

COMPUTATIONAL STUDIES OF THE EFFECTS OF PRESSURE ON REACTION KINETICS AND REACTION MECHANISMS

by

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S.1 Simulated kinetic data generated using equations E4-E8 used to calculate t-statistics found in Table 5.5 of the text.

S.3.1 Activation volumes (cm^3/mol) obtained by fitting equations E4-E8 to kinetic data generated using these equations with $\Delta V_0^\ddagger = -25 \text{ cm}^3\text{mol}^{-1}$, $\Delta\beta_0^\ddagger = 10. \text{ cm}^3\text{mol}^{-1}\text{kbar}^{-1}$, $\Delta\xi_0^\ddagger = -7.5 \text{ cm}^3\text{mol}^{-1}\text{kbar}^{-2}$ over various pressure ranges and various levels of random relative errors (see text for details). *0-1 kbar:*

Generating Equation	E4			E5			E6			E7			E8		
	1%	5%	10%	1%	5%	10%	1%	5%	10%	1%	5%	10%	1%	5%	10%
P (kbar)															
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.02	0.0282	0.0601	0.0985	0.0094	-0.0344	-0.0919	0.0243	0.0410	0.0616	-0.0008	-0.0890	-0.2114	0.0282	0.0600	0.0984
0.04	0.0454	0.0667	0.0927	0.0325	0.0018	-0.0378	0.0343	0.0113	-0.0183	0.0232	-0.0469	-0.1421	0.0206	-0.0611	-0.1736
0.06	0.0804	0.1589	0.2490	0.0579	0.0501	0.0403	0.0631	0.0764	0.0928	0.0645	0.0830	0.1057	0.0508	0.0140	-0.0341
0.08	0.0820	0.0923	0.1050	0.0931	0.1461	0.2086	0.0773	0.0689	0.0582	0.0625	-0.0080	-0.1038	0.0913	0.1372	0.1918
0.1	0.0899	0.0532	0.0053	0.0821	0.0118	-0.0836	0.0987	0.0979	0.0969	0.1090	0.1483	0.1954	0.1120	0.1624	0.2220
0.12	0.1217	0.1356	0.1528	0.1220	0.1371	0.1556	0.1352	0.2003	0.2761	0.1174	0.1140	0.1098	0.1257	0.1546	0.1895
0.14	0.1328	0.1144	0.0909	0.1400	0.1507	0.1638	0.1502	0.1999	0.2587	0.1216	0.0560	-0.0326	0.1397	0.1478	0.1578
0.16	0.1643	0.1956	0.2333	0.1715	0.2300	0.2985	0.1436	0.0905	0.0200	0.1517	0.1330	0.1090	0.1538	0.1418	0.1267
0.18	0.1874	0.2345	0.2904	0.1660	0.1283	0.0789	0.1784	0.1909	0.2063	0.1854	0.2248	0.2721	0.1761	0.1779	0.1800
0.2	0.1945	0.1970	0.2000	0.1893	0.1700	0.1454	0.2110	0.2760	0.3518	0.1930	0.1892	0.1843	0.2012	0.2274	0.2593
0.22	0.2144	0.2221	0.2316	0.2217	0.2575	0.3005	0.1989	0.1418	0.0655	0.2213	0.2552	0.2960	0.1972	0.1307	0.0408
0.24	0.2400	0.2757	0.3185	0.2216	0.1828	0.1321	0.2319	0.2351	0.2391	0.2228	0.1891	0.1453	0.2297	0.2212	0.2105
0.26	0.2401	0.2028	0.1541	0.2433	0.2184	0.1865	0.2494	0.2494	0.2494	0.2511	0.2578	0.2661	0.2619	0.3073	0.3612
0.28	0.2588	0.2236	0.1778	0.2547	0.2016	0.1310	0.2555	0.2053	0.1388	0.2749	0.3038	0.3388	0.2708	0.2797	0.2907
0.3	0.2931	0.3233	0.3598	0.2680	0.1940	0.0931	0.2846	0.2800	0.2742	0.2708	0.2090	0.1260	0.2960	0.3321	0.3754
0.32	0.3112	0.3422	0.3796	0.2921	0.2450	0.1828	0.3011	0.2906	0.2774	0.3047	0.3094	0.3152	0.2963	0.2617	0.2166
0.34	0.3258	0.3448	0.3680	0.3416	0.4186	0.5072	0.3306	0.3664	0.4095	0.3412	0.4170	0.5043	0.3198	0.3082	0.2933
0.36	0.3299	0.2941	0.2476	0.3447	0.3669	0.3940	0.3467	0.3763	0.4122	0.3354	0.3206	0.3018	0.3514	0.3937	0.4441
0.38	0.3578	0.3645	0.3728	0.3547	0.3469	0.3370	0.3681	0.4123	0.4650	0.3621	0.3838	0.4103	0.3558	0.3460	0.3337
0.4	0.3570	0.2879	0.1944	0.3528	0.2631	0.1382	0.3774	0.3900	0.4056	0.3695	0.3514	0.3282	0.3995	0.4890	0.5906
0.42	0.3925	0.3997	0.4085	0.3940	0.4043	0.4171	0.3976	0.4215	0.4506	0.3737	0.2998	0.1991	0.3930	0.3917	0.3901
0.44	0.4062	0.3995	0.3912	0.4041	0.3860	0.3630	0.3970	0.3489	0.2852	0.3962	0.3453	0.2778	0.3998	0.3548	0.2957
0.46	0.4237	0.4195	0.4142	0.4263	0.4291	0.4326	0.4344	0.4681	0.5088	0.4238	0.4167	0.4077	0.4410	0.4915	0.5513
0.48	0.4186	0.3205	0.1826	0.4307	0.3818	0.3171	0.4421	0.4396	0.4364	0.4189	0.3184	0.1767	0.4361	0.3993	0.3513
0.5	0.4663	0.4974	0.5349	0.4596	0.4606	0.4618	0.4353	0.3315	0.1846	0.4519	0.4215	0.3823	0.4691	0.4969	0.5306
0.52	0.4975	0.5826	0.6797	0.4894	0.5408	0.6016	0.4702	0.4449	0.4123	0.4657	0.4234	0.3678	0.4687	0.4267	0.3716
0.54	0.4800	0.4326	0.3701	0.4966	0.5119	0.5307	0.5065	0.5586	0.6201	0.4801	0.4284	0.3597	0.4995	0.5142	0.5324
0.56	0.5178	0.5566	0.6030	0.4998	0.4612	0.4107	0.5080	0.5016	0.4936	0.5081	0.5042	0.4992	0.5164	0.5321	0.5514
0.58	0.5188	0.4972	0.4696	0.5259	0.5270	0.5283	0.5283	0.5375	0.5488	0.5152	0.4730	0.4177	0.5335	0.5513	0.5730
0.6	0.5355	0.5164	0.4920	0.5277	0.4685	0.3893	0.5509	0.5846	0.6251	0.5510	0.5873	0.6307	0.5212	0.4177	0.2711
0.62	0.5687	0.6172	0.6747	0.5571	0.5532	0.5483	0.5659	0.5948	0.6298	0.5643	0.5892	0.6194	0.5763	0.6320	0.6974
0.64	0.5829	0.6248	0.6748	0.5867	0.6351	0.6926	0.5850	0.6253	0.6736	0.5803	0.6051	0.6353	0.5787	0.5808	0.5835
0.66	0.6011	0.6521	0.7123	0.5912	0.5955	0.6007	0.5796	0.5341	0.4742	0.6051	0.6636	0.7321	0.5784	0.5123	0.4229
0.68	0.6195	0.6804	0.7517	0.6133	0.6419	0.6765	0.6252	0.6964	0.7788	0.6159	0.6554	0.7027	0.6183	0.6495	0.6872
0.7	0.6125	0.5851	0.5498	0.6239	0.6322	0.6426	0.6295	0.6573	0.6911	0.6353	0.6886	0.7515	0.6190	0.5893	0.5508
0.72	0.6400	0.6608	0.6862	0.6245	0.5710	0.4997	0.6414	0.6545	0.6707	0.6375	0.6389	0.6407	0.6679	0.7647	0.8738
0.74	0.6543	0.6710	0.6915	0.6546	0.6606	0.6682	0.6722	0.7430	0.8250	0.6532	0.6548	0.6568	0.6682	0.7079	0.7555
0.76	0.6782	0.7284	0.7878	0.6674	0.6631	0.6576	0.6515	0.5775	0.4766	0.6736	0.6950	0.7210	0.6745	0.6779	0.6821
0.78	0.6845	0.7005	0.7201	0.6780	0.6540	0.6231	0.6883	0.7031	0.7212	0.6768	0.6492	0.6136	0.6926	0.7059	0.7223
0.8	0.7096	0.7641	0.8283	0.6989	0.6980	0.6968	0.6799	0.5956	0.4790	0.6973	0.6914	0.6840	0.7032	0.6971	0.6895
0.82	0.7079	0.6976	0.6847	0.6981	0.6303	0.5384	0.7057	0.6668	0.6160	0.7142	0.7154	0.7169	0.7067	0.6513	0.5774
0.84	0.7396	0.7950	0.8602	0.7235	0.6992	0.6680	0.7209	0.6822	0.6316	0.7375	0.7707	0.8106	0.7516	0.8142	0.8872
0.86	0.7387	0.7335	0.7270	0.7566	0.8035	0.8591	0.7556	0.7953	0.8429	0.7462	0.7551	0.7661	0.7546	0.7708	0.7907
0.88	0.7468	0.7151	0.6739	0.7631	0.7779	0.7961	0.7689	0.8026	0.8431	0.7503	0.7155	0.6701	0.7611	0.7426	0.7190
0.9	0.7673	0.7598	0.7504	0.7601	0.7013	0.6225	0.7617	0.7060	0.6317	0.7829	0.8191	0.8626	0.7886	0.8198	0.8575
0.92	0.7896	0.8135	0.8426	0.7954	0.8208	0.8516	0.7849	0.7645	0.7384	0.7847	0.7702	0.7516	0.8026	0.8299	0.8631
0.94	0.7842	0.7275	0.6518	0.7951	0.7603	0.7151	0.7798	0.6736	0.5228	0.8037	0.8068	0.8106	0.8099	0.8076	0.8048
0.96	0.8251	0.8754	0.9349	0.8101	0.7769	0.7337	0.8277	0.8607	0.9004	0.8183	0.8219	0.8263	0.8173	0.7850	0.7432
0.98	0.8402	0.8937	0.9568	0.8256	0.7968	0.7595	0.8167	0.7452	0.6479	0.8349	0.8466	0.8612	0.8412	0.8465	0.8530
1	0.8361	0.8191	0.7973	0.8452	0.8376	0.8279	0.8426	0.8195	0.7899	0.8506	0.8676	0.8886	0.8425	0.7934	0.7285

