HSC - HSC Estimates 1/6 Petri Kobylin, Lauri Mäenpää, Antti Roine September 6, 2023

16. H, S, C_p Estimates Module

16.1. Introduction

-	ISC Estimate													x
File	Species Type Organi e Not Specified Function	ic Group	Show Type Column	Freeze olumn A	°C _{Celsius}	K Kelvin	n Moles Kilogra	ms Graph	ics Brows Data	e HSC Sa base Da	ive to HSC atabase *	Help Abou	it.	
A 16	-	L301104011 oc	i sun nga		1	011103		1.		1003		nep		-
F	A	В	с	D	E	F	G	Н	1	J	К	L	M	
1 2 3	Chemical Formula	Temp °C	Species Type	Selected set of possible oxidation numbers	MW g/mol	H (2 kJ Estimate	25 °C) /mol Database	S (2 J/m Estimate	5°C) ol*K Database	C J/m Estimate	p ol*K Database	ΔG (kJ/ Estimate	25°C) mol Database	
4	AgCl	25	Inorganic		143,32	-127,68	-127,07	97,37	96,23	53,54	52,98	-110,73	-109,78	
5	FeMnO4	25	Inorganic	Set 1	174,78	-1036,85	N/A	129,90	N/A	122,67	N/A	-935,51	N/A	
6	Ba(OH)2	25	Inorganic		171,34	-934,11	-939,38	103,60	107,28	83,37	89,08	-864,88	-871,24	
7	CaAl2SiO6	25	Inorganic		218,12	-3273,61	-3310,14	137,04	135,00	164,39	165,97	-3096,10	-3132,02	4
8	C8H18(g)	25	Organic, ALKANES, N	IONE	114,23	-216,90	N/A	455,06	N/A	188,15	N/A	11,77	N/A	Ξ
9	MgSO4	25	Inorganic		120,37	-1281,54	-1261,80	95,88	91,60	96,71	96,40	-1168,53	-1147,52	
10	MgSO4*2H2O	25	Inorganic		156,40	-1906,20	-1894,90	168,56	167,36	175,02	175,73	-1675,78	-1664,12	
11	K2O	25	Inorganic		94,20	-242,78	-363,20	107,20	94,10	75,69	72,00	-205,59	-322,10	4
12	K2SO4	25	Inorganic		174,26	-1296,66	-1437,79	175,12	175,56	133,83	130,77	-1178,41	-1319,67	
13	KHCO3	25	Not Specified		100,12	-958,57	-964,84	116,34	115,50	95,54	90,36	-861,03	-867,05	4
14	NaCOOH	25	Not Specified		68,01	-640,11	N/A	93,36	N/A	76,16	N/A	-570,29	N/A	
15	NaCOOH(g)	25	Not Specified		68,01	-497,62	N/A	290,55	N/A	59,99	N/A	-486,59	N/A	4
16														
17														
18														
19	1					1								-
14 4	► ► ► Sheet1						•						+	
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Fig. 1. Estimates and HSC main database H, S, and Cp data.

The HSC database contains more than 29000 species with data on enthalpy H, entropy S, and heat capacity C_p ; these data are usually based on experimental measurements. The data have been collected from more than 3000 different sources, which may contain typos and misprints. The H, S, C_p Estimate module may be used to identify and filter these errors, because it gives a rough estimate of the H, S, and C_p values based purely on chemical formula.

The H, S, C_p Estimate module gives rough estimates of H, S, and C_p values for the chemical species that exist in the HSC database, and also for those that do not exist in this database. The estimates are based on statistical data mining methods, which utilize stoichiometric element amounts, oxidation states, interactions, etc., which may be calculated automatically from the chemical formula.

As input, it accepts almost any form of chemical formula using conventional organic or inorganic expressions. Typical entries may be:

NaBO3*4H2O, H2Sn(OH)6, (C2H5)2O, Fe0.998O, etc.

