

## THERMOCHEMICAL PROPERTIES OF THE ELEMENTS Rn, 112, 114, AND 118: II. VAPOR PRESSURE EQUATION AND VOLATILIZATION PROPERTIES

*R. Eichler, B. Eichler (PSI)*

*The vapor pressure equations for the solid and liquid state of the elements Rn, 112, 114, and 118 have been deduced, applying the critical data and the Debye temperatures. Thermochemical constants for the volatilization processes were calculated.*

The reduced vapor pressure equations are given introducing reduced parameters  $T_r = T/T_c$  and  $p_r = p/p_c$  into the typical vapor pressure equation (eqn. 1).

$$\log(p/kPa) = -\frac{A}{T} + B \quad (1)$$

Using the critical values  $T_c$  and  $p_c$  from [1] the reduced vapor pressure equations (eqn. 2) are deduced for noble gases (see Tab.1).

$$\log(p_r) = -\frac{a}{T_r} + b \quad (2)$$

**Table 1:** Coefficients of the reduced vapor pressure equations for noble gases

| State<br>element      | solid   |        | liquid  |        |
|-----------------------|---------|--------|---------|--------|
|                       | a       | b      | a       | b      |
| Ne                    | -       | -      | -2.1992 | 2.1659 |
| Ar                    | -2.6996 | 3.0130 | -2.2959 | 2.2834 |
| Kr                    | -2.7992 | 3.1985 | -2.3041 | 2.2937 |
| Xe                    | -2.8811 | 3.3361 | -2.3154 | 2.2043 |
| $\varnothing_{Ar,Xe}$ | -2.7930 | 3.1830 | -2.3050 | 2.2940 |

According to [2] the coefficients should be the same for ideal solids and liquids. This is fairly given for the heavy noble gases Ar to Xe.

Assuming the corresponding states principle to be valid for the heavy noble gases and Rn, 112, 114, and 118 the coefficients of the vapor pressure equations have been calculated for the elements Rn, 112, 114, and 118 using the predicted critical data from [3] according to eqn. 3.

$$\log(p/kPa) = -\frac{a \cdot T_c}{T} + b + \log(p_c/kPa) = -\frac{A}{T} + B \quad (3)$$

The coefficients A and B are compiled in Table 2.

**Table 2:** Coefficients of the vapor pressure equations of the elements Rn, 112, 114, and 118. Calculated enthalpies (kJ/mol) and entropies (J/molK) of phase transition at the corresponding triple points.

| state              |        | solid  |                          |                          |
|--------------------|--------|--------|--------------------------|--------------------------|
| element            | -A, K  | B      | $\Delta H_{\text{subl}}$ | $\Delta S_{\text{subl}}$ |
| <sup>222</sup> Rn  | 1012.3 | 6.983  | 19.38                    | 95.41                    |
| <sup>283</sup> 112 | 1038.8 | 6.987  | 19.89                    | 95.49                    |
| <sup>288</sup> 114 | 1118.3 | 6.999  | 21.41                    | 95.71                    |
| <sup>292</sup> 118 | 1226.1 | 7.014  | 23.45                    | 96.01                    |
| state              |        | liquid |                          |                          |
| element            | -A, K  | B      | $\Delta H_{\text{vap}}$  | $\Delta S_{\text{vap}}$  |
| <sup>222</sup> Rn  | 835.4  | 6.094  | 16                       | 78.4                     |
| <sup>283</sup> 112 | 857.3  | 6.098  | 16.41                    | 78.5                     |
| <sup>288</sup> 114 | 922.9  | 6.110  | 17.67                    | 78.7                     |
| <sup>292</sup> 118 | 1011.9 | 6.125  | 19.37                    | 79.0                     |

According to Lennard-Jones [4] the potential curves for elements revealing only van der Waals interaction in the solid state should be very similar. A constant proportionality between the depths of the potentials and the critical temperatures is expected according to eqn. 4.

$$k^\ominus = \frac{(\Delta H_{\text{subl}}^0 + U_0)}{R \cdot T_c} = 6.45 \quad (4)$$

We checked this expectation for the noble gases. Therefore, the zero point energies ( $U_0$ ) have been calculated according to eqn. 5 [5].

$$U_0 = \frac{9}{8} \cdot R \cdot \Theta_D \quad (5)$$

The Debye temperatures ( $\Theta_D$ ) are taken from [6]. The results are compiled in table 3. Indeed, the constant proportionality is deduced for the heavy noble gases as  $k^\ominus \sim 6.8$ . Hence, it is possible to calculate the sublimation enthalpies at 0 K ( $\Delta H_{\text{subl}}^0$ ) for the elements Rn, 112, 114, and 118. The results are listed in table 3.

**Table 3:** Thermochemical data of noble gases [1,2,6] and deduced data for elements Rn, 112, 114, and 118.

| Element            | $T_c$ ,<br>K | $\Theta_D$ ,<br>K | $U_0$ ,<br>J/mol | $\Delta H_{\text{subl}}^0$ ,<br>kJ/mol | $k^\ominus$ |
|--------------------|--------------|-------------------|------------------|--|-------------|
| Ne                 | 44.40        | 64                | 598.6            | 1.875                                  | 6.700       |
| Ar                 | 150.87       | 80                | 748.3            | 7.732                                  | 6.760       |
| Kr                 | 209.41       | 63                | 598.3            | 11.210                                 | 6.770       |
| Xe                 | 289.73       | 55                | 514.4            | 15.865                                 | 6.799       |
| <sup>220</sup> Rn  | 362.43       | 45.09             | 421.7            | 20.07                                  | 6.8         |
| <sup>283</sup> 112 | 371.92       | 40.20             | 376.0            | 20.65                                  | 6.8         |
| <sup>288</sup> 114 | 400.38       | 40.57             | 379.5            | 22.26                                  | 6.8         |
| <sup>292</sup> 118 | 438.99       | 41.14             | 384.8            | 24.43                                  | 6.8         |

The calculated sublimation enthalpies are used to predict the adsorption behavior of the elements 112 and 114 under the assumption that they behave as typical heavy noble gases, revealing pure van der Waals interaction with metal surfaces [7].

### REFERENCES

- [1] CRC Handbook of Chemistry and Physics; ed. D.R. Lide, CRC-Press, London (1999).
- [2] A.V. Grosse, J. Inorg. Nucl. Chem. **27**, 509 (1965).
- [3] R. Eichler et al., this report p. 7.
- [4] J.E. Lennard-Jones, Physica **4**, 941 (1937).
- [5] K. Clusius, Z. Phys. Chem. **B 31**, 459 (1936).
- [6] Landolt-Börnstein, 6-th ed., Vol. II (1), p. 378 (1971).
- [7] R. Eichler et al., this report p. 4.