Digitizing The NBS Tables of Chemical Thermodynamic Properties Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units

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1. Summary

The published book, NBS Tables of Chemical Thermodynamic Properties [1], is a collection of thermodynamic properties consisting of 103 tables with 14 330 critically evaluated species that were originally published as a series of NBS (National Bureau of Standards, now NIST, National Institute of Standards and Technology) Technical Notes [2]. This work provides this data in a more accessible spreadsheet format. Enthalpy of formation, $\Delta_f H°$, Gibbs energy of formation, $\Delta_f G°$, entropy, $S°$, heat capacity at constant pressure, $C_p°$, all at 298.15 K, and the enthalpy difference, $[H°(298) – H°(0)]$ are provided where known. Within this collection of data, there are no values given for transuranic elements, Lr to Np (Tables 77-87).

2. Data Specifications

NIST Operating Unit	Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group
Format	CSV, Excel
Instrument	N/A
Accessibility	Publicly available.
License	NIST license

3. Methods

The NBS Tables of Chemical Thermodynamic Properties [1] book was digitized (optical character recognition - OCR) into a portable document format (PDF) file. The tables within the PDF file were copied (Fig. 1) and pasted into Microsoft Word (Fig. 2). Within Word, column alignments and chemical formulas were fixed using the PDF as a guide. From Word, the data were then copied into Excel and printed. Using the original book as a guide, all tables were manually edited and corrected. After editing, the contents of the spreadsheet were checked using a Python script. State identifiers were checked for consistency and numeric values were checked for format and range. An erratum [4] was used to include corrected values in the data which is indicated with an asterisk.

The images below show the digitized results of a section of terbium and then copied into Word format.

$TbSO_4^+$	ao	254.9856	—	-1576.9	-1416.2	—	-88.	—
$Tb(SO_4)_2^-$	ao	351.0472	—	-2482.8	-2171.8	—	-21.	—
$TbNO_3^{2+}$	ao	220 9289	—	—	-768.6	—	—	—
$Tb_2P_2O_7^{2+}$	ao	491.7914	—	—	-3340.0	—	—	—
TbAs	cr	233.8456	—	-314.	—	—	—	—
TbC_2	g	182.9464	887.	885.8	831.3	10.33	268.	43.9
$Tb_2(CO_3)_3$	cr	497.8762	—	-3329.2	—	—	—	—
$Tb_2(C_2O_4)_3 \cdot 10H_2O$ oxalate	cr	762.0620	—	—	-5865.	—	—	—
$TbCH_2OHCOO^{2+}$ glycolate	ao	233.9686	—	-1335.49	—	—	—	—
$Tb(CH_2OHCOO)_2^+$	ao	309.0132	—	-1991.25	—	—	—	—
$TbMoO_4^+$	ao	318.8616	—	—	-1513.7	—	—	—

Fig. 1. A section from terbium copied from original PDF file

TbSO/ ao 254.9856 - -1576.9 -l416.2 - -88. -
Tb(SOJ2- ao 351.0472 - -2482.8 -217l.8 - -21. -
TbNO,H ao 2209289 - - -768.6 - - -
Tb2P2O/+ ao 491.7914 - - -334O.0 - - -
TbAs cr 233.8456 - -314. - - - -
TbC2 g 182.9464 887. 88S.8 831.3 10.33 268. 43.9
Tb2(C03h cr 497.8762 - -3329.2 - - - -
Tb2(C20J3·lOH20 oxolate cr 762.062O - - -5865. - - -
TbCH2OHCOOH glycolate ao 233.9686 - -1335.49 - - - -
Tb(CH20HCOOh+ ao 309.0132 - -1991.2S - - - -
TbMoO.+ ao 318.8616 - - -1513.7 - - -

Fig. 2. Same section from terbium (Fig. 1) copied from PDF file into MS Word file

The methods used to compile and evaluate the data are provided in chapters two through six of Ref. [1]. Table 1 describes each column in the Excel file.

Table 1. Description of each column in the Excel file

Heading	Description
Formula	Written in conventional manner
Solvent	Standard thermodynamic properties, may be a mixture
Name	Name of given formula
State Description	Additional information about the state of the species
State	Abbreviation identifying the state of the species information on the state definitions is given in a separate column in the spreadsheet
Molar Mass (g mol^{-1})	Molecular weight in gram per mole of substance
0 K $\Delta_f H°$ (kJ mol^{-1})	Enthalpy of formation
$\Delta_f H°$ (kJ mol^{-1})	Enthalpy of formation
$\Delta_f G°$ (kJ mol^{-1})	Gibbs energy of formation
$H°-H_0°$ (kJ mol^{-1})	Enthalpy difference
$S°$ (J mol^{-1} K^{-1})	Molar entropy
C_p (J mol^{-1} K^{-1})	Heat capacity at constant pressure

The break between the tables consist of two rows. The first row contains the table number followed by the element symbol. The second row contains the full name of element and the year it was prepared.

4. Impact

The NBS Tables of Chemical Thermodynamic Properties [1] is one of the most highly cited works in the history of NBS/NIST and is still used and cited in the academic, scientific, and engineering areas. In compliance with the Open Government Data Act [3], which "requires open government data assets to be published as machine-readable data", the NBS Tables are now accessible through CSV and Excel formats. The Excel files are provided as a convenience.

5. References

[1] Wagman DD, Evans WH, Parker VB, Schumm RH, Halow I, Bailey SM, Churney KL, Nuttall RL (1982) The NBS tables of chemical thermodynamic properties. Selected values for inorganic and C_1 and C_2 organic substances in SI units. *J. Phys. Chem. Ref. Data, Suppl.* 11 suppl. 2.

[2] Wagman DD, Evans WH, Parker VB, Halow I, Bailey SM, Schumm RH, Churney KL, Nuttall RL (1968 through 1981) Selected values of chemical thermodynamic properties. NBS Tech. Note 270-3 through 270-8.

[3] H.R.4174 - Foundations for Evidence-Based Policymaking Act of 2017 https://www.congress.gov/bill/115th-congress/house-bill/4174. Accessed 12 February 2019.

[4] Wagman DD, Evans WH, Parker VB, Schumm RH, Halow I, Bailey SM, Churney KL, Nuttall RL (1989) Erratum: The NBS tables of chemical thermodynamic properties. Selected values for inorganic and C_1 and C_2 organic substances in SI units [J. Phys. Chem. Ref. Data, Suppl. 11 suppl. 2 (1982)] J. Phys. Chem. Ref. Data, 18, 1807-1812 (1989).

6. Disclaimer

Certain software products are identified in this paper in order to specify the procedure adequately. Such identification is not intended to imply recommendation or endorsement by NIST, nor is it intended to imply that the products identified are necessarily the best available for the purpose.

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