Accessory Material

Some Stability and Stereochemical Considerations of Simple

Bicyclo[4.2.0]octanols

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1.0 Apparatus Description for ring opening of tolylbicyclooctanol 8 at 2 or 23 ^{o}C

Reactions were carried out in a vessel equipped with a guard tube (soda lime) into which a cold finger apparatus was inserted. The cold finger was attached to a Beckman Geneline™ Cooler (coolant ethylene glycol). A polystyrene insulator was placed around the vessel and a magnetic stirrer below the vessel. Approximately 50 μL aliquots were removed with a pasteur pipette every 6 min.

2.0 Calculations for study of ring opening of tolylbicyclooctanol 8 at 23 ^{o}C

Total volume = 10 mL (ethanol) + 57 μL (aqueous NaOH)=10.057 mL = 0.010057L

$[A]_o$ = [initial tolylbicyclooctanol **8**] = moles/vol (L) = 5.61 x 10^{-6}/0.010057 = 5.5782 x 10^{-4} M

$[A]$ = [tolylbicyclooctanol **8**] at time t = (% tolylbicyclooctanol **8** at time t/100) x [tolylbicyclooctanol **8**]

Pseudo first order conditions were achieved using 10 equivalents of NaOH in 10 mL of solvent at 23 ^{o}C.

Rate constant (k) = - gradient (m)

$$T\frac{1}{2} = \ln 2/k$$

Table S1. Data and calculations for ring opening of tolylbicyclooctanol 8 at 23 °C

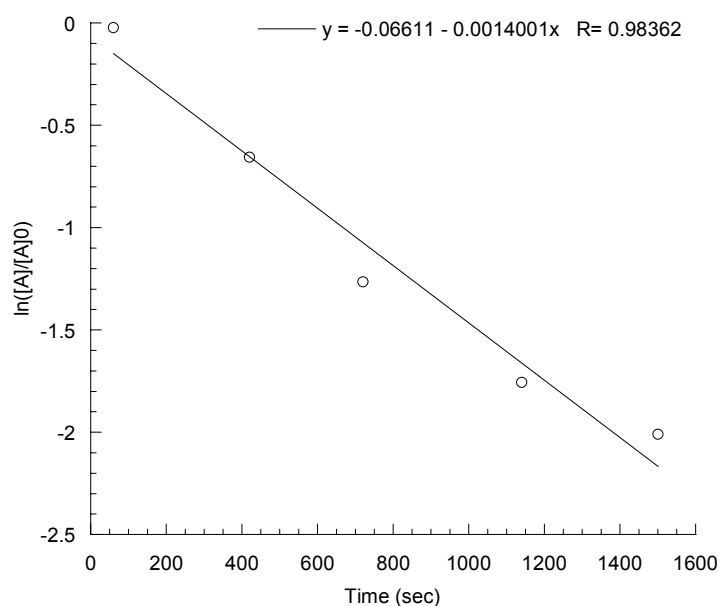| Entry	Time (s)	8 (%)	9 (%)	[A] (x 10^{-3})	[A]o (x 10^{-3})	[A]/[A]o	ln [A]/[A]o
1	60	97.73	2.27	0.5563	0.5618	0.9773	-0.0230
2	420	51.92	48.08	0.2896	0.5618	0.5192	-0.6555
3	720	28.25	71.75	0.1576	0.5618	0.2825	-1.2641
4	1140	17.29	82.71	0.0964	0.5618	0.1729	-1.7550
5	1500	13.41	86.59	0.0748	0.5618	0.1341	-2.0092
6	1920	10.72	89.28	0.0598	0.5618	0.1072	-2.2331
7	2160	9.89	90.11	0.0552	0.5618	0.0989	-2.3136
8	2520	0	100	0.0000	0.5618	-	-

y = -0.06611 - 0.0014001x R= 0.98362

Figure S1 First order plot of ring opening of tolylbicyclooctanol 8 at 23 °C

3.0 Calculations for study of ring opening of tolylbicyclooctanol 8 at 2 °C

Total volume = 20 mL (ethanol) + 113 µL (aqueous NaOH)=20.113mL = 0.020113L

[A]o = [initial tolylbicyclooctanol **8**] = moles/vol (L) = 1.12 x 10^{-5}/0.020113 = 5.5685 x 10^{-4} M

[A] = [tolylbicyclooctanol **8**] at time t = (% tolylbicyclooctanol **8** at time t/100) x [tolylbicyclooctanol **8**]

Pseudo first order conditions were achieved using 10 equivalents of NaOH in 20 mL of solvent at 2 ^{o}C.