To improve the estimated values, the user can define whether the species is inorganic or organic. In addition, if the species is defined as organic, the user can specify more accurately the form of the species depending on which kinds of functional groups it is formed of.

16.2. Basic use

E I	ISC Estimate																_ [0]	x
File	Species Type Organic	Organic Group Functional Group	ALKENES ALKANES ALKENES ene diene	•	now Type Column	Freeze Column A	Freeze Title Rows	°C Celsius	Kelvin Uni	n Moles	Kilograms	Graph	ics Brows Data	e HSC Sa base Di Tools	eve to HSC atabase *	Help Abou	it	
A4	✓ C2H4(g)		ALKYNES															
	A		yne	-	С		D	E	F		G	н	1	J.	К	L	М	-
1						Sele	cted set	MW	H	(25 °C)		S (2	5°C)	c	p	ΔG (25°C)	
2	Chemical Formula	a Te	mp °C	Spe	cies Typ	e of p	idation			kJ/mol		J/m	ol*K	J/m	ol*K	kJ/	mol	
3						nu	mbers	g/mol	Estimate	Dat	tabase	Estimate	Database	Estimate	Database	Estimate	Database	
4	C2H4(g)		25	Organic	, ALKENE	S, NONE		28,05	60,52	5	2,40	226,78	219,32	40,47	42,88	74,25	68,36	
5																		
6																		
7																		
8				-														=
10																		
11																		
12																		
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	Outotec																	

Fig. 2. Specifying additional properties for organic species ($C_2H_4(g)$ in this example).

Using the HSC Estimate module is fairly simple. First select the **Species Type** from the ribbon bar, and then type the chemical formula in the spreadsheet. Species can be also imported from the database to provide comparison cases for the estimates. Temperature parameter is used only for the Cp estimation.

For some species the solution provides different combinations of oxidation states, which result in slightly different estimated values. When available, the active set can be selected from the cell in the column D.

1	ISC Estimate									
	Species Type	Organic Group		*					°C	
HI T	e Not Specified 🔻	Functional Group	inal Group			Column	A Title Row	/S	Celsius	
Ma	ain	Estima	ation Se	ttings						
D4	✓ Set 1									
	A	В			С		D		E	
1	Chemical Form	Chemical Formula Temp °C		Spec	cies Typ	e S	elected set of possible		MW	
3							numbers		g/mol	
4	FeVO4		25	Not Spec	ified		Set 1	-	170,78	
5						Se	1			
6						Set	3			

Fig. 3. Changing the active set of oxidation numbers.

The oxidation numbers can be seen in the columns after the estimated values.

	А	N	0	Р	Q	R	S	Т	U	V	W	Х	Y	Z	AA	AB	*
1		Elemen	t Informati	ion			Elemen	t Informatio	on			Elemen	t Informati	ion			
2	Chemical Formula																
3		Elem1	Amount	Charge	Weight-%	Atom-%	Elem2	Amount	Charge	Weight-%	Atom-%	Elem3	Amount	Charge	Weight-%	Atom-%	=
4	FeVO4	V	1	5	29.83	16.67	Ee	1	3	32.70	16.67	0	4	-2	37.47	66.67	
			-		20,00	20,07		-		/	/	-		-		, ,	
5					20,00	10,07											

Fig. 4. Information about the elements found in the chemical formula.

16.3. Limitations

- 1. Superscripts and subscripts are not allowed.
- 2. The last parentheses are always reserved for species-type declarations, for example:

As(g)	Arsenic gas	С	Carbon
O2(g)	Oxygen gas	C(D)	Diamond
Fe(l)	Liquid iron	FeS2	Pyrite
OH(-a)	Aqueous OH ion	FeS2(M)	Marcasite

Example cases of the use of the last parentheses are shown below. Please note that incorrect use of the parentheses may result in estimations that are not carried out for the correct chemical formula.

