

16. H, S, C_p Estimates Module

The screenshot shows the 'H, S, Cp Estimate' window. At the top, there is a 'Species' input field containing 'Mg3Si2O5(OH)4', a 'Species Type' dropdown set to 'Inorganic', and a 'Temperature' input field set to '25'. There are checkboxes for '°C' (checked) and 'K'. An 'Estimate' button is also present. Below this is a table with columns A through M. The table contains data for 14 species, including AgCl, B3O3HF2(g), Ba(OH)2, CaAl2SiO6, Cl7H34O2(HDAG), CrO(OH)(g), Na(C2H3O3)2(-a), NaCN, MgSO4, Fe2O3, and Mg3Si2O5(OH)4. The table columns include Chemical Formula, Species Type, Temperature (°C and K), Selected set of possible oxidation numbers, Weight (MW and IW), H (25 °C) in kJ/mol (Estimate and Database), S (25 °C) in J/mol*K (Estimate and Database), and Cp in J/mol*K (Estimate and Database).

	A	B	C		D	E	F		G		H (25 °C)		I		J (25 °C)		K		L		M	
			Chemical Formula	Species Type			Temperature	Temperature	Selected set of possible oxidation numbers	Weight	Weight	Weight	Weight	Estimate	Database	Estimate	Database	Estimate	Database	Estimate	Database	Estimate
4	AgCl	Inorganic	25	298.15			143.32				-127.68	-127.07	97.37	96.23	53.54	52.98						
5	B3O3HF2(g)	Inorganic	25	298.15			119.43				-2168.31	-1987.40	340.62	329.00	112.72	103.55						
6	Ba(OH)2	Inorganic	25	298.15			171.34				-934.11	-939.38	103.60	107.28	83.37	89.08						
7	CaAl2SiO6	Inorganic	25	298.15			218.12				-3273.61	-3296.67	137.04	144.50	164.39	165.97						
8	Cl7H34O2(HDAG)	Organic, ALKANES	25	298.15			270.45				-641.53	-744.00	828.85	872.94	404.42	410.33						
9	CrO(OH)(g)	Inorganic	25	298.15			85.00				-180.12	-199.26	269.22	284.01	55.70	53.82						
10	Na(C2H3O3)2(-a)	Inorganic	25	298.15			173.08	173.08			-1598.79	-1546.74	N/A	236.81	N/A	713.30						
11	NaCN	Inorganic	25	298.15		1.00	49.01				-81.70	-87.45	64.39	115.48	54.86	68.68						
12	MgSO4	Inorganic	25	298.15			120.36				-1281.54	-1261.80	95.88	91.60	96.71	96.40						
13	Fe2O3	Inorganic	25	298.15			159.69				-781.07	-826.20	92.90	87.40	106.89	103.76						
14	Mg3Si2O5(OH)4	Inorganic	25	298.15			277.11				-4371.05	-4362.99	244.50	219.82	282.79	277.90						

Fig. 1. Estimates and HSC main database H, S, and Cp data.

The HSC 8.0 database contains more than 28000 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 Estimates 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 Estimates 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.

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, Fe_{0.998}O, 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.