S.3.2 0-5 kbar:

Generating Equation	E4			E5			E6			E7			E8		
	1%	5%	10%	1%	5%	10%	1%	5%	10%	1%	5%	10%	1%	5%	10%
P (kbar)															
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.1	0.1070	0.1388	0.1773	0.0882	0.0444	-0.0131	0.1031	0.1198	0.1403	0.0780	-0.0102	-0.1326	0.1071	0.1389	0.1773
0.2	0.1993	0.2206	0.2466	0.1865	0.1558	0.1162	0.1883	0.1653	0.1358	0.1772	0.1071	0.0119	0.1751	0.0934	-0.0191
0.3	0.3060	0.3845	0.4746	0.2837	0.2760	0.2662	0.2891	0.3024	0.3187	0.2903	0.3088	0.3315	0.2777	0.2408	0.1928
0.4	0.3761	0.3864	0.3991	0.3877	0.4407	0.5032	0.3721	0.3637	0.3530	0.3571	0.2866	0.1908	0.3877	0.4336	0.4882
0.5	0.4494	0.4127	0.3649	0.4426	0.3723	0.2769	0.4595	0.4587	0.4577	0.4694	0.5088	0.5559	0.4751	0.5254	0.5850
0.6	0.5438	0.5577	0.5749	0.5457	0.5608	0.5793	0.5593	0.6244	0.7002	0.5409	0.5376	0.5334	0.5528	0.5817	0.6166
0.7	0.6147	0.5963	0.5728	0.6245	0.6351	0.6482	0.6352	0.6849	0.7437	0.6058	0.5402	0.4516	0.6284	0.6365	0.6465
0.8	0.7034	0.7347	0.7724	0.7143	0.7728	0.8413	0.6871	0.6341	0.5636	0.6942	0.6754	0.6514	0.7017	0.6898	0.6747
0.9	0.7813	0.8284	0.8844	0.7650	0.7272	0.6779	0.7783	0.7908	0.8062	0.7838	0.8232	0.8705	0.7811	0.7828	0.7850
1	0.8410	0.8434	0.8464	0.8423	0.8231	0.7985	0.8652	0.9303	1.0061	0.8453	0.8414	0.8365	0.8611	0.8873	0.9192
1.1	0.9112	0.9188	0.9283	0.9270	0.9628	1.0057	0.9055	0.8484	0.7722	0.9254	0.9593	1.0001	0.9100	0.8435	0.7536
1.2	0.9850	1.0206	1.0635	0.9772	0.9384	0.8877	0.9892	0.9924	0.9964	0.9769	0.9432	0.8994	0.9934	0.9849	0.9742
1.3	1.0313	0.9940	0.9453	1.0476	1.0228	0.9908	1.0556	1.0556	1.0556	1.0533	1.0600	1.0683	1.0747	1.1201	1.1740
1.4	1.0944	1.0592	1.0134	1.1061	1.0530	0.9824	1.1089	1.0587	0.9922	1.1237	1.1526	1.1876	1.1309	1.1398	1.1508
1.5	1.1713	1.2015	1.2380	1.1649	1.0910	0.9901	1.1838	1.1792	1.1734	1.1644	1.1027	1.0197	1.2017	1.2378	1.2812
1.6	1.2302	1.2613	1.2987	1.2333	1.1861	1.1239	1.2446	1.2341	1.2209	1.2418	1.2464	1.2522	1.2461	1.2114	1.1664
1.7	1.2842	1.3031	1.3263	1.3255	1.4025	1.4911	1.3171	1.3529	1.3959	1.3202	1.3960	1.4833	1.3120	1.3003	1.2855
1.8	1.3259	1.2902	1.2436	1.3702	1.3924	1.4195	1.3748	1.4044	1.4403	1.3549	1.3401	1.3214	1.3845	1.4267	1.4772
1.9	1.3901	1.3968	1.4051	1.4205	1.4127	1.4028	1.4366	1.4808	1.5335	1.4209	1.4426	1.4691	1.4284	1.4186	1.4062
2	1.4241	1.3551	1.2615	1.4578	1.3681	1.2432	1.4850	1.4977	1.5133	1.4663	1.4481	1.4250	1.5101	1.5995	1.7012
2.1	1.4931	1.5003	1.5091	1.5371	1.5474	1.5602	1.5433	1.5672	1.5963	1.5072	1.4334	1.3326	1.5402	1.5389	1.5373
2.2	1.5390	1.5324	1.5240	1.5843	1.5663	1.5432	1.5798	1.5316	1.4680	1.5654	1.5145	1.4470	1.5824	1.5375	1.4783
2.3	1.5876	1.5833	1.5780	1.6427	1.6455	1.6489	1.6532	1.6869	1.7275	1.6275	1.6204	1.6115	1.6577	1.7082	1.7680
2.4	1.6122	1.5141	1.3762	1.6823	1.6334	1.5687	1.6959	1.6933	1.6901	1.6562	1.5557	1.4140	1.6856	1.6488	1.6009
2.5	1.6886	1.7197	1.7572	1.7456	1.7466	1.7478	1.7231	1.6194	1.4724	1.7217	1.6913	1.6521	1.7504	1.7782	1.8119
2.6	1.7474	1.8326	1.9297	1.8089	1.8603	1.9211	1.7912	1.7659	1.7333	1.7671	1.7247	1.6691	1.7805	1.7385	1.6834
2.7	1.7565	1.7092	1.6467	1.8488	1.8641	1.8829	1.8598	1.9119	1.9734	1.8121	1.7603	1.6916	1.8406	1.8554	1.8735
2.8	1.8200	1.8587	1.9052	1.8841	1.8454	1.7949	1.8928	1.8864	1.8784	1.8698	1.8659	1.8609	1.8859	1.9016	1.9209
2.9	1.8456	1.8240	1.7964	1.9414	1.9425	1.9438	1.9438	1.9530	1.9643	1.9058	1.8636	1.8083	1.9302	1.9480	1.9697
3	1.8861	1.8670	1.8425	1.9738	1.9146	1.8354	1.9964	2.0300	2.0705	1.9697	2.0059	2.0494	1.9441	1.8406	1.6940
3.1	1.9422	1.9907	2.0481	2.0332	2.0293	2.0244	2.0406	2.0695	2.1045	2.0102	2.0351	2.0654	2.0244	2.0801	2.1455
3.2	1.9784	2.0203	2.0704	2.0921	2.1406	2.1980	2.0882	2.1285	2.1767	2.0528	2.0776	2.1078	2.0510	2.0531	2.0558
3.3	2.0179	2.0688	2.1291	2.1254	2.1297	2.1349	2.1106	2.0651	2.0052	2.1034	2.1619	2.2305	2.0740	2.0079	1.9185
3.4	2.0567	2.1177	2.1890	2.1757	2.2043	2.2389	2.1834	2.2546	2.3370	2.1393	2.1788	2.2261	2.1362	2.1675	2.2052
3.5	2.0695	2.0421	2.0068	2.2139	2.2223	2.2326	2.2142	2.2421	2.2759	2.1832	2.2365	2.2993	2.1584	2.1286	2.0901
3.6	2.1160	2.1368	2.1622	2.2417	2.1882	2.1169	2.2521	2.2652	2.2814	2.2092	2.2105	2.2123	2.2278	2.3246	2.4337
3.7	2.1486	2.1653	2.1858	2.2984	2.3045	2.3120	2.3083	2.3791	2.4611	2.2479	2.2496	2.2516	2.2477	2.2875	2.3351
3.8	2.1903	2.2404	2.2998	2.3374	2.3331	2.3276	2.3125	2.2385	2.1375	2.2909	2.3122	2.3383	2.2729	2.2763	2.2805
3.9	2.2135	2.2295	2.2492	2.3737	2.3497	2.3189	2.3736	2.3883	2.4064	2.3160	2.2884	2.2528	2.3089	2.3223	2.3387
4	2.2551	2.3096	2.3738	2.4200	2.4191	2.4179	2.3889	2.3046	2.1880	2.3579	2.3520	2.3446	2.3367	2.3307	2.3230
4.1	2.2692	2.2590	2.2460	2.4441	2.3762	2.2844	2.4379	2.3991	2.3483	2.3957	2.3969	2.3984	2.3566	2.3013	2.2274
4.2	2.3162	2.3716	2.4368	2.4940	2.4697	2.4385	2.4759	2.4372	2.3867	2.4392	2.4724	2.5124	2.4172	2.4797	2.5528
4.3	2.3300	2.3249	2.3184	2.5511	2.5980	2.6537	2.5329	2.5726	2.6202	2.4677	2.4766	2.4877	2.4351	2.4513	2.4712
4.4	2.3524	2.3206	2.2795	2.5815	2.5963	2.6144	2.5681	2.6018	2.6423	2.4911	2.4563	2.4109	2.4557	2.4372	2.4135
4.5	2.3865	2.3791	2.3696	2.6018	2.5430	2.4643	2.5823	2.5266	2.4523	2.5425	2.5787	2.6222	2.4966	2.5278	2.5655
4.6	2.4221	2.4460	2.4751	2.6603	2.6856	2.7165	2.6265	2.6061	2.5799	2.5627	2.5481	2.5296	2.5232	2.5506	2.5838
4.7	2.4294	2.3727	2.2970	2.6827	2.6480	2.6027	2.6419	2.5357	2.3849	2.5995	2.6026	2.6064	2.5425	2.5403	2.5374
4.8	2.4826	2.5329	2.5924	2.7201	2.6869	2.6438	2.7100	2.7429	2.7827	2.6316	2.6351	2.6395	2.5612	2.5290	2.4871
4.9	2.5095	2.5630	2.6262	2.7578	2.7290	2.6917	2.7187	2.6472	2.5499	2.6651	2.6769	2.6914	2.5958	2.6011	2.6076
5	2.5169	2.4998	2.4781	2.7993	2.7917	2.7821	2.7640	2.7410	2.7114	2.6974	2.7145	2.7354	2.6071	2.5580	2.4930