Chemical formula: AIO(OH) - aluminium oxide hydroxide

AIO(OH)	Valid species, but estimated as AIO not as AIO(OH)
AIO2H	Valid species
AIO*(OH)	Invalid species
AIO*ÒH Í	Valid species
AIOOH	Valid species

16.4. Charts

Database and estimated values can be plotted to facilitate comparison. To plot the values, select the rows that you want to include in the chart and select the chart type from the ribbon bar or from the right-click menu.



Fig. 5. Plotting species in HSC Estimates.

16.5. Adding estimated species to own database

Estimated values can be utilized in other HSC modules, if the species are saved to the own database. Species can be saved either with a constant Cp value, estimated at 25 °C, or with a temperature range, specified by the user.

To add a species to the own database select a row and click "Save to HSC Database" from the ribbon bar or from the right-click menu. Selecting the "Cp at 25 °C" will open the Database editor allowing to review the species before saving. With the "Cp Range" option the Fit Cp Data window is shown with the estimated range.

Example

Estimate Na2WO4(g) and add it to the own database with the Cp estimated in the temperature range of 298.15 K - 600 K.

1. Estimate Na2WO4(g)

Type the formula to the first column in the spreadsheet.

	A	В	С
1			
2	Chemical Formula	Temp °C	Species Type
3			
4	Na2WO4(g)	25	Not Specified
5			

2. Save with a Cp range

Right-click the species and select "Save to HSC Database > Cp Range".

4	Na2WO4(g)	V	Cut		25	Not Specifie
5		60	Cut			
6			Сору			
7		Ē.	Paste			
8			Insert Row			
9		=	Delete Row			
10			Delete Now	-		
11			Browse HSC Database			
12		al	Graphics			
13		R	Save to HSC Database		a c	n at 25°C
14				- AN		
15					100	p Kange

3. Specify range parameters

Change the Max temperature to 600 and click "OK".

Parameters		
Species	Na2WO4(g)	
Tmin (K)	298,15	
Tmax (K)	600	
Steps	50 🛟	
ОК	Cancel	

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4. Fit the values to the Cp equation

Click the "Fit Cp" button to get the equation coefficients for the specified temperature range. If necessary, the range can be divided into several records for a better fit to the equation.

HSC	Cp Data											
xpe	rimental Data					F	tted Data					
Z	Import from Eq	uation				0	$T_p(T) = A + BT * 10^{-3} + CT^{-2} *$	10 ⁵ + DT ² *	10-6	•		Jpdate Specie:
	A	В	С	D	E		A	В	С	D	E	F
1		Species	Na2WO4(g)				1 Range	1	2	3	4	5
2	1	Molecular Weight	293.817				2 Tmin (K)	298.15				
3	Temperature	Cp Experimental	Cp Fitting	Error	Cp Estimate		3 Tmax (K)	600				
4	к	J/(mol*K)	J/(mol*K)		J/(mol*K)		4 Cp coefficient A J/(mol*K)	193.371				
5	298.15	121.043	121.408	-0.302			5 Cp coefficient B	-104.887				
6	304.187	122.958	123.084	-0.102			5 Cp coefficient C	-44.022				
7	310.224	124.678	124.651	0.022			7 Cp coefficient D	99.354				
8	316.261	126.237	126.124	0.090			B Cp coefficient E	0.000				
9	322.298	127.664	127.508	0.123	_		9 Cp coefficient F	0.000				
10	328.335	128.979	128.807	0.134	-		0 Average Error					
1	334.372	130.199	130.033	0.127			• • • H Hitted	1 2020	-			
12	340.409	131.336	131.190	0.112		6	Calculate C	p	s Type	Structure		Estimate C
3	346.446	132.401	132.281	0.091				Not 9	pecified •		-	
4	352.483	133.403	133.312	0.068		0	hart					
5	358.52	134.348	134.289	0.044		1		Cn He	at Capacity			
6	364.557	135.243	135.215	0.021)	op no	are cupating			
.7	370.594	136.093	136.092	0.001			155					
.8	376.631	136.901	136.926	-0.018								-
.9	382.668	137.673	137.721	-0.035			150				-	
0	388.705	138.410	138.476	-0.047						/		
1	394.742	139.117	139.197	-0.058			145 -	Fitted				
22	400.779	139.795	139.886	-0.065				1000				
:3	406.816	140.447	140.545	-0.070		1	140 -	/	Experiment	tal		
4	412.853	141.075	141.175	-0.071		0	/					
5	418.89	141.679	141.780	-0.071			\$135 -					
17	424.927	142.203	142.361	-0.069								
18	430.964	142.828	142.919	-0.064			130					
0	437.001	143.373	143.457	-0.058			175					
20	443.038	143.902	143.570	-0.031								
1	455 112	144.912	144.476	-0.042			120					
2	455.112	144.912	145.430	-0.033								
23	467 186	145.865	145 885	-0.014			×				i	
1	473 223	145.805	146 327	-0.004		-	300 350	400	450	500	550	1.
		140.377	1.4401.377						emperature	5		

