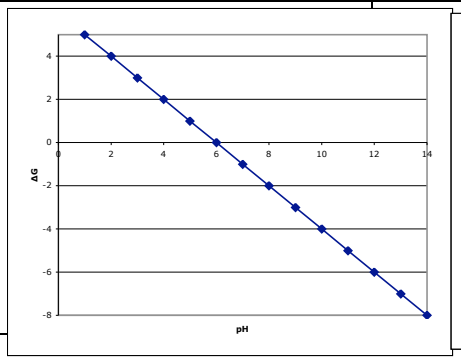
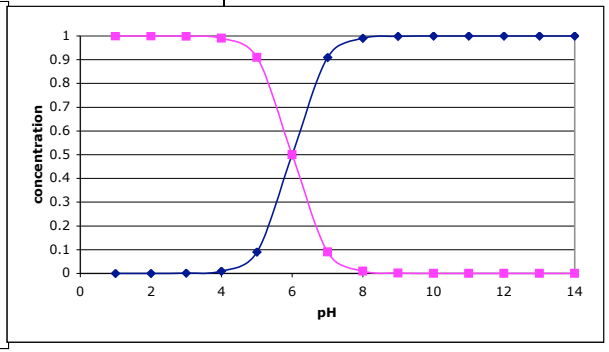
BLUE LINE: ENERGY A- AS F(PH)

PINK LINE [AH]; BLUE LINE [A-]

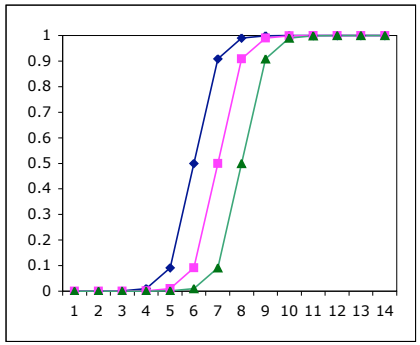
	6			
pH	dG	10(pK-pH)	<A->	<AH>
1	5	0.00001	1E-05	1
2	4	0.0001	1E-04	0.9999
3	3	0.001	0.001	0.999
4	2	0.01	0.0099	0.9901
5	1	0.1	0.0909	0.9091
6	0	1	0.5	0.5
7	-1	10	0.9091	0.0909
8	-2	100	0.9901	0.0099
9	-3	1000	0.999	0.001
10	-4	10000	0.9999	1E-04
11	-5	100000	1	1E-05
12	-6	1000000	1	1E-06
13	-7	1E+07	1	1E-07
14	-8	1E+08	1	1E-08





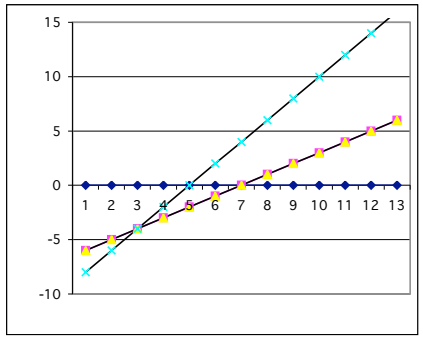
PK OF 5 (BLUE) 6 (PINK) 7 (GREEN)

	6				pK	7				pK	8			
pH	dG	10(pK-pH)	<A->	<AH>	pH	dG	10(pK-pH)	<A->	<AH>	pH	dG	10(pK-pH)	<A->	<AH>
1	5	0.00001	1E-05	1	1	6	1E-06	1E-06	0.999999	1	7	1E-07	1E-07	1
2	4	0.0001	1E-04	0.9999	2	5	1E-05	1E-05	0.99999	2	6	1E-06	1E-06	1
3	3	0.001	0.001	0.999	3	4	0.0001	1E-04	0.9999	3	5	1E-05	1E-05	1
4	2	0.01	0.0099	0.9901	4	3	0.001	0.000999	0.999001	4	4	1E-04	1E-04	1
5	1	0.1	0.0909	0.9091	5	2	0.01	0.009901	0.990099	5	3	0.001	1E-03	0.999
6	0	1	0.5	0.5	6	1	0.1	0.090909	0.9090909	6	2	0.01	0.01	0.99
7	-1	10	0.9091	0.0909	7	0	1	0.5	0.5	7	1	0.1	0.091	0.909
8	-2	100	0.9901	0.0099	8	-1	10	0.909091	0.0909091	8	0	1	0.5	0.5
9	-3	1000	0.999	0.001	9	-2	100	0.990099	0.009901	9	-1	10	0.909	0.091
10	-4	10000	0.9999	1E-04	10	-3	1000	0.999001	0.000999	10	-2	100	0.99	0.01
11	-5	100000	1	1E-05	11	-4	10000	0.9999	9.999E-05	11	-3	1000	0.999	1E-03
12	-6	1000000	1	1E-06	12	-5	100000	0.99999	1E-05	12	-4	10000	1	1E-04
13	-7	1E+07	1	1E-07	13	-6	1E+06	0.999999	1E-06	13	-5	1E+05	1	1E-05
14	-8	1E+08	1	1E-08	14	-7	1E+07	1	1E-07	14	-6	1E+06	1	1E-06



