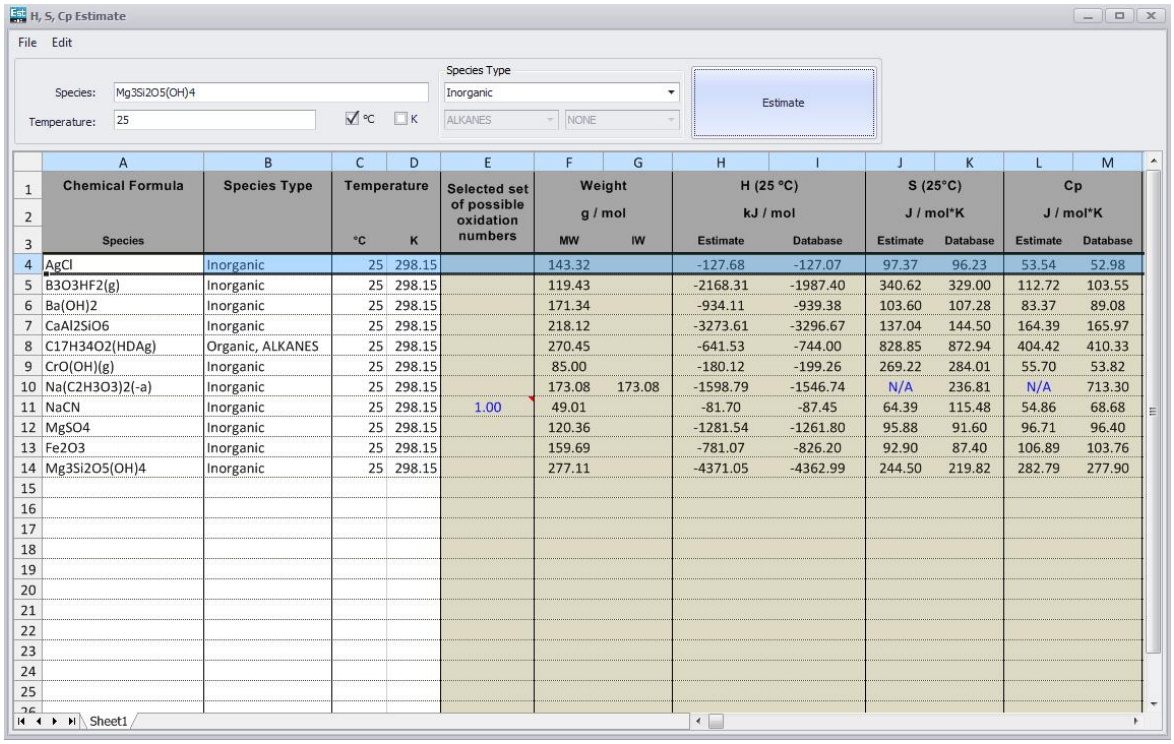
16. H, S, C_p Estimates Module



	Chemical Formula / Species	Species Type	Temperature °C	Temperature K	Selected set of possible oxidation numbers	Weight g / mol MW	Weight g / mol IW	H (25 °C) kJ / mol Estimate	H (25 °C) kJ / mol Database	S (25°C) J / mol*K Estimate	S (25°C) J / mol*K Database	Cp J / mol*K Estimate	Cp J / mol*K Database
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	C17H34O2(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.

