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**Calculation and Interpretation of the Standard Chemical Exergies of
Elements Using the Chemical Reference Species**

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Table s1 Standard molar chemical exergy, \bar{e}^{CH} (kJ/kmol), of various substances at 298.15 K and p_0

Substance	Formula	Model 1	Model 2
Nitrogen	N ₂ (g)	639	720
Oxygen	O ₂ (g)	3951	3970
Carbon dioxide	CO ₂ (g)	14176	19870
Water	H ₂ O (g)	8636	9500
Water	H ₂ O (l)	45	900
Carbon (graphite)	C (s)	404589	410260
Hydrogen	H ₂ (g)	235249	236100
Sulfur	S (s)	598158	609600
Carbon monoxide	CO (g)	269412	275100
Sulfur dioxide	SO ₂ (g)	301939	313400
Nitrogen monoxide	NO (g)	88851	88900
Nitrogen dioxide	NO ₂ (g)	55565	55600
Hydrogen peroxide	H ₂ O ₂ (g)	133587	-
Hydrogen sulfide	H ₂ S	799890	812000
Ammonia	NH ₃ (g)	336684	337900
Oxygen	O (g)	231968	233700
Hydrogen	H (g)	320822	331300
Nitrogen	N (g)	453821	-
Methane	CH₄ (g)	824348	831650
Acetylene	C₂H₂ (g)	-	1265800
Ethylene	C₂H₄ (g)	-	1361100
Ethane	C₂H₆ (g)	1482033	1495840
Propylene	C₃H₆ (g)	-	2003900
Propane	C₃H₈ (g)	-	2154000
n- Butane	C₄H₁₀ (g)	-	2805800
n- Pentane	C₅H₁₂ (g)	-	3463300
Benzene	C₆H₆ (g)	-	3303600
Octane	C₈H₁₈ (l)	-	5413100
Methanol	CH₃OH(g)	715069	722300
Methanol	CH₃OH (l)	710747	718000

Ethyl alcohol	C₂H₅OH (g)	1348328	1363900
Ethyl alcohol	C₂H₅OH (l)	1342086	1375700

Source: Ref. [18].

Table s2 Calculated standard chemical exergies of elements

Chemical element		Reference species				Chemical element	
Group	Chemical Symbol	Chemical Formula	State	E_{ch}^0 (kJ/mol)	$\Delta_f G^0$ (kJ/mol)	State	E_{ch}^0 (kJ/mol)
1 A	H	H ₂ O	g	9.4936	-228.6	H ₂ , g	236.1086
		Li ⁺	ag	-	-293.3		392.3325
	Li	LiCl	s	30.8535	-384.4	s	353.4535
		LiNO ₃	s	36.5612	-381.1		411.3462
		Na ⁺	ag	-	-261.9		336.5159
	Na	NaCl	s	20.2874	-384.1	s	342.5874
		NaNO ₃	s	21.9967	-367.0		382.6817
		K ⁺	ag	-	-283.3		367.5338
	K	KCl	s	17.8964	-408.5	s	364.5964
		KNO ₃	s	23.6041	-394.9		412.1891
		Rb ⁺	ag	-	-284.0		390.4877
	Rb	RbCl	s	33.3769	-407.8	s	379.3769
		RbNO ₃	s	39.0846	-395.8		428.5696
		Cs ⁺	ag	-	-292.0		414.3802
Cs	CsCl	s	42.9548	-414.5	s	395.6548	
	CsNO ₃	s	48.6625	-406.5		448.8475	
2 A		Be ₂ SiO ₄	s	38.1147	-2032.6		604.0874
	Be	BeO.Al ₂ O ₃	s	38.1147	-2178.6	s	431.9747
		Mg ₃ Si ₄ O ₁₀ (OH) ₂	s	17.4768	-5543.0		627.3856
	Mg	Mg ²⁺ talc	ag	-	-454.8	s	609.5076
		CaCO ₃ .MgCO ₃	s	14.7545	-2163.6		633.5245
		CaCO ₃ calcite	s	16.2890	-1128.8		728.8740
	Ca	Ca ²⁺	ag	-	-553.6	s	712.6039
		Ca(NO ₃) ₂	s	21.9967	-742.8		752.1667
		SrCO ₃	s	25.8907	-1140.1		749.7757
	Sr	SrSO ₄	s	25.8907	-1340.9	s	749.2507
	Sr ²⁺	ag	-	-559.5		730.2842	