S.3.3 0-10 kbar:

Generating Equation	E4			E5			E6			E7			E8		
	1%	5%	10%	1%	5%	10%	1%	5%	10%	1%	5%	10%	1%	5%	10%
P (kbar)															
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.2	0.2021	0.2339	0.2723	0.1833	0.1396	0.0820	0.1983	0.2150	0.2355	0.1731	0.0850	-0.0374	0.2026	0.2344	0.2728
0.4	0.3789	0.4002	0.4262	0.3665	0.3359	0.2962	0.3685	0.3455	0.3159	0.3572	0.2871	0.1919	0.3564	0.2747	0.1623
0.6	0.5609	0.6393	0.7295	0.5400	0.5323	0.5225	0.5457	0.5590	0.5754	0.5465	0.5650	0.5877	0.5365	0.4996	0.4515
0.8	0.6981	0.7084	0.7211	0.7129	0.7659	0.8284	0.6978	0.6894	0.6788	0.6819	0.6114	0.5155	0.7165	0.7624	0.8170
1	0.8314	0.7947	0.7468	0.8303	0.7600	0.6646	0.8481	0.8473	0.8463	0.8563	0.8957	0.9428	0.8674	0.9178	0.9774
1.2	0.9794	0.9934	1.0105	0.9905	1.0056	1.0241	1.0053	1.0704	1.1463	0.9843	0.9809	0.9767	1.0028	1.0317	1.0666
1.4	1.0984	1.0800	1.0566	1.1217	1.1323	1.1454	1.1339	1.1836	1.2424	1.1006	1.0350	0.9464	1.1307	1.1388	1.1488
1.6	1.2303	1.2616	1.2993	1.2599	1.3183	1.3868	1.2343	1.1813	1.1108	1.2360	1.2172	1.1932	1.2516	1.2397	1.2246
1.8	1.3468	1.3940	1.4499	1.3553	1.3175	1.2682	1.3704	1.3829	1.3983	1.3687	1.4081	1.4554	1.3741	1.3758	1.3780
2	1.4412	1.4437	1.4467	1.4743	1.4550	1.4305	1.4988	1.5639	1.6397	1.4698	1.4659	1.4611	1.4931	1.5193	1.5512
2.2	1.5426	1.5502	1.5597	1.5979	1.6337	1.6766	1.5777	1.5206	1.4444	1.5864	1.6203	1.6611	1.5773	1.5108	1.4209
2.4	1.6444	1.6800	1.7229	1.6847	1.6459	1.5952	1.6974	1.7006	1.7046	1.6715	1.6378	1.5940	1.6925	1.6841	1.6734
2.6	1.7158	1.6785	1.6298	1.7895	1.7647	1.7327	1.7974	1.7974	1.7974	1.7791	1.7858	1.7941	1.8024	1.8478	1.9017
2.8	1.8014	1.7662	1.7205	1.8806	1.8275	1.7569	1.8822	1.8320	1.7655	1.8782	1.9071	1.9421	1.8842	1.8931	1.9041
3	1.8985	1.9287	1.9652	1.9704	1.8964	1.7955	1.9866	1.9820	1.9762	1.9456	1.8838	1.8008	1.9776	2.0137	2.0571
3.2	1.9756	2.0066	2.0440	2.0682	2.0211	1.9588	2.0752	2.0648	2.0515	2.0477	2.0523	2.0581	2.0420	2.0073	1.9623
3.4	2.0457	2.0647	2.0879	2.1886	2.2656	2.3542	2.1739	2.2097	2.2528	2.1491	2.2249	2.3121	2.1254	2.1137	2.0989
3.6	2.1019	2.0662	2.0196	2.2603	2.2825	2.3096	2.2564	2.2860	2.3218	2.2052	2.1904	2.1716	2.2129	2.2552	2.3056
3.8	2.1790	2.1857	2.1940	2.3366	2.3288	2.3190	2.3415	2.3857	2.4384	2.2910	2.3127	2.3392	2.2696	2.2598	2.2474
4	2.2244	2.1554	2.0618	2.3990	2.3093	2.1844	2.4121	2.4248	2.4404	2.3549	2.3368	2.3136	2.3619	2.4514	2.5530
4.2	2.3037	2.3108	2.3197	2.5025	2.5129	2.5257	2.4914	2.5153	2.5444	2.4131	2.3392	2.2385	2.4006	2.3993	2.3977
4.4	2.3585	2.3519	2.3435	2.5733	2.5552	2.5322	2.5478	2.4996	2.4360	2.4873	2.4364	2.3689	2.4493	2.4044	2.3452
4.6	2.4150	2.4107	2.4054	2.6545	2.6573	2.6608	2.6401	2.6739	2.7145	2.5645	2.5574	2.5484	2.5293	2.5798	2.6396
4.8	2.4465	2.3485	2.2105	2.7164	2.6675	2.6028	2.7009	2.6983	2.6951	2.6071	2.5066	2.3649	2.5601	2.5234	2.4754
5	2.5290	2.5601	2.5976	2.8014	2.8024	2.8036	2.7454	2.6416	2.4946	2.6856	2.6553	2.6160	2.6260	2.6538	2.6875
5.2	2.5930	2.6781	2.7753	2.8860	2.9374	2.9982	2.8298	2.8045	2.7720	2.7432	2.7009	2.6453	2.6556	2.6136	2.5585
5.4	2.6066	2.5592	2.4967	2.9468	2.9621	2.9809	2.9142	2.9662	3.0278	2.7995	2.7478	2.6791	2.7136	2.7284	2.7465
5.6	2.6737	2.7125	2.7590	3.0024	2.9638	2.9133	2.9621	2.9558	2.9478	2.8679	2.8639	2.8589	2.7552	2.7709	2.7902
5.8	2.7025	2.6809	2.6533	3.0799	3.0810	3.0823	3.0275	3.0367	3.0480	2.9137	2.8715	2.8162	2.7944	2.8121	2.8339
6	2.7456	2.7264	2.7020	3.1321	3.0729	2.9937	3.0938	3.1275	3.1680	2.9868	3.0230	3.0665	2.8017	2.6982	2.5516
6.2	2.8037	2.8522	2.9096	3.2110	3.2071	3.2022	3.1512	3.1801	3.2151	3.0358	3.0607	3.0910	2.8739	2.9296	2.9951
6.4	2.8415	2.8834	2.9334	3.2891	3.3376	3.3950	3.2115	3.2519	3.3001	3.0864	3.1112	3.1414	2.8912	2.8933	2.8960
6.6	2.8820	2.9329	2.9932	3.3415	3.3457	3.3510	3.2462	3.2007	3.1407	3.1444	3.2028	3.2714	2.9036	2.8374	2.7481
6.8	2.9215	2.9825	3.0538	3.4106	3.4391	3.4737	3.3306	3.4018	3.4842	3.1871	3.2266	3.2739	2.9539	2.9851	3.0228
7	2.9345	2.9072	2.8719	3.4674	3.4758	3.4861	3.3728	3.4006	3.4344	3.2373	3.2906	3.3534	2.9629	2.9331	2.8946
7.2	2.9810	3.0018	3.0273	3.5137	3.4601	3.3889	3.4215	3.4346	3.4508	3.2692	3.2706	3.2723	3.0180	3.1147	3.2238
7.4	3.0133	3.0300	3.0505	3.5887	3.5948	3.6024	3.4881	3.5590	3.6410	3.3134	3.3150	3.3170	3.0224	3.0622	3.1097
7.6	3.0543	3.1044	3.1638	3.6460	3.6416	3.6361	3.5024	3.4284	3.3274	3.3613	3.3827	3.4087	3.0309	3.0343	3.0386
7.8	3.0766	3.0926	3.1123	3.7003	3.6763	3.6455	3.5732	3.5880	3.6061	3.3910	3.3635	3.3279	3.0493	3.0626	3.0790
8	3.1170	3.1715	3.2357	3.7646	3.7636	3.7624	3.5980	3.5136	3.3971	3.4372	3.4313	3.4239	3.0583	3.0522	3.0446
8.2	3.1297	3.1195	3.1065	3.8065	3.7387	3.6469	3.6561	3.6172	3.5664	3.4788	3.4800	3.4815	3.0584	3.0030	2.9291
8.4	3.1751	3.2305	3.2957	3.8742	3.8499	3.8187	3.7028	3.6641	3.6136	3.5258	3.5590	3.5990	3.0981	3.1606	3.2337
8.6	3.1871	3.1820	3.1755	3.9491	3.9960	4.0517	3.7683	3.8080	3.8556	3.5575	3.5664	3.5775	3.0942	3.1104	3.1302
8.8	3.2075	3.1758	3.1346	3.9971	4.0119	4.0301	3.8117	3.8454	3.8859	3.5838	3.5490	3.5036	3.0919	3.0734	3.0498
9	3.2395	3.2321	3.2226	4.0351	3.9763	3.8975	3.8339	3.7781	3.7038	3.6377	3.6740	3.7174	3.1091	3.1403	3.1780
9.2	3.2728	3.2967	3.3258	4.1111	4.1364	4.1673	3.8858	3.8653	3.8392	3.6602	3.6456	3.6271	3.1111	3.1384	3.1716
9.4	3.2777	3.2210	3.1453	4.1511	4.1163	4.0711	3.9087	3.8025	3.6517	3.6991	3.7021	3.7059	3.1048	3.1025	3.0997
9.6	3.3284	3.3787	3.4382	4.2059	4.1727	4.1296	3.9840	4.0169	4.0566	3.7329	3.7364	3.7408	3.0971	3.0648	3.0230
9.8	3.3526	3.4061	3.4693	4.2611	4.2322	4.1950	3.9998	3.9282	3.8309	3.7679	3.7797	3.7942	3.1043	3.1096	3.1161
10	3.3572	3.3402	3.3184	4.3200	4.3123	4.3027	4.0519	4.0288	3.9992	3.8015	3.8185	3.8395	3.0874	3.0383	2.9734

S.2 Tables of simulated kinetic data sets generated by E4-E8 used for self- and cross-fitting (see Chapter 5 text for details).