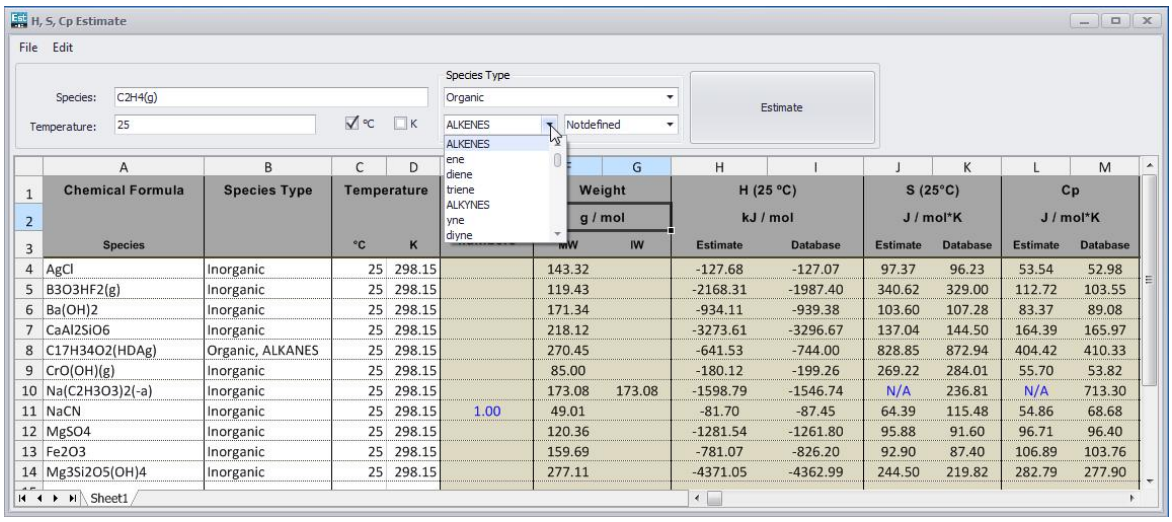
The HSC 8.0 database contains more than 28000 species with data on enthalpy H, entropy S, and heat capacity C_p; these data are usually based on experimental measurements. The data have been collected from more than 3000 different sources, which may contain typos and misprints. The H, S, C_p Estimates 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, 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.



	A	B	C	D		G	H	I	J	K	L	M
1	Chemical Formula	Species Type	Temperature			Weight	H (25 °C)		S (25°C)		Cp	
2						g / mol	kJ / mol		J / mol*K		J / mol*K	
3	Species		°C	K		IW	Estimate	Database	Estimate	Database	Estimate	Database
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
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14	Mg3Si2O5(OH)4	Inorganic	25	298.15		277.11	-4371.05	-4362.99	244.50	219.82	282.79	277.90

Sheet1

Fig. 2. Specifying additional properties for organic species (C_2H_4(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:

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

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

If you want to write the following formula;	AlO(OH)	Not valid
please write it in one of the following ways:	AlO2H	Valid
(The last parentheses are reserved for the suffix)	AlO*(OH)	Valid
	AlO*OH	Valid

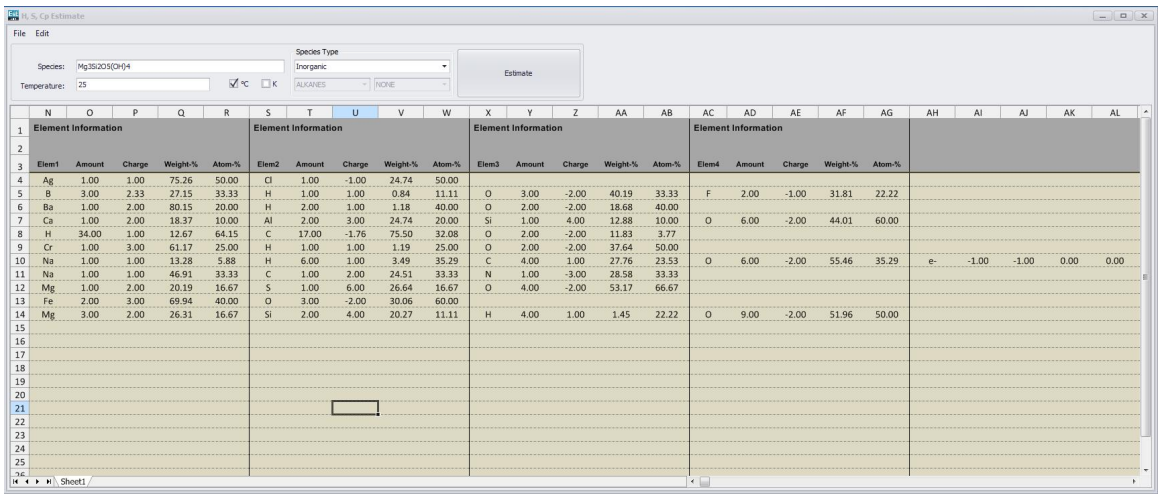

Fig. 3. Information for elements for species in **Fig. 1**.

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 Cp estimates.