			1		1	crg=	1			
	pK			7	<01>	7	<10>	4	9.212	
pH	ΔG	10^0	dG	10(-(pK-pH	dG	10(-(pK-pH	ΔG(CD)			partition
1	0	1	-6	1E+06	-6	1E+06	-8	1E+08		102000001
2	0	1	-5	100000	-5	100000	-6	1000000		1200001
3	0	1	-4	10000	-4	10000	-4	10000		30001
4	0	1	-3	1000	-3	1000	-2	100		2101
5	0	1	-2	100	-2	100	0	1		202
6	0	1	-1	10	-1	10	2	0.01		21.01
7	0	1	0	1	0	1	4	0.0001		3.0001
8	0	1	1	0.1	1	0.1	6	0.000001		1.200001
9	0	1	2	0.01	2	0.01	8	1E-08		1.02
10	0	1	3	0.001	3	0.001	10	1E-10		1.002
11	0	1	4	0.0001	4	0.0001	12	1E-12		1.0002
12	0	1	5	1E-05	5	1E-05	14	1E-14		1.00002
13	0	1	6	1E-06	6	1E-06	16	1E-16		1.000002
14	0	1	7	1E-07	7	1E-07	18	1E-18		1.0000002

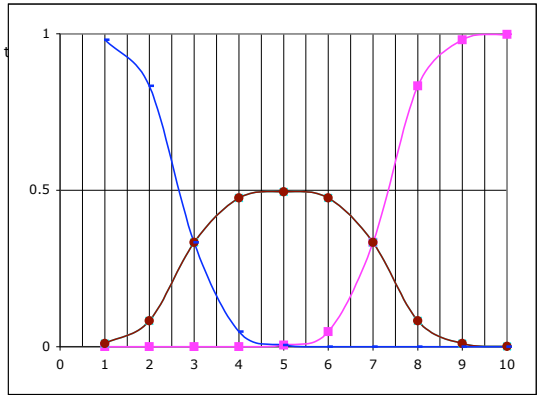
ENERGY 00 (BLUE) 10 (PINK) AND 01 (YELLOW) AND 11(CYAN)



6.8

[00] BLUE; [01] OR [10] BROWN AND [11] PINK

	<0>	<10>	<01>	<11>	t
1	9.8E-09	0.0098	0.0098	0.980	
2	8.3E-07	0.0833	0.0833	0.833	
3	3.3E-05	0.3333	0.3333	0.333	
4	0.00048	0.476	0.476	0.048	
5	0.00495	0.495	0.495	0.005	
6	0.0476	0.476	0.476	0.000	
7	0.33332	0.3333	0.3333	0.000	
8	0.83333	0.0833	0.0833	0.000	
9	0.98039	0.0098	0.0098	0.000	
10	0.998	0.001	0.001	0.000	
11	0.9998	1E-04	1E-04	0.000	
12	0.99998	1E-05	1E-05	0.000	
13	1	1E-06	1E-06	0.000	
14	1	1E-07	1E-07	0.000	



CONCENTRATION AH

	1-	-1							
1	0.990	0.990	1	1	1.980	**-4**	**-4**	**4**	**4**
2	0.917	0.917	1	1	1.833	mc4	mc3	mc4	mc3
3	0.667	0.667	1	0.91	1.333	1.000	1.000	0.928	0.917
4	0.524	0.524	1	0.5	1.047	1.000	1.000	0.687	0.667
5	0.500	0.500	1	0.09	1.000	1.000	1.000	0.523	0.522
6	0.476	0.476	1	0.01	0.953	1.000	1.000	0.497	0.501
7	0.333	0.333	1	0	0.667	1.000	1.000	0.475	0.480
8	0.083	0.083	1	0	0.167	1.000	1.000	0.314	0.334
9	0.010	0.010	0.98	0	0.020	0.990	0.991	0.072	0.082
10	0.001	0.001	0.86	0	0.002	0.503	0.837	0.009	0.010
11	0.000	0.000	0.39	0	0.000	0.011	0.017	0.001	0.000
12	0.000	0.000	0.06	0	0.000	0.000	0.000	0.000	0.000
13	0.000	0.000	0	0	0.000				
14	0.000	0.000	0	0	0.000