Table S.4.1 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E4 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-1 kbar:

Generator Equation	Error Level	1%					5%					10%				
		Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5
E4	P (kbar)															
	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.02	0.012	0.016	0.019	0.016	0.012	-0.022	0.001	0.017	-0.001	-0.022	-0.066	-0.019	0.014	-0.023	-0.066
	0.04	0.054	0.043	0.052	0.055	0.039	0.108	0.054	0.100	0.113	0.036	0.171	0.068	0.157	0.182	0.032
	0.06	0.059	0.068	0.056	0.047	0.044	0.057	0.102	0.041	-0.008	-0.023	0.055	0.142	0.022	-0.081	-0.112
	0.08	0.069	0.081	0.077	0.087	0.076	0.028	0.087	0.066	0.118	0.060	-0.026	0.094	0.052	0.154	0.041
	0.1	0.085	0.096	0.116	0.111	0.105	0.026	0.083	0.183	0.160	0.130	-0.053	0.067	0.261	0.218	0.161
	0.12	0.127	0.133	0.117	0.130	0.122	0.164	0.192	0.113	0.176	0.139	0.208	0.262	0.107	0.230	0.159
	0.14	0.136	0.155	0.142	0.150	0.134	0.131	0.221	0.158	0.199	0.119	0.125	0.299	0.178	0.257	0.100
	0.16	0.152	0.160	0.169	0.158	0.153	0.136	0.173	0.220	0.164	0.138	0.115	0.189	0.280	0.172	0.118
	0.18	0.184	0.197	0.174	0.179	0.162	0.218	0.280	0.168	0.195	0.106	0.259	0.375	0.161	0.214	0.031
	0.2	0.184	0.207	0.182	0.192	0.187	0.141	0.256	0.134	0.182	0.158	0.085	0.315	0.071	0.171	0.121
	0.22	0.224	0.217	0.212	0.226	0.195	0.266	0.233	0.211	0.277	0.120	0.317	0.253	0.210	0.338	0.018
	0.24	0.217	0.225	0.235	0.227	0.223	0.161	0.200	0.251	0.211	0.188	0.086	0.168	0.271	0.191	0.144
	0.26	0.231	0.247	0.258	0.256	0.234	0.157	0.238	0.294	0.284	0.173	0.054	0.227	0.338	0.317	0.090
	0.28	0.272	0.271	0.257	0.259	0.277	0.292	0.284	0.216	0.225	0.313	0.316	0.300	0.162	0.180	0.357
	0.3	0.290	0.278	0.261	0.280	0.277	0.306	0.250	0.159	0.256	0.243	0.326	0.212	0.013	0.225	0.198
	0.32	0.294	0.313	0.299	0.308	0.306	0.257	0.349	0.280	0.325	0.316	0.209	0.393	0.255	0.347	0.329
	0.34	0.312	0.320	0.311	0.323	0.328	0.273	0.317	0.269	0.331	0.355	0.223	0.312	0.214	0.340	0.389
	0.36	0.337	0.336	0.331	0.344	0.335	0.329	0.327	0.302	0.364	0.322	0.320	0.314	0.264	0.389	0.305
	0.38	0.363	0.355	0.351	0.350	0.354	0.390	0.349	0.330	0.327	0.346	0.423	0.341	0.303	0.296	0.336
	0.4	0.380	0.356	0.380	0.369	0.387	0.404	0.284	0.405	0.353	0.441	0.433	0.186	0.435	0.332	0.505
	0.42	0.399	0.391	0.390	0.392	0.378	0.433	0.392	0.385	0.399	0.324	0.474	0.393	0.380	0.407	0.252
	0.44	0.406	0.427	0.414	0.395	0.391	0.396	0.499	0.438	0.343	0.321	0.385	0.582	0.466	0.275	0.226
	0.46	0.410	0.434	0.421	0.422	0.430	0.350	0.468	0.406	0.409	0.451	0.269	0.509	0.387	0.393	0.477
	0.48	0.434	0.432	0.445	0.441	0.458	0.405	0.393	0.457	0.437	0.523	0.367	0.342	0.472	0.432	0.598
	0.5	0.443	0.465	0.462	0.453	0.457	0.380	0.492	0.475	0.433	0.453	0.294	0.524	0.491	0.408	0.448
	0.52	0.483	0.481	0.481	0.471	0.478	0.513	0.507	0.505	0.453	0.492	0.550	0.538	0.533	0.430	0.509
	0.54	0.478	0.507	0.490	0.479	0.483	0.420	0.565	0.484	0.425	0.451	0.344	0.634	0.476	0.355	0.408
	0.56	0.496	0.505	0.521	0.507	0.501	0.449	0.494	0.570	0.503	0.471	0.386	0.479	0.628	0.498	0.433
	0.58	0.530	0.526	0.512	0.529	0.541	0.552	0.531	0.461	0.551	0.604	0.580	0.538	0.394	0.577	0.677
	0.6	0.543	0.555	0.535	0.529	0.528	0.556	0.613	0.512	0.481	0.475	0.571	0.681	0.483	0.418	0.406
	0.62	0.568	0.556	0.562	0.578	0.569	0.615	0.554	0.584	0.662	0.620	0.671	0.552	0.610	0.758	0.681
	0.64	0.574	0.587	0.571	0.578	0.581	0.582	0.645	0.567	0.602	0.615	0.591	0.713	0.562	0.631	0.657
	0.66	0.582	0.603	0.585	0.592	0.601	0.558	0.662	0.575	0.610	0.650	0.527	0.730	0.561	0.631	0.708
	0.68	0.611	0.597	0.614	0.600	0.606	0.639	0.571	0.654	0.586	0.616	0.673	0.538	0.702	0.567	0.629
	0.7	0.617	0.619	0.616	0.612	0.623	0.607	0.620	0.603	0.585	0.640	0.595	0.621	0.586	0.550	0.661
	0.72	0.622	0.642	0.635	0.653	0.611	0.568	0.670	0.634	0.721	0.509	0.496	0.704	0.633	0.801	0.365
	0.74	0.662	0.633	0.665	0.650	0.643	0.710	0.564	0.722	0.647	0.616	0.766	0.471	0.789	0.645	0.582
	0.76	0.657	0.659	0.660	0.671	0.668	0.626	0.634	0.639	0.696	0.677	0.584	0.603	0.611	0.725	0.688
0.78	0.685	0.664	0.674	0.679	0.700	0.703	0.593	0.647	0.675	0.774	0.726	0.498	0.612	0.670	0.859	
0.8	0.702	0.681	0.685	0.705	0.684	0.729	0.622	0.644	0.744	0.635	0.761	0.542	0.590	0.789	0.570	
0.82	0.705	0.720	0.712	0.696	0.707	0.685	0.756	0.720	0.635	0.691	0.660	0.799	0.729	0.553	0.671	
0.84	0.723	0.739	0.730	0.732	0.721	0.716	0.793	0.747	0.757	0.704	0.707	0.857	0.768	0.788	0.683	
0.86	0.749	0.731	0.729	0.751	0.749	0.786	0.694	0.682	0.796	0.782	0.829	0.645	0.621	0.849	0.823	
0.88	0.752	0.757	0.763	0.728	0.754	0.744	0.766	0.795	0.613	0.752	0.733	0.778	0.833	0.448	0.750	
0.9	0.775	0.769	0.757	0.766	0.777	0.797	0.766	0.707	0.755	0.810	0.824	0.763	0.642	0.741	0.849	
0.92	0.797	0.783	0.797	0.779	0.782	0.848	0.779	0.851	0.760	0.778	0.909	0.775	0.914	0.737	0.773	
0.94	0.802	0.796	0.802	0.805	0.805	0.819	0.790	0.816	0.833	0.833	0.840	0.782	0.835	0.868	0.867	
0.96	0.791	0.823	0.809	0.802	0.827	0.700	0.864	0.796	0.758	0.886	0.574	0.913	0.779	0.700	0.955	
0.98	0.830	0.816	0.811	0.816	0.838	0.846	0.772	0.745	0.775	0.883	0.865	0.714	0.657	0.722	0.938	
1	0.841	0.835	0.847	0.854	0.848	0.842	0.814	0.874	0.905	0.876	0.844	0.787	0.906	0.965	0.911	

Table S.4.2 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E5 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-1 kbar:

Generator Equation	Error Level	1%					5%					10%				
	P (kbar)	Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5
E5	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.02	0.012	0.016	0.019	0.016	0.012	-0.022	0.001	0.017	-0.001	-0.022	-0.066	-0.019	0.014	-0.023	-0.066
	0.04	0.054	0.043	0.052	0.055	0.039	0.108	0.054	0.100	0.113	0.036	0.171	0.068	0.157	0.182	0.032
	0.06	0.059	0.068	0.056	0.047	0.044	0.057	0.102	0.041	-0.008	-0.023	0.055	0.142	0.022	-0.081	-0.112
	0.08	0.069	0.081	0.077	0.087	0.076	0.028	0.087	0.066	0.118	0.060	-0.026	0.094	0.052	0.154	0.041
	0.1	0.085	0.096	0.116	0.111	0.105	0.026	0.083	0.183	0.160	0.130	-0.053	0.067	0.261	0.218	0.161
	0.12	0.128	0.134	0.117	0.130	0.122	0.164	0.192	0.113	0.176	0.139	0.208	0.262	0.107	0.230	0.159
	0.14	0.136	0.155	0.142	0.150	0.134	0.131	0.221	0.158	0.199	0.119	0.125	0.299	0.178	0.257	0.100
	0.16	0.152	0.160	0.169	0.158	0.153	0.136	0.173	0.220	0.164	0.138	0.115	0.189	0.280	0.172	0.118
	0.18	0.184	0.197	0.174	0.179	0.162	0.218	0.280	0.168	0.195	0.106	0.259	0.375	0.161	0.214	0.031
	0.2	0.184	0.207	0.182	0.192	0.187	0.141	0.256	0.134	0.183	0.158	0.085	0.315	0.071	0.171	0.121
	0.22	0.224	0.217	0.212	0.226	0.195	0.266	0.233	0.211	0.277	0.120	0.318	0.254	0.210	0.338	0.018
	0.24	0.217	0.225	0.235	0.227	0.223	0.161	0.200	0.251	0.211	0.188	0.086	0.169	0.271	0.191	0.144
	0.26	0.232	0.247	0.259	0.256	0.235	0.157	0.239	0.295	0.284	0.173	0.055	0.228	0.338	0.317	0.090
	0.28	0.273	0.271	0.257	0.259	0.277	0.292	0.284	0.216	0.225	0.314	0.316	0.300	0.162	0.180	0.357
	0.3	0.290	0.279	0.262	0.280	0.277	0.306	0.250	0.159	0.256	0.243	0.326	0.213	0.014	0.225	0.198
	0.32	0.295	0.313	0.299	0.308	0.306	0.257	0.350	0.280	0.326	0.316	0.209	0.393	0.256	0.347	0.329
	0.34	0.312	0.321	0.311	0.323	0.328	0.274	0.317	0.269	0.331	0.356	0.224	0.313	0.214	0.340	0.389
	0.36	0.337	0.337	0.332	0.344	0.336	0.330	0.327	0.302	0.364	0.323	0.320	0.315	0.264	0.389	0.306
	0.38	0.364	0.355	0.351	0.351	0.355	0.391	0.349	0.330	0.327	0.347	0.424	0.341	0.304	0.297	0.337
	0.4	0.380	0.357	0.380	0.370	0.388	0.404	0.285	0.405	0.354	0.442	0.434	0.187	0.436	0.333	0.505
	0.42	0.400	0.392	0.390	0.393	0.378	0.434	0.392	0.386	0.399	0.325	0.475	0.393	0.381	0.407	0.253
	0.44	0.406	0.427	0.415	0.396	0.392	0.397	0.500	0.438	0.344	0.322	0.386	0.583	0.467	0.275	0.227
	0.46	0.411	0.434	0.422	0.422	0.431	0.351	0.468	0.407	0.410	0.452	0.270	0.510	0.388	0.393	0.478
	0.48	0.435	0.433	0.446	0.442	0.459	0.406	0.394	0.458	0.438	0.524	0.368	0.343	0.473	0.433	0.599
	0.5	0.444	0.466	0.463	0.454	0.458	0.381	0.493	0.476	0.434	0.454	0.296	0.525	0.492	0.409	0.449
	0.52	0.484	0.483	0.482	0.472	0.480	0.515	0.508	0.506	0.454	0.494	0.551	0.539	0.535	0.432	0.511
	0.54	0.479	0.508	0.491	0.480	0.485	0.422	0.566	0.485	0.427	0.452	0.345	0.635	0.478	0.356	0.409
	0.56	0.498	0.506	0.522	0.508	0.502	0.450	0.495	0.571	0.504	0.472	0.388	0.481	0.630	0.499	0.434
	0.58	0.531	0.527	0.513	0.531	0.542	0.554	0.533	0.463	0.552	0.605	0.582	0.540	0.395	0.578	0.679
0.6	0.545	0.557	0.536	0.530	0.529	0.558	0.615	0.514	0.483	0.477	0.573	0.682	0.484	0.420	0.408	
0.62	0.570	0.558	0.564	0.580	0.571	0.617	0.556	0.585	0.664	0.622	0.673	0.554	0.612	0.760	0.683	
0.64	0.576	0.589	0.573	0.580	0.583	0.584	0.647	0.569	0.604	0.617	0.593	0.715	0.564	0.633	0.659	
0.66	0.584	0.605	0.588	0.595	0.603	0.560	0.664	0.577	0.612	0.652	0.529	0.732	0.563	0.633	0.710	
0.68	0.613	0.600	0.616	0.602	0.609	0.641	0.574	0.656	0.588	0.619	0.675	0.540	0.704	0.569	0.631	
0.7	0.619	0.622	0.619	0.615	0.626	0.610	0.623	0.605	0.588	0.643	0.598	0.623	0.589	0.552	0.664	
0.72	0.624	0.645	0.637	0.655	0.614	0.570	0.673	0.637	0.724	0.512	0.498	0.706	0.636	0.804	0.368	
0.74	0.665	0.636	0.668	0.653	0.646	0.713	0.567	0.725	0.650	0.619	0.769	0.474	0.792	0.648	0.585	
0.76	0.661	0.662	0.663	0.675	0.671	0.629	0.638	0.642	0.699	0.680	0.588	0.606	0.614	0.728	0.692	
0.78	0.689	0.667	0.677	0.683	0.703	0.707	0.597	0.650	0.678	0.777	0.729	0.501	0.616	0.673	0.862	
0.8	0.706	0.685	0.689	0.709	0.687	0.732	0.625	0.648	0.747	0.638	0.764	0.546	0.594	0.793	0.574	
0.82	0.709	0.724	0.716	0.700	0.711	0.689	0.760	0.724	0.639	0.695	0.664	0.803	0.733	0.557	0.675	
0.84	0.728	0.743	0.734	0.736	0.725	0.720	0.797	0.751	0.762	0.708	0.711	0.861	0.773	0.793	0.687	
0.86	0.754	0.735	0.733	0.756	0.753	0.790	0.698	0.687	0.800	0.787	0.834	0.649	0.626	0.854	0.828	
0.88	0.757	0.762	0.768	0.733	0.759	0.749	0.771	0.799	0.618	0.757	0.738	0.783	0.838	0.453	0.754	
0.9	0.780	0.774	0.762	0.771	0.782	0.802	0.771	0.712	0.760	0.815	0.829	0.768	0.647	0.747	0.854	
0.92	0.802	0.788	0.803	0.784	0.788	0.854	0.785	0.856	0.766	0.784	0.914	0.780	0.919	0.742	0.778	
0.94	0.808	0.802	0.807	0.811	0.811	0.825	0.796	0.822	0.839	0.839	0.845	0.788	0.840	0.873	0.872	
0.96	0.797	0.829	0.815	0.808	0.833	0.706	0.870	0.802	0.764	0.892	0.580	0.919	0.785	0.706	0.961	
0.98	0.837	0.822	0.817	0.823	0.844	0.852	0.778	0.751	0.782	0.890	0.871	0.720	0.663	0.728	0.944	
1	0.847	0.842	0.854	0.860	0.854	0.849	0.821	0.880	0.911	0.883	0.851	0.794	0.913	0.972	0.917	

Table S.4.3 Simulated kinetic data, $\ln(k/k_0)$, generated using equation **E6** with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-1 kbar:

Generator Equation	Error Level	1%					5%					10%				
		Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5
E6	P (kbar)															
	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.02	0.012	0.016	0.019	0.016	0.012	-0.022	0.001	0.017	-0.001	-0.022	-0.066	-0.019	0.014	-0.023	-0.066
	0.04	0.054	0.043	0.052	0.055	0.039	0.108	0.054	0.100	0.113	0.036	0.171	0.068	0.157	0.182	0.032
	0.06	0.059	0.068	0.056	0.047	0.044	0.057	0.102	0.041	-0.008	-0.023	0.055	0.142	0.022	-0.081	-0.112
	0.08	0.069	0.081	0.077	0.087	0.076	0.028	0.087	0.066	0.118	0.060	-0.026	0.094	0.052	0.154	0.041
	0.1	0.085	0.096	0.116	0.111	0.105	0.026	0.083	0.183	0.160	0.130	-0.053	0.067	0.261	0.218	0.161
	0.12	0.128	0.134	0.117	0.130	0.122	0.164	0.192	0.113	0.176	0.139	0.208	0.262	0.107	0.230	0.159
	0.14	0.136	0.155	0.142	0.150	0.134	0.131	0.221	0.158	0.199	0.119	0.125	0.299	0.178	0.257	0.100
	0.16	0.152	0.160	0.169	0.158	0.153	0.136	0.173	0.220	0.164	0.138	0.115	0.189	0.280	0.172	0.118
	0.18	0.184	0.197	0.174	0.179	0.162	0.218	0.280	0.168	0.195	0.106	0.259	0.375	0.161	0.214	0.031
	0.2	0.184	0.207	0.182	0.192	0.187	0.141	0.256	0.134	0.183	0.158	0.085	0.315	0.071	0.171	0.121
	0.22	0.224	0.217	0.212	0.226	0.195	0.266	0.233	0.211	0.277	0.120	0.318	0.254	0.210	0.338	0.018
	0.24	0.218	0.225	0.235	0.227	0.223	0.161	0.200	0.251	0.211	0.188	0.086	0.169	0.271	0.191	0.144
	0.26	0.232	0.247	0.259	0.256	0.235	0.157	0.239	0.295	0.284	0.173	0.055	0.228	0.338	0.317	0.090
	0.28	0.273	0.271	0.258	0.259	0.277	0.292	0.284	0.216	0.225	0.314	0.316	0.300	0.162	0.180	0.357
	0.3	0.290	0.279	0.262	0.280	0.277	0.306	0.250	0.159	0.256	0.243	0.326	0.213	0.014	0.225	0.198
	0.32	0.295	0.313	0.299	0.308	0.306	0.258	0.350	0.280	0.326	0.316	0.209	0.394	0.256	0.347	0.329
	0.34	0.312	0.321	0.311	0.323	0.328	0.274	0.317	0.269	0.331	0.356	0.224	0.313	0.214	0.341	0.389
	0.36	0.337	0.337	0.332	0.344	0.336	0.330	0.327	0.302	0.364	0.323	0.321	0.315	0.264	0.389	0.306
	0.38	0.364	0.355	0.352	0.351	0.355	0.391	0.349	0.331	0.327	0.347	0.424	0.342	0.304	0.297	0.337
	0.4	0.380	0.357	0.381	0.370	0.388	0.404	0.285	0.406	0.354	0.442	0.434	0.187	0.436	0.333	0.505
	0.42	0.400	0.392	0.390	0.393	0.379	0.434	0.392	0.386	0.399	0.325	0.475	0.393	0.381	0.407	0.253
	0.44	0.406	0.428	0.415	0.396	0.392	0.397	0.500	0.438	0.344	0.322	0.386	0.583	0.467	0.276	0.227
	0.46	0.411	0.435	0.422	0.423	0.431	0.351	0.469	0.407	0.410	0.452	0.270	0.510	0.388	0.394	0.478
	0.48	0.436	0.433	0.446	0.442	0.460	0.406	0.394	0.458	0.438	0.524	0.369	0.343	0.473	0.434	0.599
	0.5	0.444	0.466	0.463	0.455	0.459	0.381	0.493	0.476	0.435	0.454	0.296	0.526	0.492	0.409	0.449
	0.52	0.484	0.483	0.482	0.472	0.480	0.515	0.508	0.506	0.454	0.494	0.552	0.540	0.535	0.432	0.511
	0.54	0.479	0.508	0.492	0.480	0.485	0.422	0.567	0.485	0.427	0.452	0.346	0.635	0.478	0.356	0.410
	0.56	0.498	0.507	0.522	0.509	0.502	0.451	0.495	0.572	0.505	0.473	0.388	0.481	0.630	0.500	0.435
	0.58	0.532	0.527	0.514	0.531	0.542	0.554	0.533	0.463	0.553	0.606	0.582	0.540	0.396	0.578	0.679
	0.6	0.545	0.557	0.537	0.531	0.530	0.558	0.615	0.514	0.483	0.477	0.573	0.683	0.485	0.420	0.408
	0.62	0.571	0.558	0.564	0.581	0.572	0.618	0.557	0.586	0.664	0.623	0.673	0.555	0.612	0.760	0.683
	0.64	0.577	0.590	0.574	0.581	0.583	0.584	0.648	0.570	0.604	0.618	0.594	0.716	0.565	0.633	0.659
	0.66	0.585	0.606	0.588	0.595	0.603	0.561	0.664	0.577	0.612	0.652	0.530	0.733	0.564	0.634	0.710
	0.68	0.614	0.600	0.617	0.603	0.609	0.642	0.574	0.657	0.588	0.619	0.676	0.540	0.705	0.570	0.632
	0.7	0.620	0.623	0.619	0.616	0.627	0.610	0.623	0.606	0.588	0.644	0.598	0.624	0.589	0.553	0.664
	0.72	0.625	0.645	0.638	0.656	0.614	0.571	0.673	0.637	0.725	0.512	0.499	0.707	0.636	0.805	0.368
	0.74	0.666	0.637	0.669	0.653	0.647	0.713	0.568	0.726	0.651	0.620	0.769	0.474	0.793	0.648	0.585
	0.76	0.661	0.663	0.664	0.675	0.672	0.630	0.638	0.642	0.699	0.681	0.588	0.607	0.615	0.729	0.692
0.78	0.689	0.668	0.678	0.684	0.704	0.708	0.598	0.651	0.679	0.778	0.730	0.502	0.616	0.674	0.863	
0.8	0.707	0.686	0.690	0.710	0.688	0.733	0.626	0.649	0.748	0.639	0.765	0.546	0.595	0.794	0.574	
0.82	0.710	0.724	0.717	0.700	0.711	0.690	0.760	0.724	0.640	0.696	0.664	0.804	0.733	0.558	0.676	
0.84	0.729	0.744	0.735	0.737	0.726	0.721	0.798	0.752	0.762	0.709	0.712	0.862	0.773	0.793	0.688	
0.86	0.755	0.736	0.734	0.757	0.754	0.791	0.699	0.688	0.801	0.788	0.835	0.650	0.627	0.854	0.829	
0.88	0.758	0.763	0.768	0.734	0.760	0.750	0.772	0.800	0.619	0.758	0.739	0.784	0.839	0.454	0.755	
0.9	0.781	0.775	0.763	0.772	0.783	0.803	0.772	0.713	0.761	0.816	0.830	0.769	0.648	0.748	0.855	
0.92	0.803	0.789	0.804	0.785	0.789	0.855	0.786	0.857	0.767	0.785	0.915	0.781	0.920	0.743	0.779	
0.94	0.809	0.803	0.808	0.812	0.812	0.826	0.797	0.823	0.840	0.840	0.846	0.789	0.841	0.874	0.873	
0.96	0.798	0.830	0.816	0.809	0.835	0.707	0.871	0.803	0.765	0.893	0.581	0.920	0.786	0.707	0.962	
0.98	0.838	0.823	0.818	0.824	0.846	0.853	0.779	0.753	0.783	0.891	0.873	0.721	0.664	0.729	0.945	
1	0.849	0.843	0.855	0.861	0.856	0.850	0.822	0.882	0.912	0.884	0.852	0.795	0.914	0.973	0.919	

Table S.4.4 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E7 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-1 kbar:

Generator Equation	Error Level	1%					5%					10%				
		Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5
E7	P (kbar)															
	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.02	0.012	0.016	0.019	0.016	0.012	-0.022	0.001	0.017	-0.001	-0.022	-0.066	-0.019	0.014	-0.023	-0.066
	0.04	0.054	0.043	0.052	0.055	0.039	0.108	0.054	0.100	0.113	0.036	0.171	0.068	0.157	0.182	0.032
	0.06	0.059	0.068	0.056	0.047	0.044	0.057	0.102	0.041	-0.008	-0.023	0.055	0.142	0.022	-0.081	-0.112
	0.08	0.069	0.081	0.077	0.087	0.076	0.028	0.087	0.066	0.118	0.060	-0.026	0.094	0.052	0.154	0.041
	0.1	0.085	0.096	0.116	0.111	0.105	0.026	0.083	0.183	0.160	0.130	-0.053	0.067	0.261	0.218	0.161
	0.12	0.128	0.134	0.117	0.130	0.122	0.164	0.192	0.113	0.176	0.139	0.208	0.262	0.107	0.230	0.159
	0.14	0.136	0.155	0.142	0.150	0.134	0.131	0.221	0.158	0.199	0.119	0.125	0.299	0.178	0.257	0.100
	0.16	0.152	0.160	0.169	0.158	0.153	0.136	0.173	0.220	0.164	0.138	0.115	0.189	0.280	0.172	0.118
	0.18	0.184	0.197	0.174	0.179	0.162	0.218	0.280	0.168	0.195	0.106	0.259	0.375	0.161	0.214	0.031
	0.2	0.184	0.207	0.182	0.192	0.187	0.141	0.256	0.134	0.183	0.158	0.085	0.315	0.071	0.171	0.121
	0.22	0.224	0.217	0.212	0.226	0.195	0.266	0.233	0.211	0.277	0.120	0.318	0.254	0.210	0.338	0.018
	0.24	0.217	0.225	0.235	0.227	0.223	0.161	0.200	0.251	0.211	0.188	0.086	0.169	0.271	0.191	0.144
	0.26	0.232	0.247	0.259	0.256	0.235	0.157	0.239	0.295	0.284	0.173	0.054	0.228	0.338	0.317	0.090
	0.28	0.273	0.271	0.257	0.259	0.277	0.292	0.284	0.216	0.225	0.314	0.316	0.300	0.162	0.180	0.357
	0.3	0.290	0.279	0.262	0.280	0.277	0.306	0.250	0.159	0.256	0.243	0.326	0.213	0.014	0.225	0.198
	0.32	0.295	0.313	0.299	0.308	0.306	0.257	0.350	0.280	0.326	0.316	0.209	0.393	0.256	0.347	0.329
	0.34	0.312	0.321	0.311	0.323	0.328	0.274	0.317	0.269	0.331	0.356	0.224	0.313	0.214	0.340	0.389
	0.36	0.337	0.337	0.332	0.344	0.336	0.330	0.327	0.302	0.364	0.323	0.320	0.315	0.264	0.389	0.306
	0.38	0.363	0.355	0.351	0.351	0.355	0.391	0.349	0.330	0.327	0.347	0.423	0.341	0.304	0.297	0.337
	0.4	0.380	0.357	0.380	0.370	0.388	0.404	0.285	0.405	0.354	0.442	0.434	0.187	0.436	0.333	0.505
	0.42	0.400	0.391	0.390	0.393	0.378	0.434	0.392	0.386	0.399	0.325	0.475	0.393	0.381	0.407	0.253
	0.44	0.406	0.427	0.415	0.396	0.392	0.397	0.499	0.438	0.344	0.322	0.386	0.583	0.467	0.275	0.227
	0.46	0.411	0.434	0.422	0.422	0.431	0.351	0.468	0.407	0.410	0.452	0.270	0.509	0.388	0.393	0.478
	0.48	0.435	0.433	0.446	0.442	0.459	0.406	0.394	0.458	0.438	0.524	0.368	0.343	0.473	0.433	0.599
	0.5	0.444	0.466	0.463	0.454	0.458	0.381	0.493	0.476	0.434	0.454	0.295	0.525	0.491	0.409	0.449
	0.52	0.484	0.483	0.482	0.472	0.480	0.514	0.508	0.506	0.454	0.493	0.551	0.539	0.534	0.431	0.510
	0.54	0.479	0.508	0.491	0.480	0.485	0.422	0.566	0.485	0.427	0.452	0.345	0.635	0.477	0.356	0.409
	0.56	0.498	0.506	0.522	0.508	0.502	0.450	0.495	0.571	0.504	0.472	0.388	0.481	0.630	0.499	0.434
0.58	0.531	0.527	0.513	0.531	0.542	0.554	0.533	0.463	0.552	0.605	0.582	0.540	0.395	0.578	0.679	
0.6	0.545	0.557	0.536	0.530	0.529	0.557	0.615	0.513	0.483	0.477	0.573	0.682	0.484	0.420	0.408	
0.62	0.570	0.558	0.563	0.580	0.571	0.617	0.556	0.585	0.664	0.622	0.673	0.554	0.612	0.759	0.682	
0.64	0.576	0.589	0.573	0.580	0.583	0.584	0.647	0.569	0.604	0.617	0.593	0.715	0.564	0.633	0.658	
0.66	0.584	0.605	0.587	0.594	0.603	0.560	0.664	0.577	0.612	0.652	0.529	0.732	0.563	0.633	0.710	
0.68	0.613	0.599	0.616	0.602	0.608	0.641	0.573	0.656	0.588	0.619	0.675	0.540	0.704	0.569	0.631	
0.7	0.619	0.622	0.618	0.615	0.626	0.610	0.622	0.605	0.587	0.643	0.597	0.623	0.588	0.552	0.663	
0.72	0.624	0.644	0.637	0.655	0.613	0.570	0.672	0.636	0.724	0.511	0.498	0.706	0.635	0.804	0.367	
0.74	0.665	0.636	0.668	0.652	0.646	0.712	0.567	0.725	0.650	0.619	0.769	0.473	0.792	0.647	0.584	
0.76	0.660	0.662	0.663	0.674	0.671	0.629	0.637	0.641	0.698	0.680	0.587	0.606	0.614	0.728	0.691	
0.78	0.688	0.667	0.677	0.682	0.703	0.707	0.596	0.650	0.678	0.777	0.729	0.501	0.615	0.673	0.862	
0.8	0.705	0.684	0.689	0.709	0.687	0.732	0.625	0.647	0.747	0.638	0.764	0.545	0.593	0.793	0.573	
0.82	0.709	0.723	0.716	0.699	0.710	0.689	0.759	0.723	0.638	0.695	0.663	0.802	0.732	0.557	0.675	
0.84	0.727	0.743	0.733	0.736	0.725	0.720	0.797	0.751	0.761	0.708	0.711	0.860	0.772	0.792	0.686	
0.86	0.753	0.735	0.733	0.755	0.753	0.790	0.698	0.686	0.800	0.786	0.833	0.649	0.625	0.853	0.827	
0.88	0.757	0.761	0.767	0.732	0.758	0.748	0.771	0.799	0.617	0.756	0.737	0.782	0.837	0.452	0.754	
0.9	0.779	0.773	0.762	0.771	0.782	0.801	0.770	0.712	0.760	0.814	0.828	0.767	0.646	0.746	0.853	
0.92	0.802	0.787	0.802	0.784	0.787	0.853	0.784	0.855	0.765	0.783	0.914	0.780	0.918	0.741	0.777	
0.94	0.807	0.801	0.807	0.810	0.810	0.824	0.795	0.821	0.838	0.838	0.845	0.787	0.840	0.873	0.872	
0.96	0.796	0.828	0.814	0.807	0.833	0.705	0.869	0.801	0.763	0.891	0.579	0.918	0.784	0.705	0.960	
0.98	0.836	0.821	0.816	0.822	0.844	0.851	0.777	0.751	0.781	0.889	0.871	0.719	0.662	0.727	0.943	
1	0.847	0.841	0.853	0.859	0.854	0.848	0.820	0.880	0.910	0.882	0.850	0.793	0.912	0.971	0.917	

