

Problem set 10

Due May 19, 2026

1. Given the characteristic rotational temperature of the dihydrogen molecule, $\Theta_r^{H_2} = 85.3$ K, compute numerically and plot in the range of temperatures from 30 K (above hydrogen boiling point) to 300 K the following quantities for gaseous hydrogen:
 - (a) The equilibrium fractions of ortho- and para-hydrogen.
 - (b) The heat capacity of the ortho-hydrogen.
 - (c) The heat capacity of the para-hydrogen.
 - (d) The heat capacity of the equilibrium mixture of ortho- and para-hydrogen.
 - (e) The heat capacity of the mixture of ortho- and para-hydrogen with fractions of these species frozen at those corresponding to high temperatures.

Express the heat capacity in gas-constant (R) units

2. Overlay on the plot of point 1e the experimental heat capacity determined by sound-velocity measurements in R. E. Cornish, E. D. Eastman, *J. Am. Chem. Soc.*, **1928**, 50, 627-652. For more data you can refer to the publication by H. W. Wooley, R. B. Scott, F. G. Brickwedge, *J. Res. Natl. Bur. Stand.*, **1948**, 41, 379-495 at https://nvlpubs-1nist-1gov-19fb4771816d8.hansolo.bg.ug.edu.pl/nistpubs/jres/041/jresv41n5p379_A1b.pdf (caution: a large pdf file).

For more discussion about the problems with the theoretical description of the properties of gaseous hydrogen at low temperatures see C. A. Gearhart, *Arch. Hist. Exact Sci.*, **2010**, 64, 113-202.