

16. FORMULA WEIGHTS

	A	B	C	D	E	F	G	H	I
1	DB	ROUGH ESTIMATES	T	H	kcal/mol	S	cal/(mol*K)	Cp	cal/(mol*K)
2	No	Chemical Formula	°C	Estimate	Database	Estimate	Database	Estimate	Database
3	2	AgCl	25.00	-32.35	-30.37	25.40	23.00	13.07	12.66
4	2	B3O3HF2(g)	25.00	-464.35	-475.00	81.73	78.63	25.80	24.75
5	2	Ba(OH)2	25.00	-228.58	-224.52	25.53	25.64	18.89	21.29
6	2	CaAl2SiO6	25.00	-780.73	-787.92	35.84	34.54	41.38	39.67
7	2	C17H34O2(HDAg)	25.00	-166.37	-177.82	197.79	208.64	96.58	98.07
8	2	CrO(OH)(g)	25.00	-46.70	-47.63	67.35	67.88	13.41	12.86
9	2	Na(C2H3O3)2(-a)	25.00	-384.92	-369.68	N/A	56.60	N/A	170.48
10	2	NaCN	25.00	-18.51	-20.90	18.75	27.60	13.48	16.41
11	2	MgSO4	25.00	-306.92	-301.58	28.49	21.89	26.24	23.04
12	2	Fe2O3	25.00	-183.50	-197.47	28.20	20.89	26.01	24.80
13	2	Mg3Si2O5(OH)4	25.00	-1041.15	-1042.78	62.20	52.54	64.79	66.42

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

The HSC 7.0 database contains more than 25000 species with enthalpy H, entropy S, and heat capacity Cp data; this data is usually based on experimental measurements. The data has been collected from more than 3000 different sources, which may contain typos and misprints. The new HSC Estimates module may be used to identify and filter these errors, because it gives a rough estimate of the H, S, and Cp values based purely on chemical formula.

The new HSC Estimates module gives rough estimates of H, S and Cp 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.

You can collect several results on the sheet. **Clear** will clear the whole sheet. You can print the results using **Print**. The Formula Weight option uses the same routine for calculating the formula weights and elemental composition as all other calculation options in the HSC. Therefore you can test the correct formula formats in this option. **Copy** will copy the results into the clipboard.

You can select mol or kg units for column E as well as the total amount from the box at top right corner of the form. By pressing mouse right button you can, for example, modify number format.

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. **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;
please write it in one of the following ways:
(Last parenthesis are reserved for suffix)

AIO(OH)	Not valid
AIO2H	Valid
AIO*(OH)	Valid
AIO*OH	Valid

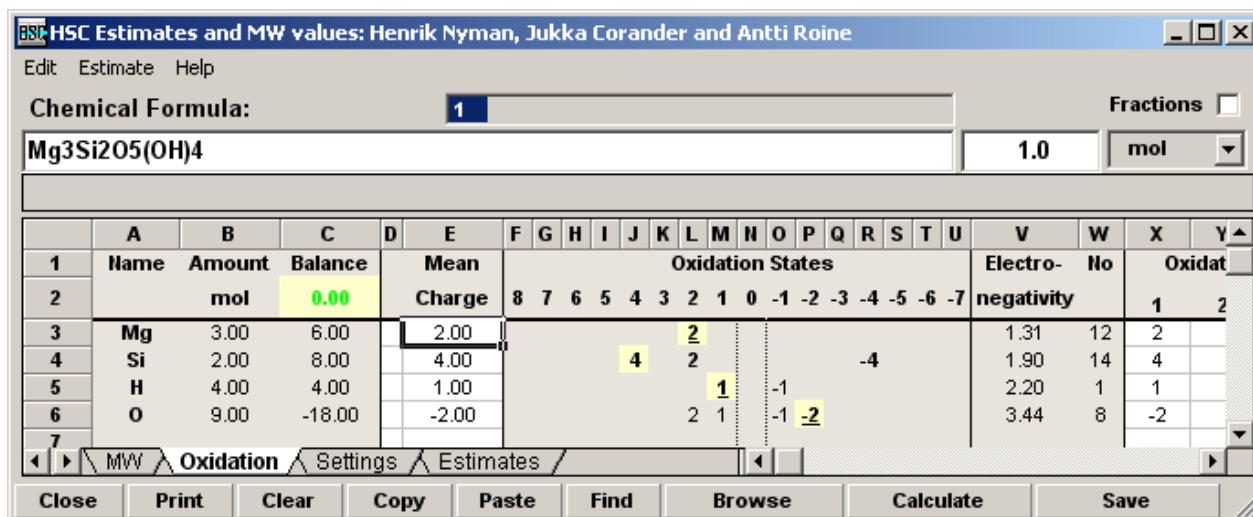


Fig. 2. Oxidation states for elements in the selected chemical compound.

HSC 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.