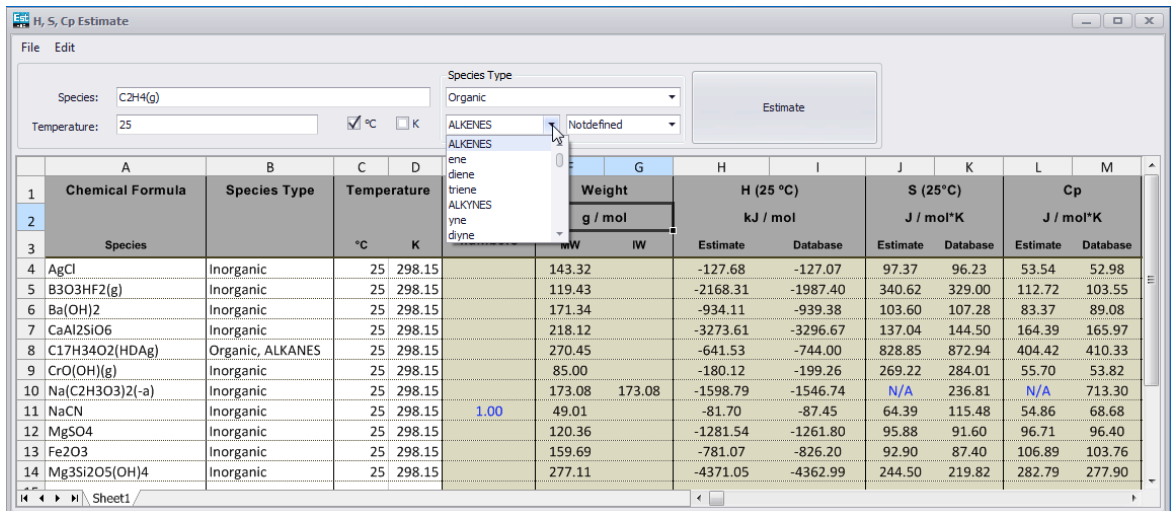


Fig. 2. Specifying additional properties for organic species (C₂H₄(g) in this example).

It is easy to use this module. To type chemical formulae in the **Species** field, select **Species Type** if you know it and click **Estimate**. You can collect several results on the sheet. You can print the results using **File - Print**. The HSC Estimates module uses the same routine for calculating the formula weights and elemental composition as all other calculation options in HSC. Therefore you can test the correct formula formats in this option. **Edit - Copy** will copy the results into the clipboard.

You can modify the sheet by clicking the right mouse button.

Limitations:

- Superscripts and subscripts are not allowed.
- Inner parentheses are not allowed, for example: H₂(Sn(OH)₆) is not a valid formula. Use H₂Sn(OH)₆ instead.
- The last parentheses are always reserved for species-type declarations, for example:

As(g)	Arsenic gas	C	Carbon
O ₂ (g)	Oxygen gas	C(D)	Diamond
Fe(l)	Liquid iron	FeS ₂	Pyrite
OH(-a)	Aqueous OH ion	FeS ₂ (M)	Marcasite

If you want to write the following formula;
 please write it in one of the following ways:
 (The last parentheses are reserved for the suffix) AIO*(OH)
 AIO(OH) Not valid
 AIO2H Valid
 AIO*(OH) Valid
 AIO*OH Valid

Element Information					Element Information					Element Information					Element Information					
Elem1	Amount	Charge	Weight-%	Atom-%	Elem2	Amount	Charge	Weight-%	Atom-%	Elem3	Amount	Charge	Weight-%	Atom-%	Elem4	Amount	Charge	Weight-%	Atom-%	
Ag	1.00	1.00	75.26	50.00	Cl	1.00	-1.00	24.74	50.00											
B	3.00	2.33	27.15	33.33	H	1.00	1.00	0.84	11.11	O	3.00	-2.00	40.19	33.33	F	2.00	-1.00	31.81	22.22	
Ba	1.00	2.00	80.15	20.00	H	2.00	1.00	1.18	40.00	O	2.00	-2.00	18.68	40.00						
Ca	1.00	2.00	18.37	10.00	Al	2.00	3.00	24.74	20.00	Si	1.00	4.00	12.88	10.00	O	6.00	-2.00	44.01	60.00	
H	34.00	1.00	12.67	64.15	C	17.00	-1.76	75.50	32.08	O	2.00	-2.00	11.83	3.77						
Cr	1.00	3.00	61.17	25.00	H	1.00	1.00	1.19	25.00	O	2.00	-2.00	37.64	50.00						
Na	1.00	1.00	13.28	5.88	H	6.00	1.00	3.49	35.29	C	4.00	1.00	27.76	23.53	O	6.00	-2.00	55.46	35.29	
Na	1.00	1.00	46.91	33.33	C	1.00	2.00	24.51	33.33	N	1.00	-3.00	28.58	33.33						
Mg	1.00	2.00	20.19	16.67	S	1.00	6.00	26.64	16.67	O	4.00	-2.00	53.17	66.67						
Fe	2.00	3.00	69.94	40.00	O	3.00	-2.00	30.06	60.00											
Mg	3.00	2.00	26.31	16.67	Si	2.00	4.00	20.27	11.11	H	4.00	1.00	1.45	22.22	O	9.00	-2.00	51.96	50.00	

Fig. 3. Information for elements for species in Fig. 1.

H, S, C_p 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. This module is quite easy to use: the user types in the formula and the program gives the formula weight, oxidation states, and H, S, and C_p estimates.