Rate constant (k) = - gradient (m)

T½ = ln 2/k

Table S2. Data and calculations for ring opening of tolylbicyclooctanol 8 at 2 ^{o}C

Entry	Time (s)	8 (%)	9 (%)	[A] (x 10^{-3})	[A]o (x 10^{-3})	[A]/[A]o	ln [A]/[A]o
1	420	88.01	11.99	0.4901	0.5569	0. 8801	-0.12772
2	780	83.46	16.54	0.4648	0.5569	0. 8346	-0.18080
3	1140	78.56	21.44	0.4375	0.5569	0. 7856	-0.24131
4	1500	74.13	25.87	0.4128	0.5569	0. 7413	-0.29935
5	1860	69.78	30.22	0.3886	0.5569	0. 6978	-0.35982
6	2280	65.17	34.83	0.3629	0.5569	0. 6517	-0.42817
7	2640	62.21	37.79	0.3464	0.5569	0. 6221	-0.47465
8	3000	58.37	41.63	0.3251	0.5569	0. 5837	-0.53837
9	3420	54.31	45.69	0.3025	0.5569	0.5431	-0.61046
10	3840	52.46	47.54	0.2921	0.5569	0.5246	-0.64512
11	4200	49.35	50.65	0.2748	0.5569	0.4935	-0.70623
12	7200	34.92	65.08	0.1945	0.5569	0.3492	-1.0521
13	9720	26.63	73.37	0.1483	0.5569	0.2663	-1.3231
14	12240	22.53	77.47	0.1255	0.5569	0.2253	-1.4903
15	15600	18.35	81.56	0.022	0.5569	0.1835	-1.6955

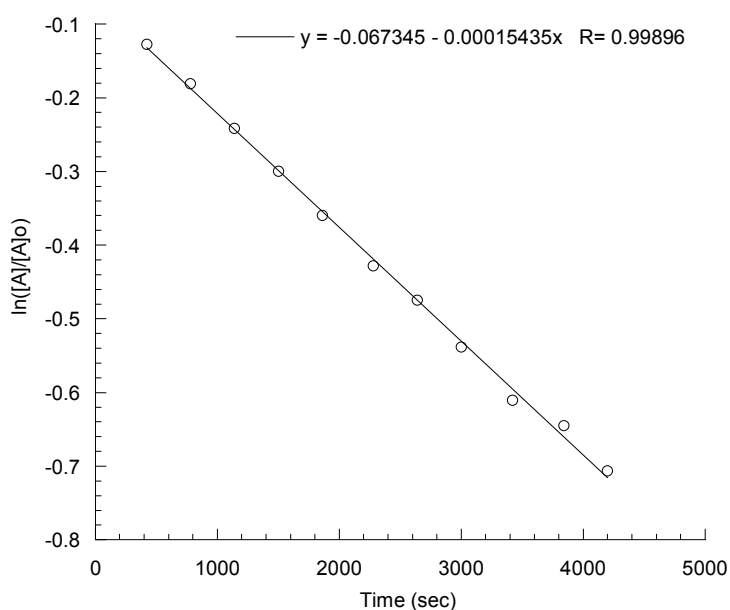y = -0.067345 - 0.00015435x   R= 0.99896

Figure S2 First order plot of ring opening of tolylbicyclooctanol 8 at 2 ^{o}C

4. ^{1}H NMR spectrum of bicyclo[4.2.0]octan-1-ol 2 in CDCl$_3$

CH$_2$Cl$_2$