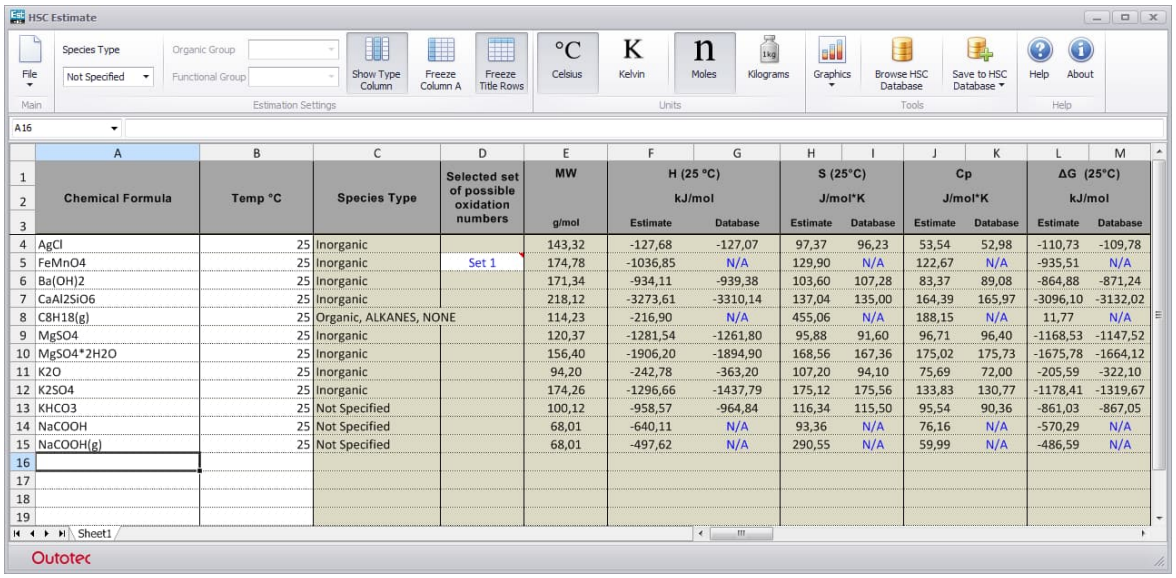
16. H, S, C_p Estimates Module

16.1. Introduction



	Chemical Formula	Temp °C	Species Type	Selected set of possible oxidation numbers	MW	H (25 °C) kJ/mol		S (25°C) J/mol*K		Cp J/mol*K		ΔG (25°C) kJ/mol	
					g/mol	Estimate	Database	Estimate	Database	Estimate	Database	Estimate	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
8	C8H18(g)	25	Organic, ALKANES, NONE		114,23	-216,90	N/A	455,06	N/A	188,15	N/A	11,77	N/A
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
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
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

