

## Appendix F

# Comment on the data for ZrO(g) and ZrO<sub>2</sub>(g)

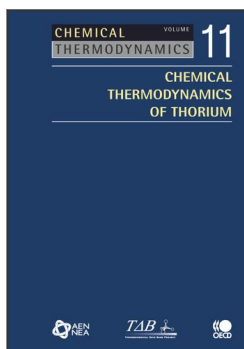
There may be some problems with the data for ZrO(g) and ZrO<sub>2</sub>(g) selected in the NEA-TDB review of zirconium by Brown *et al.* [2005BRO/CUR]. The values given by Brown *et al.* are based on the assessment in the third edition of the Janaf tables [1985CHA/DAV], modified for the slightly different values of  $\Delta_f H_m^\circ$ (ZrO<sub>2</sub>, cr, 298.15 K) used in the two reviews. However, the assessments in [1985CHA/DAV] for these species were made in December 1965 and thus predate a number of detailed experimental studies made in 1970s. Indeed, their values of the Gibbs energies of formation of both ZrO(g) and ZrO<sub>2</sub>(g) are based solely on an early mass-spectrometric study by Chupka *et al.* [1957CHU/BER].

The later assessment of [1982GLU/GUR] quotes seven studies of the thermodynamics of ZrO(g) and six for ZrO<sub>2</sub>(g), in both cases dating from 1957 to 1979. There seem to be no more recent experimental data on the vaporisation of these species. The values of  $\Delta_f H_m^\circ$ (ZrO, g, 298.15 K) derived by [1982GLU/GUR] vary from 45.9 to 108.9 kJ·mol<sup>-1</sup> (selected value (83.89 ± 11.00) kJ·mol<sup>-1</sup>), and those for  $\Delta_f H_m^\circ$ (ZrO<sub>2</sub>, g, 298.15 K) vary from -298 to -349 kJ·mol<sup>-1</sup> (selected value -(318.31 ± 15.00) kJ·mol<sup>-1</sup>). These selected values, especially that for ZrO(g), are appreciably different from the values in [1985CHA/DAV] and [2005BRO/CUR], as shown in Table F-1, which summarises the data for ZrO(g), ZrO<sub>2</sub>(cr) and ZrO<sub>2</sub>(g) from the three assessments.

Because of the considerable uncertainty in the value of  $\Delta_f H_m^\circ$ (ZrO, g, 298.15 K), this review has not utilised the data for the gaseous reaction Th(g) + ZrO(g) ⇌ ThO(g) + Zr(g) given by Ackermann and Rauh [1974ACK/RAU], as noted in Section VII.1.1.2.

Table F-1: Comparison of assessed data for ZrO(g), ZrO<sub>2</sub>(cr) and ZrO<sub>2</sub>(g)

Property	[1982GLU/GUR]	[1985CHA/DAV]	[2005BRO/CUR]
<b>ZrO(g)</b>			
$\Delta_f H_m^\circ$ (298.15 K) (kJ·mol <sup>-1</sup> )	83.89 ± 11.00	58.6 ± 50.2	56.200 ± 27.008
$S_m^\circ$ (298.15 K) (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	228.184	227.6 ± 8.4	227.6 ± 8.4
$C_{p,m}^\circ$ (298.15 K) (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	34.374	30.845	30.8 ± 1.0
<b>ZrO<sub>2</sub>(cr)</b>			
$\Delta_f H_m^\circ$ (298.15 K) (kJ·mol <sup>-1</sup> )	-1100.3 ± 1.3	-1097.463 ± 1.700	-1100.6 ± 1.3
$S_m^\circ$ (298.15 K) (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	50.39	50.359 ± 0.330	50.19 ± 0.62
$C_{p,m}^\circ$ (298.15 K) (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	55.92	56.191	55.96 ± 0.79
<b>ZrO<sub>2</sub>(g)</b>			
$\Delta_f H_m^\circ$ (298.15 K) (kJ·mol <sup>-1</sup> )	-318.31 ± 15.00	-305.4 ± 12.6	-289.600 ± 47.018
$S_m^\circ$ (298.15 K) (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	264.631	260.48 ± 4.2	273.7 ± 5.0
$C_{p,m}^\circ$ (298.15 K) (J·K <sup>-1</sup> ·mol <sup>-1</sup> )	42.487	46.061	46.1 ± 1.0



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