	64.1143	773.6546	36.4602	578.2173	477.6428
135	1195.7133	69.9848	817.9603	40.4392	584.0877	473.6638
140	1237.7041	76.0688	862.2091	44.6396	590.1718	469.4634
145	1278.2057	82.3592	906.3525	49.0611	596.4622	465.0418
150	1317.2291	88.8483	950.3479	53.7029	602.9513	460.4001
155	1354.7957	95.5290	994.1554	58.5642	609.6320	455.5388
160	1390.9306	102.3939	1037.7434	63.6440	616.4968	450.4589
165	1425.6644	109.4359	1081.0795	68.9412	623.5388	445.1618
170	1459.0339	116.6482	1124.1386	74.4543	630.7512	439.6486
175	1491.0764	124.0241	1166.8977	80.1819	638.1270	433.9211
180	1521.8317	131.5568	1209.3366	86.1227	645.6597	427.9803
185	1551.3424	139.2400	1251.4388	92.2748	653.3429	421.8282
190	1579.6525	147.0680	1293.1885	98.6364	661.1710	415.4665
195	1606.8052	155.0346	1334.5748	105.2059	669.1376	408.8970
200	1632.8446	163.1341	1375.5861	111.9814	677.2370	402.1215
205	1657.8147	171.3613	1416.2142	118.9610	685.4643	395.1420
210	1681.7589	179.7105	1456.4531	126.1429	693.8135	387.9601
215	1704.7177	188.1770	1496.2962	133.5249	702.2800	380.5781
220	1726.7354	196.7559	1535.7411	141.1050	710.8589	372.9979
225	1747.8509	205.4427	1574.7835	148.8814	719.5457	365.2216

230	1768.1043	214.2329	1613.4227	156.8521	728.3359	357.2509
235	1787.5328	223.1223	1651.6579	165.0149	737.2252	349.0881
240	1806.1731	232.1068	1689.4880	173.3679	746.2098	340.7351
245	1824.0618	241.1827	1726.9158	181.9091	755.2857	332.1939
250	1841.2312	250.3463	1763.9403	190.6363	764.4493	323.4667
255	1857.7139	259.5937	1800.5658	199.5477	773.6967	314.5552
260	1873.5431	268.9222	1836.7929	208.6412	783.0252	305.4618
265	1888.7462	278.3279	1872.6260	217.9148	792.4309	296.1882
270	1903.3531	287.8085	1908.0674	227.3667	801.9115	286.7363
273	1912.2613	293.8181	1930.1965	233.4120	807.9211	280.6910
275	1917.3905	297.3606	1943.1214	236.9947	811.4636	277.1082
277	1923.2589	301.4892	1958.0767	241.1885	815.5922	272.9145
280	1930.8849	306.9812	1977.7921	246.7971	821.0842	267.3059
285	1943.8606	316.6685	2012.0828	256.7718	830.7714	257.3311
290	1956.3406	326.4190	2045.9994	266.9172	840.5219	247.1858
294	1965.0326	333.4777	2070.1896	274.3264	847.5807	239.7766
295	1968.3485	336.2309	2079.5451	277.2310	850.3338	236.8719
296	1970.6957	338.2004	2086.2100	279.3140	852.3034	234.7890
298	1975.6802	342.4429	2100.4902	283.8146	856.5458	230.2883
300	1979.9048	346.1017	2112.7241	287.7119	860.2046	226.3911
310	2001.7445	366.0112	2178.0055	309.1666	880.1142	204.9363
320	2022.0103	386.1310	2241.8826	331.2670	900.2340	182.8360
330	2040.8385	406.4463	2304.3953	353.9994	920.5493	160.1036
340	2058.3531	426.9433	2365.5834	377.3502	941.0462	136.7528
350	2074.6661	447.6092	2425.4878	401.3065	961.7122	112.7964
360	2089.8784	468.4330	2484.1492	425.8555	982.5360	88.2474
370	2104.0812	489.4031	2541.6050	450.9852	1003.5061	63.1178
373	2108.3599	496.0374	2559.4604	459.0193	1010.1404	55.0837
380	2117.3578	510.5112	2597.8959	476.6834	1024.6142	37.4196
390	2129.7822	531.7476	2653.0577	502.9389	1045.8506	11.1640
400	2141.4233	553.1037	2707.1269	529.7406	1067.2066	-15.6377
425	2167.4877	606.9734	2837.7529	599.0644	1121.0763	-84.9614
