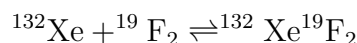


Problem set 11**Due May 26, 2026**

1. Consider the reaction of 1 mole of gaseous fluorine-19 ($^{19}\text{F}_2$) with 1 mole of gaseous xenon (^{132}Xe) to give 1 mole of gaseous xenon difluoride ($^{132}\text{Xe}^{19}\text{F}_2$) (a symmetric linear molecule).

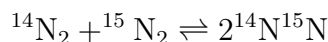


- (a) Derive the formula for the energy of this reaction. The dissociation energies of the molecules involved with zero-point oscillation energies subtracted (D_o) and their vibrational wave numbers ($\bar{\nu}$), along with the degeneracies of the respective vibrational modes, are listed in the table below.

Molecule	D_o [kJ/mol]	$\bar{\nu}$ [cm^{-1}]
$^{19}\text{F}_2$	154.8	894
$^{132}\text{Xe}^{19}\text{F}_2$	267.8	214 (2), 515 (1), 555 (1)

- (b) Make a plot of the energy of this reaction as a function of temperature from $T = 300$ K to $T = 2000$ K.

2. Consider the isotope-exchange reaction between $^{14}\text{N}_2$ and $^{15}\text{N}_2$.



- (a) Based on the formula for the equilibrium constant for the isotopic-exchange reaction between hydrogen and deuterium to form hydrogen-deuterium, derive the formula for the gas-phase equilibrium constant of this reaction. The characteristic vibrational temperature of the $^{14}\text{N}_2$ molecule is $\Theta_\nu = 3374$ K.

- (b) Make the Arrhenius plot $\log K = f(1/T)$.

3. The data of the time course of the $^{14}\text{N}_2 - ^{15}\text{N}_2$ isotope-exchange reaction catalyzed by iron and methylamine (Joris & Taylor, *J. Chem. Phys.*, 7, 893, 1939) at two temperatures are in the table below.

- (a) Calculate the fractions of all three dinitrogen species at each point.

- (b) Insert the calculated fractions into the expression for the isotope-exchange equilibrium constant, and calculate the apparent equilibrium constant at each point.
- (c) Check if the apparent equilibrium constant approaches that calculated from the first principles at long time and comment on the result.

T [°C]	time [h]	quantity/1000 units of $^{14}\text{N}_2$	
		$^{14}\text{N}^{15}\text{N}$	$^{15}\text{N}_2$
465	2	100.5	51.50
	17	125.8	39.00
	37	163.0	22.60
	60	194.0	14.00
500	2	108.0	48.00
	8	142.0	38.00
	21	184.0	20.00
	26	197.5	17.40
	35	202.0	13.40
	46	207.0	13.25