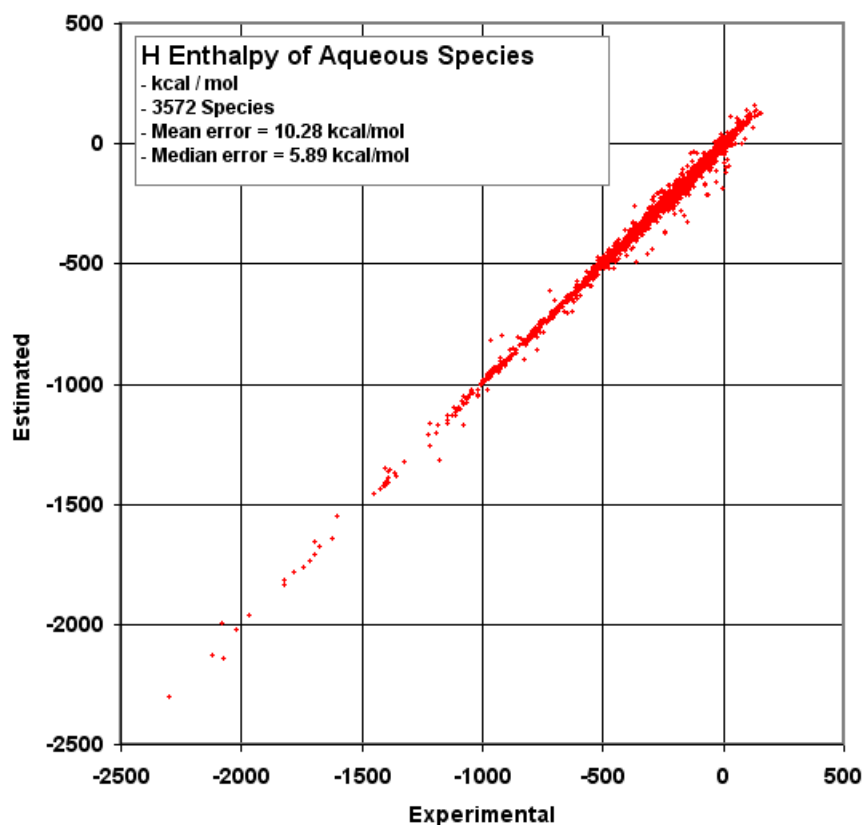


Fig. 3. Enthalpy of aqueous species in HSC main database compared to estimated data.

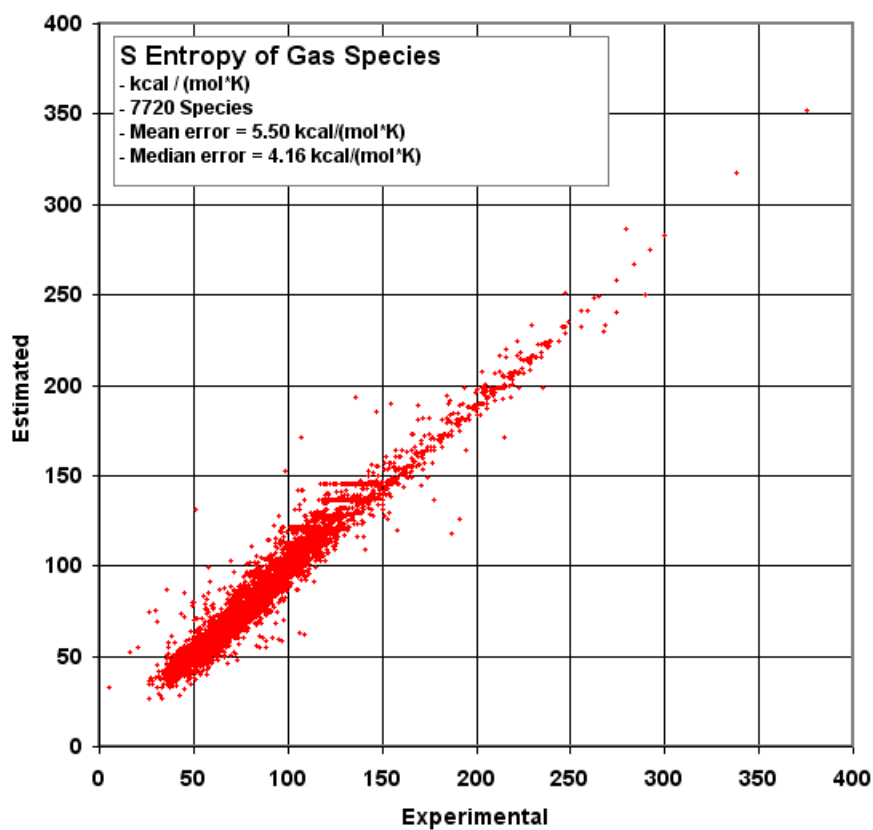


Fig. 4. Entropy of gas species in HSC database compared to estimated data.