450	2189.8446	661.4461	2962.2918	671.5765	1175.5490	-157.4736
475	2209.1434	716.4388	3081.2201	747.1313	1230.5418	-233.0283
500	2225.9029	771.8822	3194.9701	825.5934	1285.9852	-311.4905
525	2240.5398	827.7163	3303.9343	906.8389	1341.8193	-392.7359
550	2253.3891	883.8930	3408.4677	990.7523	1397.9959	-476.6493
575	2264.7251	940.3726	3508.8895	1077.2271	1454.4755	-563.1242
600	2274.7715	997.1185	3605.4925	1166.1640	1511.2214	-652.0610
650	2291.7065	1111.2953	3788.2654	1351.0619	1625.3983	-836.9589
700	2305.3306	1226.2325	3958.6148	1544.7812	1740.3354	-1030.6783
750	2316.4455	1341.7852	4118.0581	1746.7395	1855.8882	-1232.6365
800	2325.6255	1457.8435	4267.8606	1956.4242	1971.9465	-1442.3213
850	2333.2907	1574.3216	4409.0868	2173.3801	2088.4245	-1659.2772
900	2339.7552	1691.1518	4542.6428	2397.2019	2205.2547	-1883.0990
950	2345.2544	1808.2791	4669.2977	2627.5268	2322.3821	-2113.4239
1000	2349.9713	1925.6622	4789.7160	2864.0249	2439.7652	-2349.9219
1050	2354.0462	2043.2643	4904.4729	3106.4008	2557.3673	-2592.2978
1100	2357.5899	2161.0574	5014.0665	3354.3825	2675.1604	-2840.2796
1150	2360.6912	2279.0146	5118.9357	3607.7259	2793.1175	-3093.6230
1200	2363.4192	2397.1184	5219.4657	3866.2014	2911.2213	-3352.0984
1250	2365.8320	2515.3505	5315.9938	4129.6024	3029.4535	-3615.4995
1300	2367.9763	2633.6955	5408.8262	4397.7361	3147.7985	-3883.6331
1350	2369.8895	2752.1419	5498.2313	4670.4248	3266.2448	-4156.3218
1400	2371.6056	2870.6799	5584.4503	4947.5016	3384.7828	-4433.3987

1450	2373.1480	2989.2989	5667.7002	5228.8161	3503.4019	-4714.7132
1500	2374.5415	3107.9903	5748.1780	5514.2226	3622.0933	-5000.1196
1550	2375.8036	3226.7492	5826.0592	5803.5878	3740.8522	-5289.4849
1600	2376.9502	3345.5680	5901.5067	6096.7845	3859.6710	-5582.6815
1650	2377.9953	3464.4418	5974.6653	6393.6958	3978.5447	-5879.5929
1700	2378.9498	3583.3647	6045.6696	6694.2099	4097.4677	-6180.1070
1750	2379.8245	3702.3331	6114.6426	6998.2255	4216.4360	-6484.1225
1800	2380.6285	3821.3448	6181.6967	7305.6393	4335.4478	-6791.5363
1850	2381.3685	3940.3942	6246.9323	7616.3606	4454.4971	-7102.2576
1900	2382.0511	4059.4783	6310.4485	7930.2997	4573.5812	-7416.1967
1950	2382.6822	4178.5961	6372.3318	8247.3745	4692.6991	-7733.2715
2000	2383.2676	4297.7449	6432.6644	8567.5021	4811.8478	-8053.3992
2050	2383.8097	4416.9206	6491.5195	8890.6122	4931.0236	-8376.5092
2100	2384.3144	4536.1234	6548.9694	9216.6283	5050.2264	-8702.5253
2150	2384.7850	4655.3503	6605.0791	9545.4821	5169.4533	-9031.3791
2200	2385.2231	4774.6013	6659.9100	9877.1098	5288.7043	-9363.0068
2250	2385.6330	4893.8707	6713.5169	10211.4459	5407.9736	-9697.3429
2300	2386.0163	5013.1632	6765.9557	10548.4401	5527.2661	-10034.3371
2350	2386.3764	5132.4711	6817.2729	10888.0202	5646.5741	-10373.9172
2400	2386.7131	5251.7984	6867.5183	11230.1474	5765.9013	-10716.0445
2450	2387.0307	5371.1410	6916.7344	11574.7544	5885.2440	-11060.6514
2500	2387.3284	5490.4982	6964.9603	11921.7927	6004.6012	-11407.6898
2550	2387.6094	5609.8718	7012.2399	12271.2239	6123.9747	-11757.1209