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

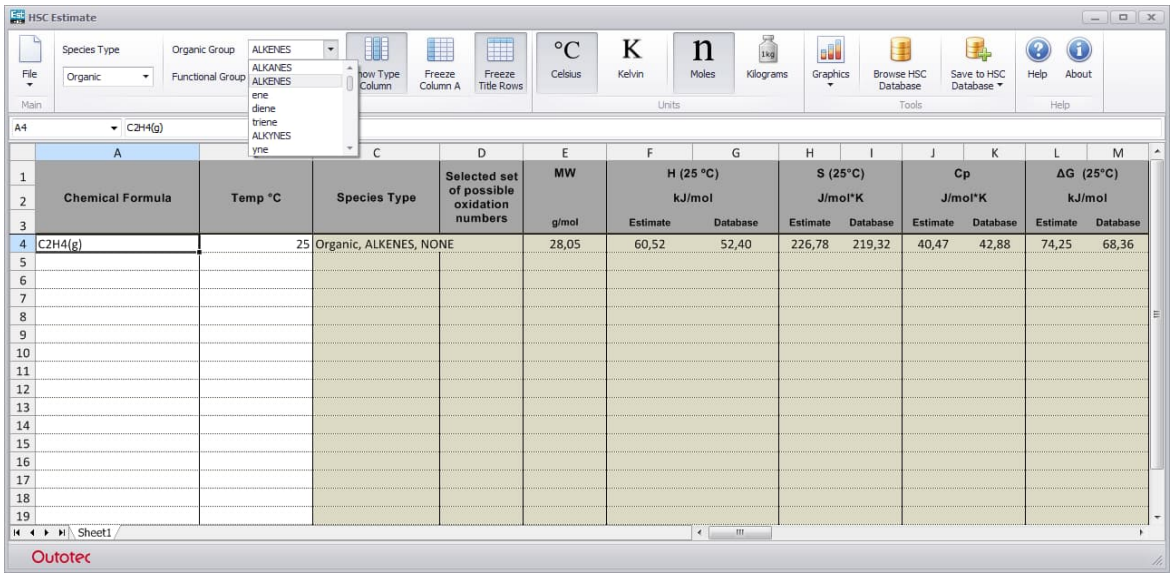


Fig. 2. Specifying additional properties for organic species (C_2H_4(g) in this example).

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.

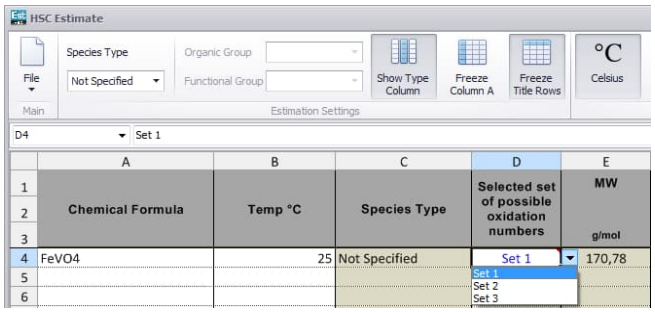


Fig. 3. Changing the active set of oxidation numbers.

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

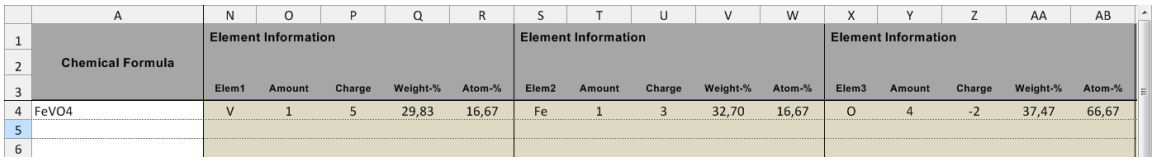


Fig. 4. Information about the elements found in the chemical formula.

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	C	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: AlO(OH) - aluminium oxide hydroxide

AlO(OH)	Valid species, but estimated as AlO not as AlO(OH)
AlO2H	Valid species
AlO*(OH)	Invalid species
AlO*OH	Valid species
AlOOH	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.