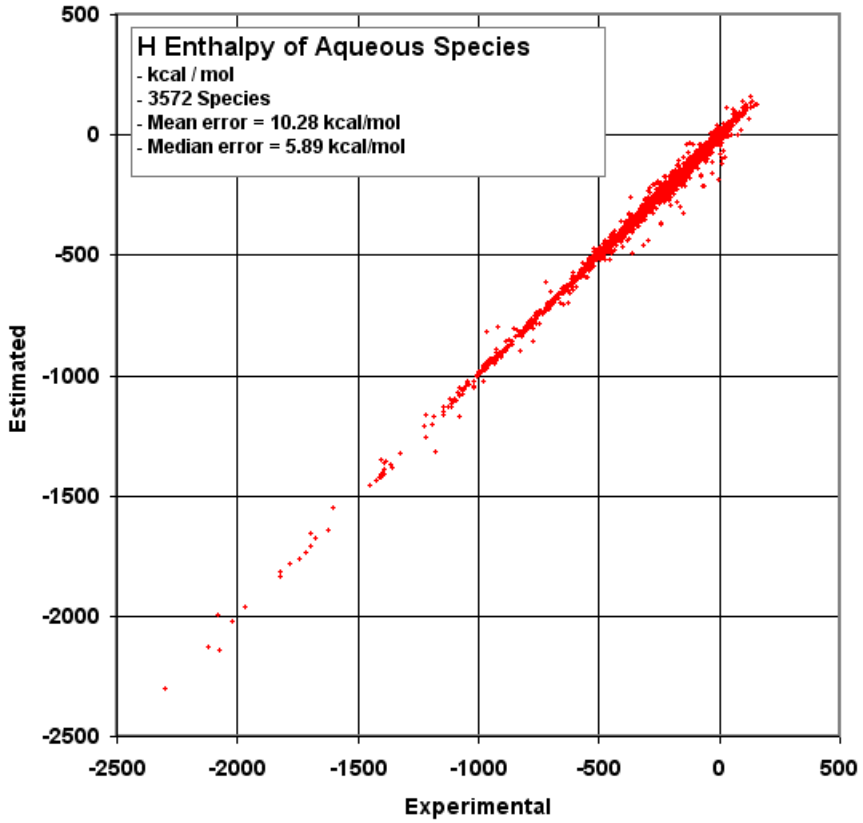

Fig. 4. Enthalpy of aqueous species on the HSC main database compared to estimated data.

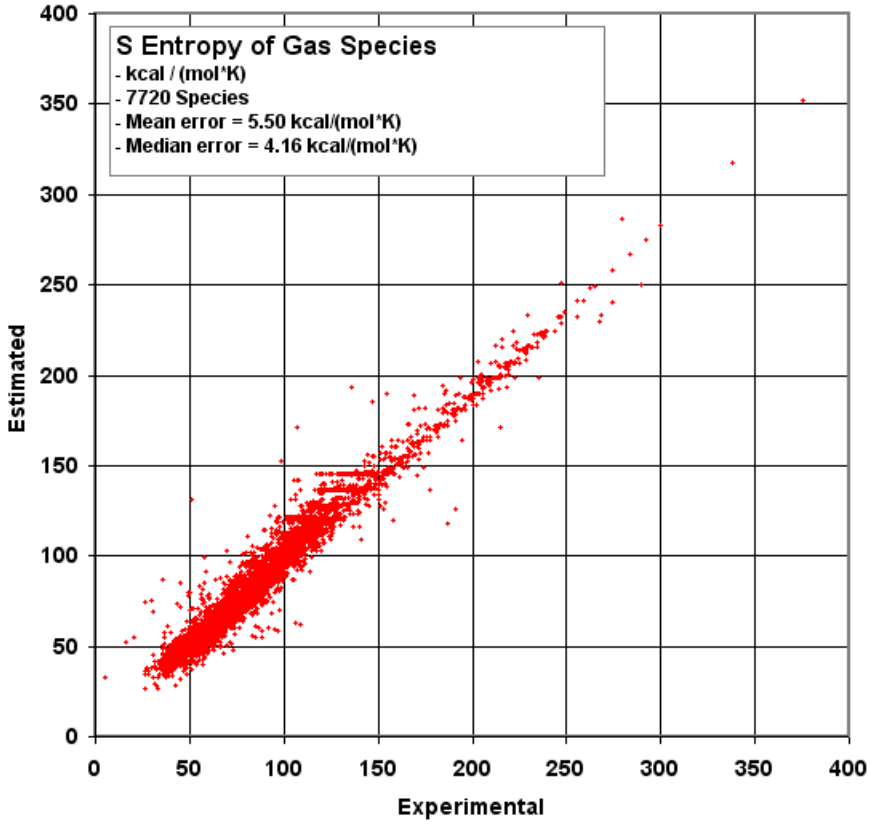

Fig. 5. Entropy of gas species on the HSC database compared to estimated data.