2600	2387.8738	5729.2588	7058.6033	12622.9997	6243.3618	-12108.8967
2650	2388.1241	5848.6575	7104.0911	12977.0718	6362.7604	-12462.9689
2700	2388.3610	5968.0696	7148.7334	13333.3921	6482.1726	-12819.2891
2750	2388.5839	6087.4914	7192.5601	13691.9219	6601.5944	-13177.8189
2800	2388.7967	6206.9257	7235.6001	14052.6322	6721.0287	-13538.5292
2850	2388.9971	6326.3707	7277.8827	14415.4652	6840.4737	-13901.3622
2900	2389.1875	6445.8253	7319.4329	14780.4016	6959.9283	-14266.2986
2950	2389.3687	6565.2876	7360.2762	15147.3931	7079.3906	-14633.2901
3000	2389.5409	6684.7596	7400.4378	15516.4108	7198.8626	-15002.3079

Thermodynamic Properties for empirical formula $\text{Ce}_{31}\text{NiO}_{64}$ unit

Zero-point energy = 515.99 kJ/mol

T K	C_v $\text{J K}^{-1} \text{mol}^{-1}$	$E(T) - E(0)$ kJ mol^{-1}	$S(T)$ $\text{J K}^{-1} \text{mol}^{-1}$	$-(A(T) - E(0))$ kJ mol^{-1}	$E(T)$ kJ mol^{-1}	$A(T)$ kJ mol^{-1}
0	0.0000	0.0000	0.0000	0.0000	515.9904	515.9904
1	0.0000	0.0000	0.0000	0.0000	515.9904	515.9904
2	0.0001	0.0000	0.0000	0.0000	515.9904	515.9904
3	0.0041	0.0000	0.0004	0.0000	515.9904	515.9904
4	0.0367	0.0000	0.0049	0.0000	515.9904	515.9904
5	0.1406	0.0002	0.0226	0.0000	515.9906	515.9904
10	2.7403	0.0057	0.6945	0.0014	515.9961	515.9891
15	9.9871	0.0351	2.9840	0.0096	516.0255	515.9808
20	25.0687	0.1186	7.6864	0.0351	516.1090	515.9553
25	50.9762	0.3041	15.8556	0.0923	516.2945	515.8981
30	87.2732	0.6458	28.2163	0.2007	516.6362	515.7897
35	131.5683	1.1901	44.9103	0.3817	517.1806	515.6087
40	181.3578	1.9706	65.6800	0.6566	517.9610	515.3338

45	234.6985	3.0096	90.0932	1.0445	519.0000	514.9459
50	290.2372	4.3212	117.6808	1.5629	520.3116	514.4275
55	347.0643	5.9141	148.0011	2.2260	521.9045	513.7644
60	404.5662	7.7929	180.6618	3.0467	523.7833	512.9437
65	462.3174	9.9601	215.3242	4.0359	525.9505	511.9545
70	520.0074	12.4160	251.6980	5.2028	528.4064	510.7876
75	577.3951	15.1596	289.5341	6.5553	531.1500	509.4351
80	634.2824	18.1890	328.6174	8.1002	534.1794	507.8902
85	690.4985	21.5013	368.7612	9.8432	537.4917	506.1472
90	745.8919	25.0926	409.8012	11.7893	541.0831	504.2012
95	800.3278	28.9586	451.5925	13.9425	544.9490	502.0479
100	853.6867	33.0941	494.0056	16.3062	549.0845	499.6842
105	905.8644	37.4934	536.9245	18.8833	553.4838	497.1071
110	956.7708	42.1506	580.2453	21.6761	558.1410	494.3143
115	1006.3328	47.0589	623.8741	24.6862	563.0493	491.3042
120	1054.4913	52.2115	667.7257	27.9151	568.2019	488.0753
125	1101.2031	57.6013	711.7242	31.3637	573.5918	484.6267
130	1146.4357	63.2210	755.8003	35.0325	579.2114	480.9579
135	1190.1733	69.0630	799.8920	38.9216	585.0534	477.0688
140	1232.4069	75.1202	843.9438	43.0313	591.1106	472.9591
145	1273.1422	81.3846	887.9051	47.3610	597.3750	468.6294
150	1312.3900	87.8490	931.7325	51.9101	603.8394	464.0804
155	1350.1712	94.5059	975.3854	56.6780	610.4963	459.3124
160	1386.5106	101.3483	1018.8295	61.6635	617.3387	454.3269
165	1421.4390	108.3686	1062.0326	66.8657	624.3590	449.1247
170	1454.9930	115.5603	1104.9687	72.2833	631.5507	443.7071
175	1487.2101	122.9163	1147.6130	77.9149	638.9067	438.0755