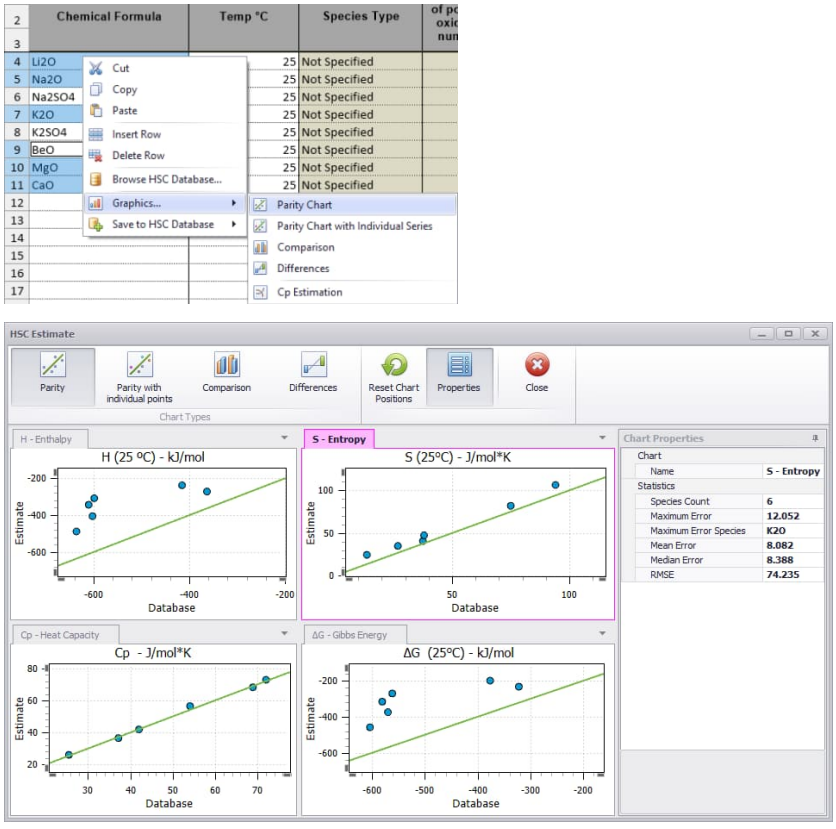


Fig. 5. Plotting species in HSC Estimates.

16.5. Adding estimated species to own database

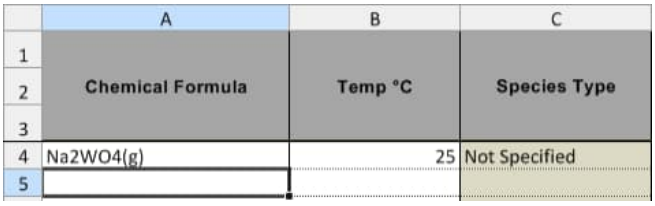
Estimated values can be utilized in other HSC modules, if the species are saved to the own database. Species can be saved either with a constant Cp value, estimated at 25 °C, or with a temperature range, specified by the user.

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.

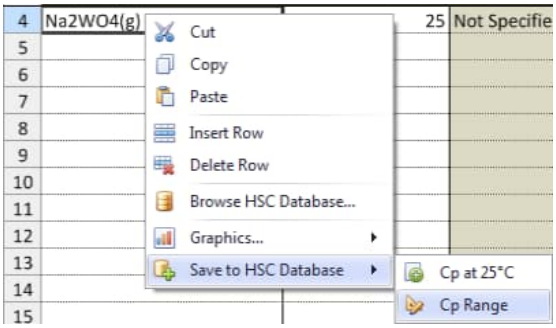
Example

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

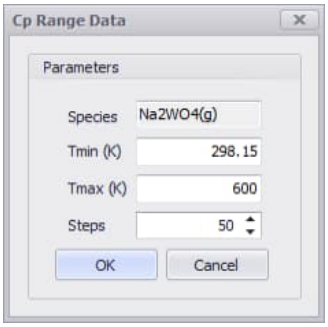
1. **Estimate Na2WO4(g)**
   Type the formula to the first column in the spreadsheet.



2. **Save with a Cp range**
   Right-click the species and select “Save to HSC Database > Cp Range”.

