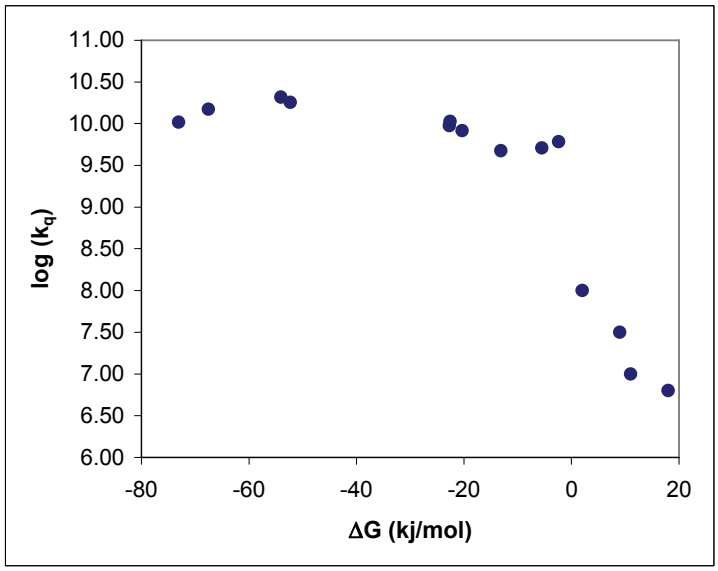
	A	B	C	D	E	F
1	ΔG (J/mol)	log kq	log kq fit		A	5.00E+10
2	-22730	9.98	10.03		λ	40000
3	-5510	9.71	9.33		kd	2.00E+10
4	-22580	10.03	10.03			
5	-13140	9.68	9.75		X2	2.778965
6	-2400	9.78	9.11			
7	-67540	10.17	9.72			
8	-54060	10.32	10.08			
9	-20340	9.92	9.98			
10	-73080	10.02	9.43			
11	-52300	10.26	10.10			
12	2000	8.00	8.73			
13	9000	7.50	8.04			
14	11000	7.00	7.82			
15	18000	6.80	6.98			
16						
17						

Values in column A and B are the class experimental data and are plotted below



$$k_q = \frac{1}{k_d} + \frac{1}{K_a k_{el}} \qquad K_a \approx 1 \qquad \text{where} \quad k_{el} = A \exp\left[-\frac{(\lambda + \Delta G)^2}{4\lambda RT} \right]$$

$$\log(k_q) = \log\left(\frac{1}{1/k_d + 1/k_{el}} \right)$$

The fitted values are calculated using the parameters in column F and the equations above

Cell C2 has the following equation:
=LOG(1/(1/$F$3+1/($F$1*EXP(-1*(($F$2+**A2**)^2)/(4*$F$2*8.314*295)))))