5. After fitting, save the coefficients

Click "Update Species" to save the coefficients to the Database and close the Cp Fit dialog.

C _p ($(T) = A + BT * 10^{-3} + CT^{-2} *$	$10^{5} + DT^{2} *$	10-6			Jpdate Species
	A	В	С	D	E	F
1	Range	1	2	3	4	5
2	Tmin (K)	298.15				
3	Tmax (K)	600				
4	Cp coefficient A J/(mol*K)	193.371				
5	Cp coefficient B	-104.887				
6	Cp coefficient C	-44.022				
7	Cp coefficient D	99.354				
8	Cp coefficient E	0.000				
9	Cp coefficient F	0.000				
10	Average Error					
• •	Fitted			•		

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6. Save the species

Finally, review the data for the new species and click "Save".

Database Editor												. 🗆 🗙
File Edit Add New F T Species S	Remove Save Cancel	Joules Calories	Kelvin Cel	C Main C	Database	Own Database	Find by Elements	Diagrams	DB Merg	PE Fit Cp Data	() Help	About
Menu		Unit	Temperatu	re	Database	e Selection		To	ols		Info	
							Select A	li l				
Elements			Possible Spec	ties	- 5	🖉 Gases	V Liquids		1	ndude Organics		
Formula Na2WO4(g)			Start With		- 6	🛛 Gas Ions	Aqueou	s Ions	Ran	oe Of Carbon &	tome	
Stoichiometry			Free Ratio		- 6	Z Condensed	Aqueou	s Neutrals		ge of calcorn	1991119	
Keywords			Structural For	mula, Che	+	Z Electrons	V Fluids					
	Basic Data - Diodated on	14.2.2017]										
Na2WO4(n)	Formula Na7M	04(a)		CAS				40 formation at	209 15 V	-1248 563		k1/mol
	Structural Formula		Mol	ecular Weight	293.817	6	a/mol	S° at	298.15 K	412.671		1/(mol*K)
	Chemical Name			Melting Point	0.000		к	Co at	298.15 K	121,408		J/(mol*K)
	Common Name			Boiling Point	0.000		к	ΔG° at	298, 15 K	-1182,404		k3/mol
	Temperature Ranges	$C_p(T) = A + BT * 10^{\circ}$	$-3 + CT^{-2} + 1$	$10^{5} + DT^{2} *$	10-6							
	A1 -	Range										
	Range	1	2	3		4	5	6		7	8	9 ^
	Tmin (K)	298.15										
	Tmax (K)	600.00										
	Phase	g										
	H kJ / mol	-1248.564										
	SJ/(mol*K)	412.671										
	Cp coefficient A J/(moi	-104.887										
	Cp coefficient C	-44.022										
	Cp coefficient D	99.354										
	Density g/l (0 *C, 1 atm)	0.000										
	Color	0										
	Solubility in H2O g/I	0.000										
	Reference	HSC Estimate										
	Reliability Class	4										
	Coloring Couries . 0					*****						
Outotec Database	s in use 🔻											