Table S.4.5 Simulated kinetic data, $\ln(k/k_0)$, generated using equation **E8** with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-1 kbar:

Generator Equation	Error Level	1%					5%					10%				
		Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5	Set 1	Set 2	Set 3	Set 4	Set 5
E8	P (kbar)															
	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.02	0.012	0.016	0.020	0.016	0.012	-0.022	0.001	0.017	-0.001	-0.022	-0.066	-0.019	0.014	-0.023	-0.066
	0.04	0.054	0.043	0.052	0.055	0.039	0.108	0.054	0.100	0.113	0.036	0.171	0.068	0.157	0.182	0.032
	0.06	0.059	0.068	0.056	0.047	0.044	0.057	0.102	0.041	-0.008	-0.022	0.055	0.142	0.022	-0.081	-0.112
	0.08	0.069	0.081	0.077	0.087	0.076	0.028	0.087	0.066	0.118	0.060	-0.026	0.094	0.052	0.154	0.041
	0.1	0.085	0.096	0.116	0.112	0.105	0.026	0.083	0.184	0.160	0.131	-0.053	0.067	0.261	0.218	0.161
	0.12	0.128	0.134	0.117	0.130	0.123	0.164	0.193	0.113	0.176	0.139	0.208	0.262	0.107	0.230	0.160
	0.14	0.136	0.155	0.142	0.150	0.134	0.131	0.222	0.158	0.199	0.119	0.125	0.299	0.179	0.257	0.100
	0.16	0.153	0.160	0.170	0.158	0.153	0.136	0.173	0.220	0.164	0.138	0.115	0.190	0.280	0.172	0.119
	0.18	0.184	0.198	0.174	0.180	0.162	0.218	0.280	0.169	0.195	0.106	0.259	0.375	0.162	0.214	0.032
	0.2	0.184	0.207	0.183	0.192	0.187	0.142	0.257	0.135	0.183	0.159	0.086	0.316	0.071	0.171	0.121
	0.22	0.224	0.217	0.213	0.226	0.195	0.267	0.234	0.212	0.278	0.121	0.318	0.254	0.210	0.339	0.019
	0.24	0.218	0.226	0.236	0.228	0.223	0.162	0.201	0.252	0.212	0.189	0.087	0.169	0.272	0.192	0.145
	0.26	0.232	0.248	0.259	0.257	0.235	0.158	0.239	0.295	0.285	0.174	0.055	0.228	0.339	0.318	0.091
	0.28	0.273	0.272	0.258	0.260	0.278	0.293	0.285	0.217	0.226	0.314	0.317	0.301	0.163	0.181	0.358
	0.3	0.291	0.280	0.263	0.281	0.278	0.307	0.251	0.160	0.257	0.244	0.327	0.214	0.015	0.226	0.199
	0.32	0.296	0.314	0.300	0.309	0.307	0.259	0.351	0.281	0.327	0.318	0.210	0.395	0.257	0.348	0.330
	0.34	0.313	0.322	0.313	0.325	0.330	0.275	0.318	0.271	0.332	0.357	0.225	0.314	0.216	0.342	0.390
	0.36	0.339	0.338	0.333	0.346	0.337	0.331	0.328	0.304	0.366	0.324	0.322	0.316	0.266	0.390	0.307
	0.38	0.365	0.357	0.353	0.352	0.356	0.392	0.351	0.332	0.329	0.348	0.425	0.343	0.305	0.298	0.338
	0.4	0.382	0.359	0.382	0.372	0.390	0.406	0.287	0.407	0.355	0.444	0.435	0.189	0.438	0.334	0.507
	0.42	0.402	0.394	0.392	0.395	0.380	0.436	0.394	0.388	0.401	0.327	0.477	0.395	0.383	0.409	0.255
	0.44	0.408	0.430	0.417	0.398	0.394	0.399	0.502	0.440	0.346	0.324	0.388	0.585	0.469	0.277	0.229
	0.46	0.413	0.437	0.424	0.425	0.433	0.353	0.471	0.409	0.412	0.454	0.272	0.512	0.390	0.396	0.480
	0.48	0.438	0.436	0.448	0.444	0.462	0.409	0.397	0.460	0.440	0.526	0.371	0.346	0.476	0.436	0.601
	0.5	0.447	0.469	0.465	0.457	0.461	0.383	0.496	0.478	0.437	0.457	0.298	0.528	0.494	0.412	0.451
	0.52	0.487	0.485	0.485	0.475	0.482	0.517	0.511	0.509	0.457	0.496	0.554	0.542	0.537	0.434	0.513
	0.54	0.482	0.511	0.494	0.483	0.488	0.425	0.569	0.488	0.430	0.455	0.348	0.638	0.481	0.359	0.412
	0.56	0.501	0.510	0.525	0.511	0.505	0.454	0.498	0.575	0.508	0.476	0.391	0.484	0.633	0.503	0.437
	0.58	0.535	0.530	0.517	0.534	0.545	0.557	0.536	0.466	0.556	0.609	0.585	0.543	0.399	0.581	0.682
	0.6	0.549	0.560	0.540	0.534	0.533	0.561	0.618	0.517	0.486	0.481	0.577	0.686	0.488	0.423	0.411
	0.62	0.574	0.561	0.567	0.584	0.575	0.621	0.560	0.589	0.668	0.626	0.677	0.558	0.616	0.763	0.686
	0.64	0.580	0.593	0.577	0.584	0.587	0.588	0.651	0.573	0.608	0.621	0.597	0.719	0.568	0.637	0.663
	0.66	0.588	0.609	0.592	0.599	0.607	0.564	0.668	0.581	0.616	0.656	0.533	0.737	0.567	0.638	0.714
	0.68	0.617	0.604	0.621	0.607	0.613	0.645	0.578	0.661	0.592	0.623	0.679	0.544	0.709	0.574	0.636
	0.7	0.624	0.626	0.623	0.620	0.631	0.614	0.627	0.610	0.592	0.648	0.602	0.628	0.593	0.557	0.668
	0.72	0.629	0.649	0.642	0.660	0.618	0.575	0.677	0.641	0.729	0.516	0.503	0.711	0.640	0.809	0.372
	0.74	0.670	0.641	0.673	0.657	0.651	0.718	0.572	0.730	0.655	0.624	0.774	0.478	0.797	0.653	0.590
	0.76	0.666	0.668	0.668	0.680	0.676	0.634	0.643	0.647	0.704	0.685	0.593	0.611	0.620	0.733	0.697
0.78	0.694	0.672	0.683	0.688	0.709	0.712	0.602	0.656	0.684	0.782	0.735	0.507	0.621	0.678	0.868	
0.8	0.711	0.690	0.695	0.714	0.693	0.738	0.631	0.653	0.753	0.644	0.770	0.551	0.599	0.799	0.579	
0.82	0.715	0.729	0.722	0.705	0.716	0.695	0.765	0.729	0.644	0.701	0.669	0.809	0.738	0.563	0.681	
0.84	0.734	0.749	0.740	0.742	0.731	0.726	0.803	0.757	0.767	0.714	0.717	0.867	0.779	0.799	0.693	
0.86	0.760	0.741	0.739	0.762	0.759	0.796	0.704	0.693	0.807	0.793	0.840	0.656	0.632	0.860	0.834	
0.88	0.764	0.768	0.774	0.739	0.765	0.755	0.777	0.806	0.624	0.763	0.744	0.789	0.844	0.459	0.761	
0.9	0.786	0.780	0.769	0.778	0.789	0.808	0.777	0.719	0.767	0.821	0.835	0.774	0.653	0.753	0.860	
0.92	0.809	0.795	0.809	0.791	0.795	0.860	0.791	0.863	0.772	0.790	0.921	0.787	0.926	0.749	0.785	
0.94	0.815	0.809	0.814	0.818	0.818	0.831	0.803	0.829	0.846	0.845	0.852	0.795	0.847	0.880	0.879	
0.96	0.804	0.836	0.822	0.815	0.840	0.713	0.877	0.809	0.771	0.899	0.587	0.926	0.792	0.713	0.968	
0.98	0.844	0.829	0.824	0.830	0.852	0.859	0.785	0.759	0.789	0.897	0.879	0.727	0.670	0.735	0.951	
1	0.855	0.849	0.861	0.868	0.862	0.856	0.828	0.888	0.919	0.890	0.858	0.801	0.920	0.979	0.925	