		BaSO ₄	s	30.6888	-1362.2		775.3488
	Ba	Ba ²⁺	ag	-	-560.8	s	747.5280
		Ba(NO ₃) ₂	s	36.3965	-792.6		816.3665
	Ra	RaSO ₄	s	77.2010	-1365.6	s	825.2610
3 A		B(OH) ₃	ag	-	-968.8		628.4922
	B	B(OH) ₃	s	39.3810	-968.9	s	648.1760
		Al ₂ SiO ₅	s	15.3196	-2625.9		888.3473
	Al	Al ₂ O ₃	s	17.0498	-1582.3	s	796.6974
	Ga	Ga ₂ O ₃	s	37.2472	-998.3	s	514.7961
	In	In ₂ O ₃	s	48.6876	-830.7	s	436.7163
	Tl	Tl ₂ O ₄	s	50.3807	-347.3	s, α	194.8704
4 A		CO ₂	g	19.8666	-394.4		410.2966
	C	HCO ₃ ⁻	ag	-	-586.8	s, graphite	407.8725
	Si	SiO ₂ , α quartz	s	2.2344	-856.3	s	854.5644
	Ge	GeO ₂	s	40.0862	-521.4	s	557.5162
	Sn	SnO ₂	s	36.1656	-515.8	s, white	547.9956
		PbCl ₂	ag	-	-297.2		232.8273
	Pb	PbCO ₃	s	39.8566	-625.5	s	249.1416
		PbCl(OH)	s	45.5643	-480.4		344.1293
5 A	N	N ₂	g	0.7201	0	N ₂ , g	0.7201
		HPO ₄ ²⁻	ag	-	-1089.2	s, white	861.3134
	P	Ca ₃ (PO ₄) ₂	s	20.7661	-3873.5		870.5930
		HAsO ₄ ²⁻	ag	-	-714.7		494.6214
	As	As ₂ O ₅	s	50.1581	-782.4	s	411.3166
	Sb	Sb ₂ O ₅	s	56.8861	-829.2	s	438.0806
		BiO ⁺	ag	-	-146.4		274.5675
	Bi	Bi ₂ O ₃	s	54.5784	-493.7	s	271.1617

Table s2-contd

Chemical element		Reference species				Chemical element	
Group	Chemical Symbol	Chemical Formula	State	E_{ch}^0 (kJ/mol)	$\Delta_f G^0$ (kJ/mol)	State	E_{ch}^0 (kJ/mol)
6 A	O	O ₂	g	3.9743	0	O ₂ , g	3.9743
		SO ₄ ²⁻	ag	-	-744.5		609.4389
	S	CaSO ₄ ·2H ₂ O	s	24.3172	-1797.4	s, rhombic	625.2072
		SeO ₄ ²⁻	ag	-	-441.3		346.3662
	Se	SeO ₂	s	51.7604	-171.4	s	219.1904
	Te	TeO ₂	s	62.9170	-270.3	s	329.2470

7 A		CaF ₂ .3Ca ₃ (PO ₄) ₂	s	26.5394	-12985.3		585.3994
	F	F ⁻	ag	-	-278.8	F ₂ , g	466.2229
		CaF ₂	s	26.5394	-1175.6		489.7394
		Cl ⁻	ag	-	-131.2		123.5176
	Cl	NaCl	s	20.5496	-384.1	Cl ₂ , g	136.0992
	Br	Br ⁻	ag	-	-104.0	Br ₂ , l	101.2298
		IO ₃ ⁻	ag	-	-128.0		174.7380
8 A	I	KIO ₃	s	47.2446	-418.4	I ₂ , s	186.1792
	He	He	g	30.3648	0	g	30.3648
	Ne	Ne	g	27.1557	0	g	27.1557
	Ar	Ar	g	11.6927	0	g	11.6927
	Kr	Kr	g	34.3543	0	g	34.3543
	Xe	Xe	g	40.3317	0	g	40.3317
1 B		Cu ²⁺	ag	-	+65.5		134.2576
	Cu	CuCO ₃	s	29.8506	-519.9	s	133.5356
		CuCl ₂ .3Cu(OH) ₂	s	35.5583	-1340.7		129.8483
		AgCl ₂ ⁻	ag	-	-215.5		70.2640
	Ag	AgCl	s	51.3692	-109.8	s	99.3692
		Au	s	50.6070	0		50.6070
2 B	Au	AuCl ₂ ⁻	ag	-	-151.2	s	15.4841
		Zn ²⁺	ag	-	-147.1		339.0544
	Zn	ZnCO ₃	s	29.2682	-731.5	s	344.5532
		Zn(NO ₃) ₂ .6H ₂ O	s	38.9653	-1773.1		370.9253
		CdCl ₂	ag	-	-359.4		293.7967
	Cd	CdCO ₃	s	45.1686	-669.4	s	298.3536
3 B		CdCl ₂ .5/2H ₂ O	s	54.8658	-944.1		280.1533
		HgCl ₄ ²⁻	ag	-	-446.9		115.8324
	Hg	HgCl ₂	s	52.8875	-178.6	l	107.8875
	Sc	Sc ₂ O ₃	s	36.6907	-1819.4	s, α	925.0678
	Y	Y(OH) ₃	s	34.2462	-1291.4	s, α	965.5412
	4 B	Ti	TiO ₂	s	21.6197	-888.8	s
		ZrSiO ₄	s	26.3274	-1919.1		1082.8874
Zr		ZrO ₂	s	28.0455	-1042.8	s, α	1066.8755
5 B	Hf	HfO ₂	s	39.6074	-1088.2	s, α	1123.8374
	V	V ₂ O ₅	s	31.0200	-1419.5	s	720.2975
	Nb	Nb ₂ O ₅	s	38.9653	-1766.0	s	897.5202
	Ta	Ta ₂ O ₅	s	46.3912	-1911.2	s	973.8331
		K ₂ Cr ₂ O ₇	s	33.4840	-1882.0		584.1945
	Cr	Cr ₂ O ₃	s	35.2094	-1058.1	s	543.6772
		MoO ₄ ²⁻	ag	-	-836.3	s	730.1665