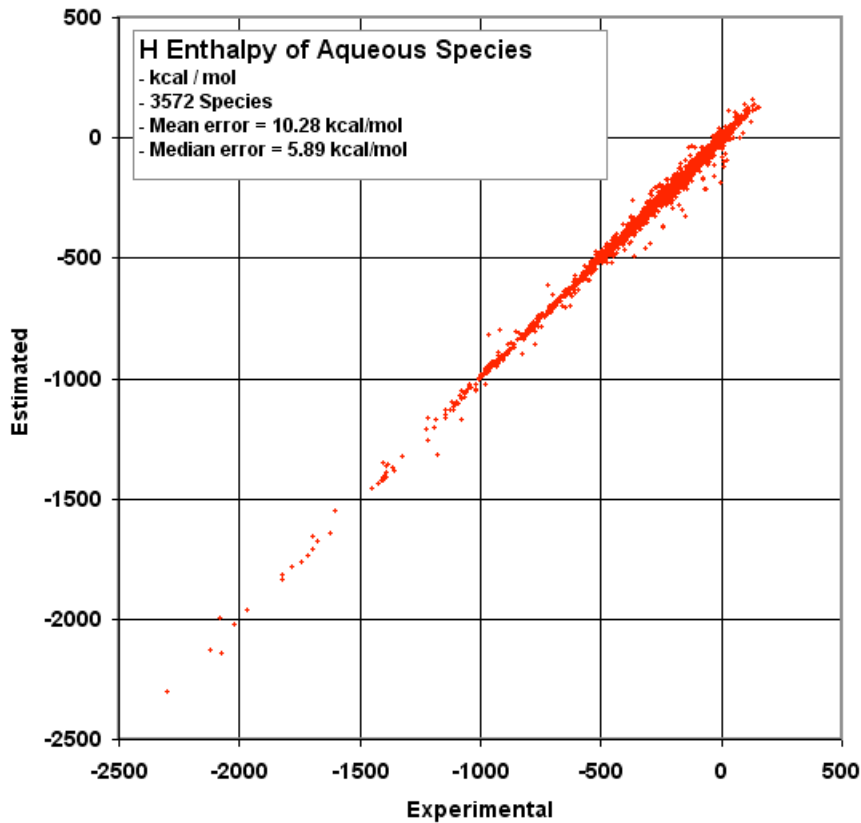


Fig. 4. Enthalpy of aqueous species on the HSC main database compared to estimated data.

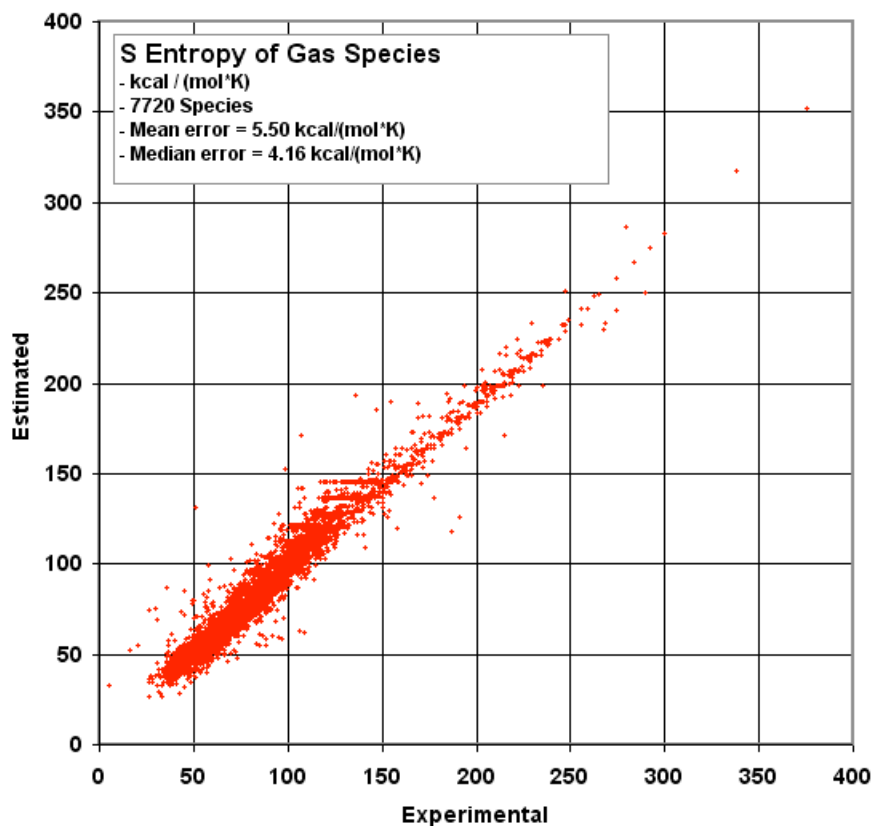


Fig. 5. Entropy of gas species on the HSC database compared to estimated data.