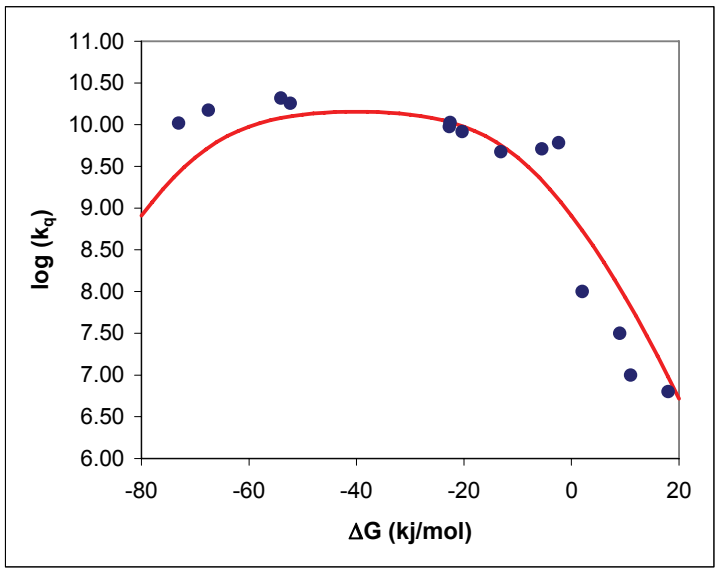
	A	B	C	D	E	F	G	H
1	ΔG (J/mol)	log kq	log kq fit		A	5.00E+10	ΔG	log kq
2	-22730	9.98	10.03		λ	40000	20000	6.71
3	-5510	9.71	9.33		kd	2.00E+10	18000	6.98
4	-22580	10.03	10.03				16000	7.23
5	-13140	9.68	9.75		X2	2.778965	14000	7.47
6	-2400	9.78	9.11				12000	7.71
7	-67540	10.17	9.72				10000	7.93
8	-54060	10.32	10.08				8000	8.15
9	-20340	9.92	9.98				6000	8.35
10	-73080	10.02	9.43				4000	8.55
11	-52300	10.26	10.10				2000	8.73
12	2000	8.00	8.73				0	8.91
13	9000	7.50	8.04				-2000	9.07
14	11000	7.00	7.82				-4000	9.23
15	18000	6.80	6.98				-6000	9.37
16							-8000	9.49
17							-10000	9.61
							-12000	9.70

To make a smooth plot of the fitted parameters, new data must be generated (column G and H)
Enter a range of ΔG in column G

Cell H2 has the following equation:
=LOG(1/(1/$F$3+1/($F$1*EXP(-1*(($F$2+**G2**)^2)/(4*$F$2*8.314*295)))))

The goodness of the fit is given by the χ^2 parameter in cell F5

Cell F5 has the following equation:
=SUMXMY2(B2:B100,C2:C100)



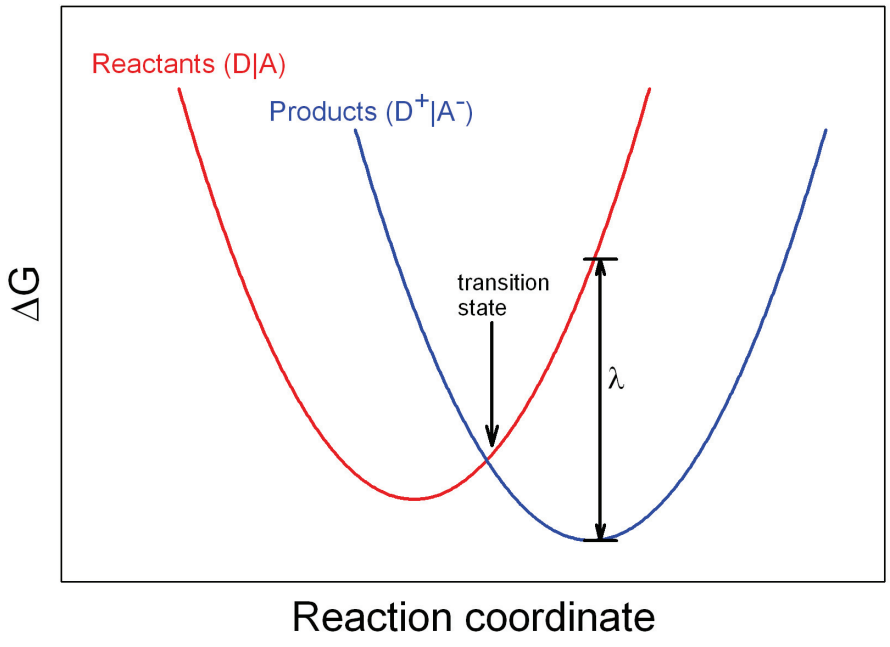
The goal is to vary the parameters A, λ and k_d to obtain the best fit to the experimental data (i.e. minimum value of χ^2)