180	1518.1318	130.4301	1189.9455	83.7588	646.4205	432.2316
185	1547.8005	138.0955	1231.9488	89.8136	654.0859	426.1768
190	1576.2602	145.9060	1273.6061	96.0777	661.8964	419.9128
195	1603.5534	153.8560	1314.9051	102.5491	669.8464	413.4413
200	1629.7267	161.9395	1355.8358	109.2260	677.9299	406.7644
205	1654.8224	170.1514	1396.3890	116.1068	686.1418	399.8837
210	1678.8854	178.4861	1436.5573	123.1892	694.4765	392.8012
215	1701.9590	186.9385	1476.3347	130.4716	702.9289	385.5188
220	1724.0839	195.5039	1515.7164	137.9519	711.4943	378.0385
225	1745.3009	204.1777	1554.7015	145.6280	720.1681	370.3624
230	1765.6498	212.9553	1593.2850	153.4981	728.9457	362.4923
235	1785.1706	221.8327	1631.4686	161.5600	737.8231	354.4304
240	1803.8974	230.8056	1669.2497	169.8119	746.7960	346.1785
245	1821.8667	239.8703	1706.6309	178.2518	755.8607	337.7386
250	1839.1152	249.0230	1743.6122	186.8775	765.0134	329.1129
255	1855.6727	258.2601	1780.1960	195.6872	774.2505	320.3032
260	1871.5709	267.5785	1816.3850	204.6786	783.5689	311.3118
265	1886.8413	276.9747	1852.1806	213.8501	792.9651	302.1403
270	1901.5123	286.4458	1887.5879	223.1998	802.4362	292.7907
273	1910.4595	292.4497	1909.6954	229.1804	808.4401	286.8100
275	1915.6103	295.9888	1922.6078	232.7253	811.9792	283.2651
277	1921.5037	300.1136	1937.5499	236.8750	816.1040	279.1154
280	1929.1622	305.6008	1957.2469	242.4250	821.5912	273.5654
285	1942.1935	315.2795	1991.5085	252.2970	831.2699	263.6934
290	1954.7260	325.0219	2025.3960	262.3394	841.0123	253.6510
294	1963.4545	332.0746	2049.5655	269.6743	848.0651	246.3161
295	1966.7837	334.8258	2058.9143	272.5502	850.8162	243.4403
296	1969.1400	336.7937	2065.5734	274.6124	852.7842	241.3780

298	1974.1462	341.0327	2079.8436	279.0688	857.0231	236.9216
300	1978.3882	344.6888	2092.0684	282.9278	860.6792	233.0626
310	2000.3169	364.5835	2157.3016	304.1757	880.5740	211.8147
320	2020.6650	384.6896	2221.1337	326.0688	900.6800	189.9216
330	2039.5681	404.9920	2283.6057	348.5935	920.9824	167.3969
340	2057.1524	425.4763	2344.7572	371.7363	941.4667	144.2541
350	2073.5295	446.1307	2404.6284	395.4841	962.1211	120.5063
360	2088.8000	466.9431	2463.2582	419.8244	982.9335	96.1660
370	2103.0577	487.9035	2520.6857	444.7450	1003.8939	71.2454
373	2107.3521	494.5340	2538.5319	452.7132	1010.5244	63.2772
380	2116.3842	509.0010	2576.9491	470.2339	1024.9914	45.7565
390	2128.8560	530.2278	2632.0860	496.2798	1046.2182	19.7106
400	2140.5403	551.5752	2686.1328	522.8717	1067.5656	-6.8813
425	2166.7003	605.4236	2816.7089	591.6700	1121.4140	-75.6796
450	2189.1387	659.8790	2941.2054	663.6556	1175.8694	-147.6652
475	2208.5073	714.8544	3060.0963	738.6826	1230.8448	-222.6921
500	2225.3268	770.2823	3173.8163	816.6163	1286.2727	-300.6259
525	2240.0152	826.1029	3282.7531	897.3325	1342.0933	-381.3421
550	2252.9085	882.2670	3387.2632	980.7162	1398.2574	-464.7257
575	2264.2844	938.7350	3487.6651	1066.6603	1454.7254	-550.6699
600	2274.3657	995.4703	3584.2489	1155.0665	1511.4607	-639.0760
650	2291.3581	1109.6279	3766.9928	1338.9016	1625.6183	-822.9111
700	2305.0288	1224.5496	3937.3180	1531.5562	1740.5400	-1015.5658