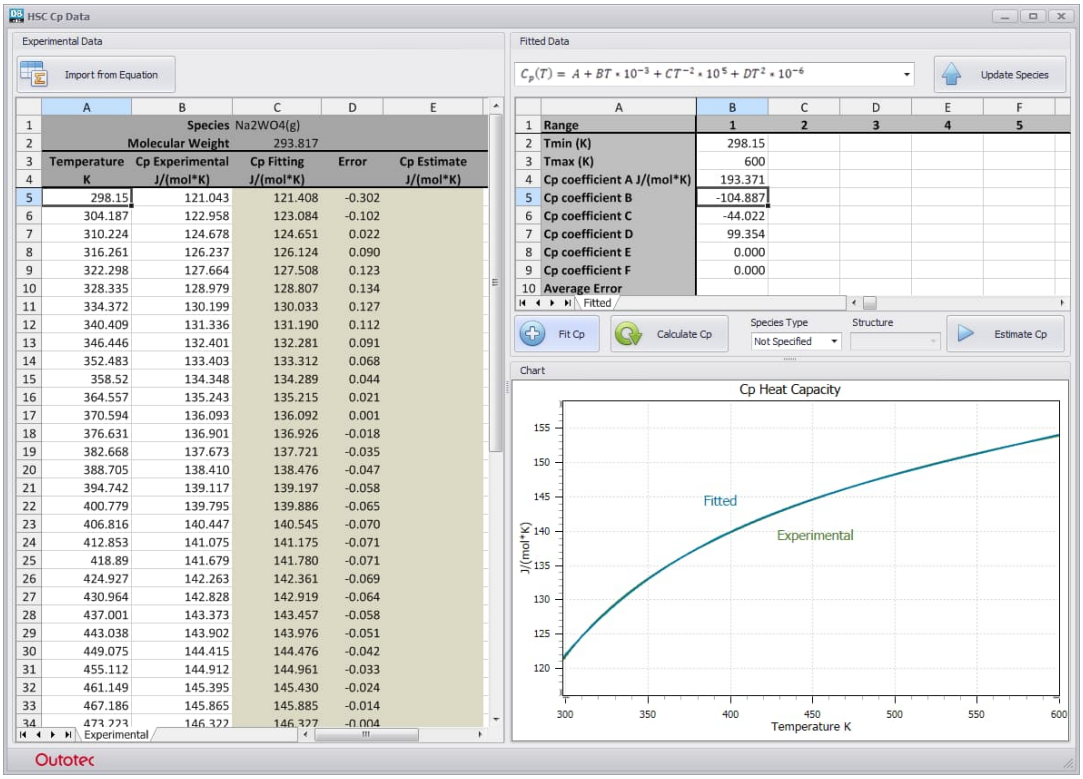


3. **Specify range parameters**
   Change the Max temperature to 600 and click “OK”.



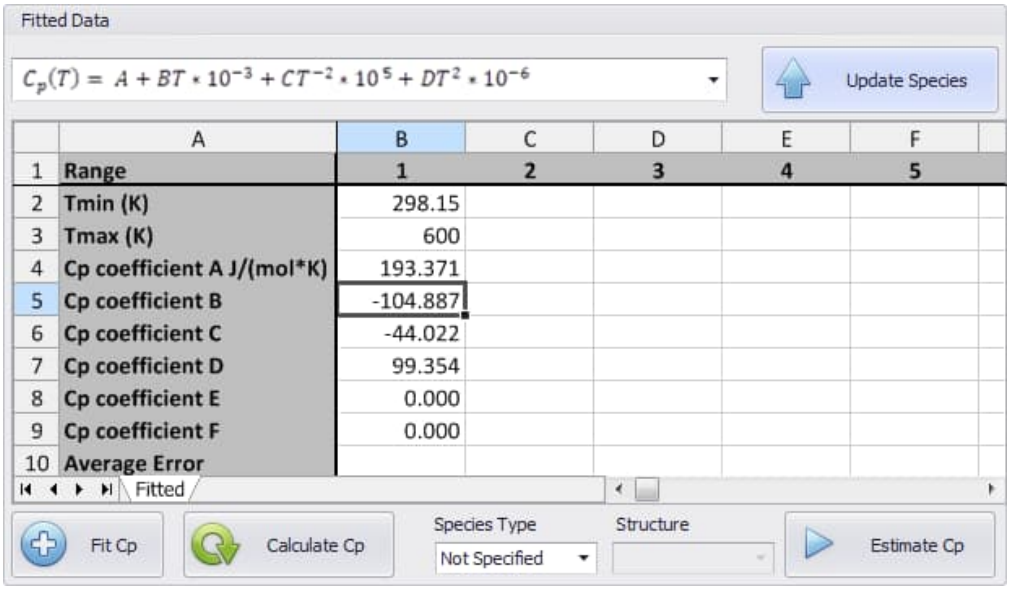
4. Fit the values to the Cp equation

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.



5. After fitting, save the coefficients

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



6. Save the species

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