Since the diffusion limited rate can be estimated from the Debye equation we will fix the value of k_d

$$k_d \approx \frac{8RT}{3000\eta} \quad (\text{R} = 8.31\times10^7 \text{ erg mol}^{-1} \text{ K}^{-1}, \ \eta \text{ in poise})$$

A is the frequency factor (how often the system crosses the transition state)
Estimate 5×10^{10} s^{-1}

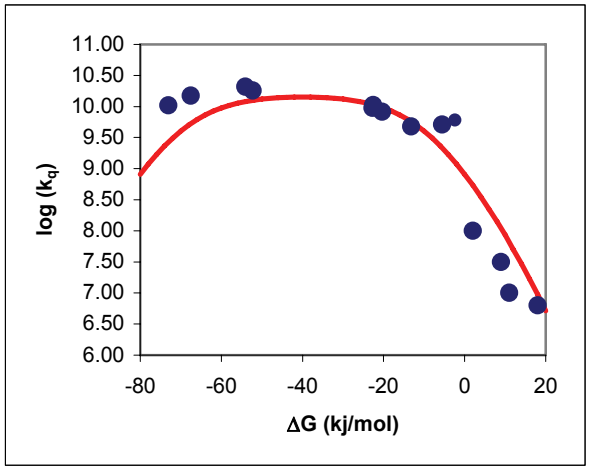
λ is the reorganization energy (reorder after charge transfer)
Estimate 40 kJ



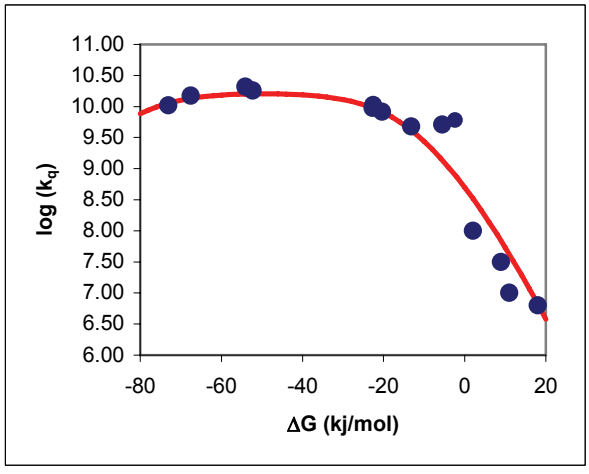
Excel Solver Add-In

	A	B	C	D	E	F	G	H
1	ΔG (J/mol)	log kq	log kq fit		A	5.00E+10	ΔG	log kq
2	-22730	9.98	10.03		λ	40000	20000	6.71
3	-5510	9.71	9.33		kd	2.00E+10	18000	6.98
4	-22580	10.03	10.03				16000	7.23
5	-13140	9.68	9.75		X2	2.778965	14000	7.47
6	-2400	9.78	9.11				12000	7.71

1. Under the **Tools** menu select **Solver**. A pop-up window will appear. *
2. In the box labeled **Set Target Cell** type in **$F$5**
3. Below this select **Equal To** the **min** function since we are trying to minimize the value in cell F5.
4. In the box labeled **By Changing Cells** type **$F$1:$F$2** . This allows the solver to vary the values for A and λ to minimize the sum of chi squared.
5. Click the **Options** button and check the box labeled **Use automatic scaling** then click **OK**.
6. Now click on **Solve**. The program will alter your guess values to fit the data to minimize chi squared.
7. A new pop-up will appear asking if you want to keep the new values or revert to your original values. Select **keep solver solution** and click the **OK** button.
8. The best fit values for A and λ will now be in cells F1 and F2. The fitted values should match very closely to the experimental data (see below). If they do not, then you need to make better guesses for A and λ to start with. Enter new guess values and repeat the procedure.



BEFORE FIT



AFTER FIT

* If you do not see Solver as an option, the add-in needs to be installed. To do this select "Add-Ins" under the "Tools" menu and check the solver add-in. Note: You may need the Excel installation disk to add this feature.