750	2316.1811	1340.0878	4096.7413	1732.4492	1856.0783	-1216.4588
800	2325.3919	1456.1336	4246.5272	1941.0678	1972.1240	-1425.0774
850	2333.0828	1572.6001	4387.7409	2156.9566	2088.5905	-1640.9662
900	2339.5681	1689.4206	4521.2845	2379.7113	2205.4110	-1863.7209
950	2345.0857	1806.5393	4647.9311	2608.9671	2322.5297	-2092.9767
1000	2349.8183	1923.9147	4768.3410	2844.3971	2439.9051	-2328.4067
1050	2353.9065	2041.5090	4883.0904	3085.7039	2557.4994	-2569.7135
1100	2357.4626	2159.2944	4992.6782	3332.6176	2675.2849	-2816.6271
1150	2360.5731	2277.2468	5097.5417	3584.8900	2793.2372	-3068.8996
1200	2363.3102	2395.3448	5198.0658	3842.2964	2911.3352	-3326.3060
1250	2365.7314	2513.5711	5294.5906	4104.6274	3029.5615	-3588.6370
1300	2367.8832	2631.9123	5387.4196	4371.6901	3147.9027	-3855.6996
1350	2369.8030	2750.3548	5476.8214	4643.3078	3266.3452	-4127.3174
1400	2371.5233	2868.8879	5563.0371	4919.3165	3384.8783	-4403.3261
1450	2373.0715	2987.5021	5646.2845	5199.5591	3503.4926	-4683.5687
1500	2374.4691	3106.1916	5726.7590	5483.8946	3622.1820	-4967.9041
1550	2375.7354	3224.9457	5804.6385	5772.1869	3740.9362	-5256.1965
1600	2376.8853	3343.7606	5880.0836	6064.3154	3859.7511	-5548.3250
1650	2377.9338	3462.6315	5953.2396	6360.1539	3978.6219	-5844.1635
1700	2378.8916	3581.5516	6024.2422	6659.5980	4097.5420	-6143.6076
1750	2379.7696	3700.5180	6093.2136	6962.5416	4216.5084	-6446.5512
1800	2380.5762	3819.5259	6160.2660	7268.8844	4335.5163	-6752.8939
1850	2381.3186	3938.5723	6225.5008	7578.5337	4454.5627	-7062.5433
1900	2382.0029	4057.6555	6289.0154	7891.4018	4573.6459	-7375.4114
1950	2382.6365	4176.7704	6350.8970	8207.4037	4692.7608	-7691.4133
2000	2383.2235	4295.9172	6411.2287	8526.4613	4811.9077	-8010.4709
2050	2383.7681	4415.0911	6470.0838	8848.4975	4931.0815	-8332.5071
2100	2384.2736	4534.2919	6527.5321	9173.4417	5050.2823	-8657.4513
2150	2384.7459	4653.5169	6583.6409	9501.2254	5169.5073	-8985.2350
2200	2385.1857	4772.7660	6638.4710	9831.7812	5288.7564	-9315.7908
2250	2385.5965	4892.0334	6692.0780	10165.0521	5408.0238	-9649.0617
2300	2385.9814	5011.3220	6744.5143	10500.9657	5527.3125	-9984.9753

2350	2386.3423	5130.6290	6795.8323	10839.4747	5646.6194	-10323.4843
2400	2386.6807	5249.9543	6846.0760	11180.5214	5765.9448	-10664.5309
2450	2386.9991	5369.2951	6895.2905	11524.0573	5885.2855	-11008.0669
2500	2387.2976	5488.6522	6943.5171	11870.0343	6004.6427	-11354.0439
2550	2387.5795	5608.0248	6990.7943	12218.3945	6124.0152	-11702.4041
2600	2387.8455	5727.4090	7037.1593	12569.0897	6243.3994	-12053.0993
2650	2388.0958	5846.8057	7082.6464	12922.0909	6362.7961	-12406.1004
2700	2388.3336	5966.2179	7127.2870	13277.3401	6482.2083	-12761.3497
2750	2388.5581	6085.6387	7171.1136	13634.7989	6601.6291	-13118.8085
2800	2388.7701	6205.0711	7214.1545	13994.4286	6721.0615	-13478.4382
2850	2388.9721	6324.5151	7256.4355	14356.2003	6840.5055	-13840.2098
2900	2389.1634	6443.9668	7297.9856	14720.0657	6959.9572	-14204.0752
2950	2389.3446	6563.4282	7338.8289	15085.9765	7079.4186	-14569.9861
3000	2389.5176	6682.9001	7378.9880	15453.9233	7198.8905	-14937.9329