6 B	Mo	CaMoO ₄	s	43.7411	-1434.7		758.1011
		MoO ₃	s	68.2534	-668.0		732.2834
		WO ₄ ²⁻	ag	-	-920.5		827.4555
	W	CaWO ₄	s	45.4028	-1538.5	s	863.5628
		WO ₃	s	69.3275	-764.1		827.4725

Table s2-contd

Chemical element		Reference species				Chemical element	
Group	Chemical Symbol	Chemical Formula	State	E_{ch}^0 (kJ/mol)	$\Delta_f G^0$ (kJ/mol)	State	E_{ch}^0 (kJ/mol)
7 B	Mn	MnO ₂	s	26.4738	-465.1		487.6038
		Mn ²⁺	ag	-	-228.1	s	422.0829
		Re ₂ O ₇	s	65.2761	-1066.0		560.6756
Re	ReO ₂	s	63.5579	-368.2	s	427.7879	
8 B	Fe	Fe ₂ O ₃	s	12.7867	-742.2	s, α	374.5158
		RuO ₂	s	69.4556	-253.1		318.5856
	Ru	Ru	s	67.7301	0	s	67.7301
	Os	OsO ₄	s	71.1738	-304.9	s	368.1338
		CoFe ₂ O ₄	s	37.3664	-1032.6		309.2264
	Co	Co ₃ O ₄	s	40.0862	-774.0	s	268.9740
		Co ²⁺	ag	-	-54.4		248.6258
	Rh	Rh ₂ O ₃	s	65.5478	-299.8		179.6964
		Rh	s	62.1153	0	s	62.1153
	Ir	IrO ₂	s	65.3240	-185.6	s	246.9540
		Ni ²⁺	ag	-	-45.6		232.7103
	Ni	NiO	s	32.8448	-211.7	s	242.5598
		NiCl ₂ ·6H ₂ O	s	38.5525	-1713.5		199.9425
		Pd	PdO	s	58.1948	-82.5	s
	PtO ₂		s	61.3833	-83.7		141.1133
Pt	Pt	s	59.6651	0	s	59.6651	
Lanthanides and actinides	La	La(OH) ₃	s	35.5290	-1319.2		994.6240
		LaCl ₃ ·7H ₂ O	s	42.9548	-2713.3	s, α	904.2598
	Ce	CeO ₂	s	33.8783	-1024.6	s, γ	1054.5082
	Pr	Pr(OH) ₃	s	38.8357	-1284.9	s, α	963.6307
		Nd(OH) ₃	s	35.8911	-1294.3		970.0861
	Nd	NdCl ₃ ·6H ₂ O	s	43.3606	-2460.6	s, α	890.0506
		Sm(OH) ₃	s	39.7631	-1314.0		993.6581
	Sm	SmCl ₃ ·6H ₂ O	s	47.1798	-2456.4	s, α	889.6698
		Eu(OH) ₃	s	43.7756	-1320.1		1003.7706
	Eu	EuCl ₃ ·6H ₂ O	s	51.2015	-2366.1	s	803.3915

	Gd(OH) ₃	s	40.1578	-1288.9		968.9528
Gd	GdCl ₃ ·6H ₂ O	s	47.5810	-2451.8	s, α	885.4710
	Tb(OH) ₃	s	44.3317	-1314.2		998.4267
Tb	TbCl ₃ ·6H ₂ O	s	51.7604	-2440.9	s, α	878.7504
	Dy(OH) ₃	s	41.7322	-1294.3		975.9272
Dy	DyCl ₃ ·6H ₂ O	s	49.1581	-2451.8	s, α	887.0481
	Ho(OH) ₃	s	44.0061	-1294.8		978.7011
Ho	HoCl ₃ ·6H ₂ O	s	51.4294	-2460.2	s, α	897.7194
	Er(OH) ₃	s	41.8733	-1291.0		972.7683
Er	ErCl ₃ ·6H ₂ O	s	49.3046	-2454.3	s	889.6946
	Tm(OH) ₃	s	46.3451	-1265.5		951.7401
Tm	Tm ₂ O ₃	s	48.0665	-1794.5	s	918.3058
	Yb(OH) ₃	s	41.8733	-1262.5		944.2683
Yb	YbCl ₃ ·6H ₂ O	s	49.3046	-2429.2	s, α	864.5946
	Lu(OH) ₃	s	46.2584	-1259.6		945.7534
Lu	LuCl ₃ ·6H ₂ O	s	53.6843	-2411.2	s	850.9743
Th	ThO ₂	s	37.4826	-1169.2	s, α	1202.7126
	UO ₃ ·H ₂ O	s	44.6730	-1395.9		1196.5330
U	UO ₃	s	44.6730	-1145.7	s	1184.4180
Pu	PuO ₂	s	108.878	-995.1	s	1100.0083