Partial answers to microprojects

Part 1: Equilibrium

1.1 (c) 18.30 $cm^3\,mol^{-1}$, 5789 $cm^3\,mol^{-1}$.

1.2 (a) 501 K; (b) virial: 0.455 $L\,mol^{-1}$, 0.598 $L\,mol^{-1}$; perfect: 0.496 $L\,mol^{-1}$, 0.621 $L\,mol^{-1}$; (c) $\pi_T = 2.91\ kJ\,L^{-1}$, $\Delta S_m = -40.4\ J\,K^{-1}\,mol^{-1}$, $\Delta H_m = -0.99\ kJ\,mol^{-1}$, $\Delta G_m = +14.1\ kJ\,mol^{-1}$.

1.4 $\Delta_f H^{\ominus}(Na^+, aq) = -240.65\ kJ\,mol^{-1}$.

1.5 (a) $\Delta_{sub}H(1\ Torr) = +80.84\ kJ\,mol^{-1}$, $\Delta_{sub}S(1\ Torr) = +201.1\ J\,K^{-1}\,mol^{-1}$; (b) $\Delta_{atom}H = +11\,525 \pm 5\ kJ\,mol^{-1}$.

1.8 (b) $-24.9\ kJ\,mol^{-1}$.

1.9 (e) 45.1 kPa for methanol in TAME, 25.3 kPa for TAME in methanol; (f) 6.16 kPa.

1.10 (a) $F(1500\ K) = 3$, $F(1100\ K) = 2$; (c) 0.67 g Pb per g Cu; 0.050 g Cu per g Pb.

1.12 (a) $p(450°C) = 156.5$ bar, $p(400°C) = 81.8$ bar; (b) $p(450°C) = 132.5$ bar, $p(400°C) = 210$ bar.

1.13 (a) mp(SiO_2) = 1934.1 K, mp(Si) = 1715.5 K; (c) 5.3 per cent carbon impurity.

1.14 (b) maximum carbon mass in ocean $\approx 2.67 \times 10^{12}$ tonne.

1.15 (b) $E^{\ominus} = 2.05$ V, $\Delta_r G^{\ominus} = -395.6\ kJ\,mol^{-1}$, $\Delta_r H^{\ominus} = -586.21\ kJ\,mol^{-1}$, $\Delta_r S^{\ominus} = -639.29\ J\,K^{-1}\,mol^{-1}$; $E^{\ominus}(15°C) = 2.083$ V; $E(25°C, Q) = 2.185$ V; (c) pH = 5: 1.0997 V; pH = 8: 0.745 V; $E(PbSO_4/Pb) = -0.3588$ V.

1.16 $pK_a(25°C) = 6.736$; $a_0 = -14.102$, $a_1 = 2461$ K, $a_2 = 2.209$.

Part 2: Structure

2.1 (b) 255.1 K; (c) 281.9 K, 81.1 per cent.

2.3 (b) 3*s* radial nodes: $\rho = 3 \pm 3^{1/2}$, no nodal plane; $3p_x$ radial nodes: $\rho = 0$ and 4, *yz* nodal plane ($\phi = 90°$); $3d_{xy}$ radial node: $\rho = 0$ only, *xz* nodal plane ($\phi = 0$) and *yz* nodal plane ($\phi = 90°$); (c) $13.5a_0/Z$.

2.4 (b) $n_{max} \approx 29$.

2.5 (c) $A/hc = 46\,119\ cm^{-1}$, $B = 1.4275$, $C = 2.3896$, $D = 88.99$ pm, $\varepsilon/hc = 1750\ cm^{-1}$.

2.6 (b) $\nu = 2169.2\ cm^{-1}$, $x\nu = 13.13\ cm^{-1}$, $B = 1.94\ cm^{-1}$, $\alpha = 0.0174\ cm^{-1}$, $D_J = 6.19 \times 10^{-6}\ cm^{-1}$; (c) $I_e = 1.444 \times 10^{-46}\ kg\,m^2$, $R_e = 112.63$ pm, $D_e = 89\,595\ cm^{-1}$, $D_0 = 88\,574\ cm^{-1}$, $I_{v=0} = 1.451 \times 10^{-46}\ kg\,m^2$, $I_{v=1} = 1.464 \times 10^{-46}\ kg\,m^2$, $R_{v=0} = 112.88$ pm, $R_{v=1} = 113.39$ pm.

2.7 (c) $h \leq 30$ m.

2.9 (b) $E_{min} = -15.367$ eV, $R_e = 131.864$ pm, $D_e = 1.7612$ eV.

2.10 (a) $E_{min} = -15.96$ eV, $R_e = 106.009$ pm, $D_e = 2.354$ eV, $\eta = 1.238$.

2.11 (b) $\beta \approx -21\,135\ cm^{-1}$; (c) $E_{deloc} = 1.5176\beta$.

Part 3: Change

3.1 (b) $J_0 = 7.55\ mmol\,m^{-2}\,h^{-1}$.

3.2 (b) $\Lambda_m^0 = 391.347\ S\,cm^2\,mol^{-1}$, $K_a = 0.157$.

3.3 (b) $\log(A) = 11.09$, $E_a = 73.8\ kJ\,mol^{-1}$; at 293.15 K: $\Delta^\ddagger H = 71.4\ kJ\,mol^{-1}$, $\Delta^\ddagger S = -40.8\ J\,K^{-1}\,mol^{-1}$; (c) $a = 0.411$, $b = -0.192$, $c = 1.369 \times 10^{-3}\ K^{-1}$.

3.4 (a) $a = 1$, $b = 0.5$; (b) $k(433.15\ K) = 0.077\ cm^{3/2}\,s^{-1}\,mol^{-1/2}$, $A = 5.002 \times 10^{16}\ cm^{3/2}\,s^{-1}\,mol^{-1/2}$, $E_a = 147.7\ kJ\,mol^{-1}$.

3.5 (a) 0.012 per cent ozone.

3.6 (a) period ≈ 5 years; (b) attractor: $[X] = 22.35$, $[Y] = 21.88$.

3.7 For x^{-1} versus c^{-1} regression: $r = 0.99836$, coefficient of variation = 7.381, $x_{max} = 0.380$, $K = 0.351\ L\,mg^{-1}$, specific surface area $= 658\ m^2\,g^{-1}$.