Table S.4.6 Simulated kinetic data, $\ln(k/k_0)$, generated using equation **E4** with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-5 kbar:

Generator Equation	Error Level	1%					5%					10%					
		P (kbar)	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.1	0.111	0.105	0.094	0.099	0.108	0.159	0.131	0.075	0.101	0.144	0.215	0.161	0.050	0.104	0.188	
	0.2	0.200	0.193	0.186	0.208	0.190	0.225	0.187	0.153	0.260	0.175	0.256	0.180	0.110	0.323	0.156	
	0.3	0.286	0.284	0.286	0.289	0.277	0.291	0.280	0.287	0.302	0.241	0.296	0.274	0.288	0.318	0.194	
	0.4	0.386	0.362	0.351	0.388	0.388	0.436	0.316	0.258	0.442	0.445	0.494	0.256	0.127	0.506	0.512	
	0.5	0.461	0.445	0.464	0.465	0.428	0.471	0.390	0.486	0.493	0.294	0.483	0.317	0.512	0.526	0.096	
	0.6	0.539	0.554	0.541	0.540	0.559	0.533	0.606	0.545	0.539	0.629	0.526	0.668	0.549	0.539	0.711	
	0.7	0.628	0.619	0.625	0.615	0.605	0.662	0.617	0.646	0.596	0.548	0.702	0.615	0.672	0.573	0.471	
	0.8	0.691	0.686	0.697	0.691	0.700	0.673	0.646	0.703	0.672	0.720	0.650	0.594	0.711	0.648	0.744	
	0.9	0.771	0.777	0.762	0.764	0.744	0.777	0.807	0.731	0.744	0.639	0.784	0.843	0.692	0.718	0.490	
	1.0	0.831	0.841	0.836	0.833	0.852	0.791	0.845	0.818	0.802	0.897	0.740	0.851	0.795	0.762	0.950	
	1.1	0.920	0.921	0.906	0.916	0.912	0.962	0.968	0.894	0.945	0.925	1.012	1.023	0.879	0.979	0.941	
	1.2	0.973	0.959	0.972	0.958	0.993	0.961	0.886	0.957	0.883	1.056	0.947	0.788	0.937	0.780	1.131	
	1.3	1.019	1.043	1.052	1.038	1.037	0.930	1.053	1.097	1.027	1.022	0.807	1.065	1.151	1.014	1.002	
	1.4	1.124	1.123	1.130	1.098	1.095	1.202	1.201	1.231	1.079	1.064	1.292	1.291	1.345	1.054	1.024	
	1.5	1.165	1.157	1.178	1.166	1.161	1.169	1.129	1.231	1.176	1.152	1.175	1.094	1.295	1.187	1.140	
	1.6	1.236	1.227	1.220	1.232	1.224	1.287	1.245	1.211	1.269	1.231	1.348	1.267	1.199	1.314	1.240	
	1.7	1.294	1.312	1.284	1.292	1.297	1.349	1.434	1.303	1.343	1.362	1.415	1.569	1.326	1.403	1.439	
	1.8	1.326	1.344	1.331	1.341	1.329	1.292	1.382	1.318	1.367	1.306	1.248	1.428	1.301	1.399	1.277	
	1.9	1.400	1.407	1.403	1.390	1.394	1.446	1.476	1.457	1.397	1.414	1.501	1.557	1.522	1.405	1.439	
	2.0	1.436	1.443	1.427	1.444	1.432	1.419	1.450	1.372	1.457	1.398	1.398	1.459	1.299	1.473	1.353	
	2.1	1.505	1.510	1.496	1.494	1.496	1.559	1.582	1.515	1.505	1.516	1.622	1.665	1.539	1.518	1.541	
	2.2	1.543	1.524	1.547	1.544	1.545	1.550	1.453	1.571	1.558	1.561	1.560	1.356	1.601	1.575	1.581	
	2.3	1.581	1.602	1.591	1.581	1.565	1.549	1.654	1.602	1.549	1.467	1.508	1.716	1.615	1.508	1.328	
	2.4	1.634	1.653	1.648	1.647	1.646	1.630	1.719	1.696	1.691	1.690	1.624	1.796	1.754	1.743	1.741	
	2.5	1.686	1.665	1.682	1.694	1.669	1.709	1.601	1.685	1.744	1.622	1.736	1.515	1.690	1.803	1.559	
	2.6	1.716	1.730	1.728	1.736	1.742	1.678	1.751	1.739	1.780	1.805	1.630	1.777	1.753	1.832	1.880	
	2.7	1.753	1.772	1.748	1.755	1.761	1.693	1.787	1.661	1.702	1.733	1.612	1.805	1.542	1.632	1.697	
	2.8	1.823	1.819	1.803	1.818	1.826	1.874	1.854	1.776	1.848	1.889	1.934	1.897	1.742	1.884	1.962	
	2.9	1.843	1.848	1.863	1.844	1.863	1.813	1.836	1.908	1.814	1.912	1.774	1.820	1.962	1.775	1.969	
	3.0	1.884	1.912	1.907	1.908	1.907	1.858	1.992	1.971	1.972	1.969	1.824	2.084	2.046	2.047	2.042	
3.1	1.925	1.920	1.933	1.941	1.921	1.904	1.879	1.947	1.984	1.883	1.878	1.826	1.964	2.035	1.835		
3.2	1.979	1.981	1.959	1.976	1.972	2.024	2.033	1.925	2.011	1.989	2.077	2.095	1.881	2.052	2.010		
3.3	1.994	2.017	1.998	2.010	2.010	1.948	2.063	1.968	2.031	2.032	1.889	2.118	1.930	2.056	2.059		
3.4	2.043	2.040	2.046	2.044	2.040	2.053	2.036	2.067	2.055	2.038	2.065	2.030	2.093	2.069	2.036		
3.5	2.078	2.085	2.068	2.063	2.076	2.085	2.122	2.036	2.009	2.074	2.093	2.165	1.993	1.937	2.072		
3.6	2.121	2.101	2.103	2.136	2.116	2.160	2.063	2.072	2.230	2.138	2.208	2.013	2.031	2.337	2.164		
3.7	2.137	2.155	2.147	2.127	2.144	2.105	2.196	2.159	2.055	2.140	2.064	2.246	2.174	1.956	2.136		
3.8	2.181	2.176	2.177	2.160	2.191	2.198	2.171	2.178	2.088	2.245	2.218	2.165	2.179	1.990	2.308		
3.9	2.211	2.211	2.209	2.200	2.230	2.219	2.219	2.206	2.163	2.306	2.229	2.228	2.202	2.115	2.394		
4.0	2.251	2.240	2.228	2.238	2.222	2.292	2.238	2.176	2.224	2.142	2.340	2.236	2.107	2.207	2.032		
4.1	2.265	2.283	2.274	2.272	2.268	2.236	2.325	2.285	2.273	2.253	2.200	2.375	2.298	2.275	2.233		
4.2	2.285	2.307	2.301	2.298	2.304	2.216	2.328	2.299	2.281	2.313	2.123	2.354	2.295	2.261	2.324		
4.3	2.326	2.355	2.331	2.320	2.330	2.306	2.446	2.329	2.271	2.323	2.279	2.550	2.326	2.206	2.315		
4.4	2.348	2.353	2.353	2.353	2.360	2.298	2.324	2.322	2.325	2.358	2.232	2.287	2.282	2.288	2.355		
4.5	2.392	2.373	2.372	2.396	2.390	2.408	2.309	2.304	2.428	2.395	2.428	2.223	2.213	2.466	2.403		
4.6	2.417	2.399	2.423	2.397	2.436	2.422	2.329	2.450	2.317	2.511	2.429	2.235	2.483	2.207	2.598		
4.7	2.444	2.438	2.437	2.444	2.443	2.446	2.418	2.413	2.448	2.443	2.448	2.393	2.382	2.453	2.442		
4.8	2.469	2.479	2.444	2.469	2.464	2.469	2.517	2.333	2.468	2.444	2.468	2.562	2.176	2.466	2.417		
4.9	2.508	2.488	2.488	2.496	2.494	2.557	2.457	2.459	2.495	2.486	2.615	2.416	2.421	2.495	2.475		
5.0	2.517	2.516	2.533	2.512	2.506	2.498	2.494	2.580	2.472	2.445	2.475	2.466	2.635	2.421	2.362		

Table S.4.7 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E5 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-5 kbar:

Generator Equation	Error Level	1%					5%					10%				
	P (kbar)	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E5	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.1	0.111	0.105	0.094	0.099	0.108	0.159	0.131	0.075	0.101	0.144	0.215	0.161	0.050	0.104	0.188
	0.2	0.200	0.193	0.186	0.208	0.190	0.225	0.187	0.153	0.260	0.175	0.256	0.180	0.110	0.323	0.156
	0.3	0.287	0.285	0.286	0.289	0.277	0.291	0.280	0.287	0.302	0.241	0.296	0.274	0.289	0.318	0.194
	0.4	0.387	0.363	0.352	0.388	0.389	0.436	0.317	0.258	0.443	0.446	0.495	0.256	0.128	0.507	0.513
	0.5	0.462	0.446	0.465	0.466	0.429	0.472	0.391	0.487	0.494	0.295	0.484	0.318	0.514	0.527	0.097
	0.6	0.541	0.555	0.543	0.542	0.560	0.535	0.608	0.546	0.541	0.631	0.528	0.670	0.551	0.540	0.712
	0.7	0.630	0.621	0.627	0.617	0.608	0.664	0.620	0.649	0.599	0.551	0.705	0.617	0.675	0.576	0.474
	0.8	0.695	0.689	0.701	0.695	0.704	0.676	0.650	0.707	0.676	0.724	0.653	0.597	0.715	0.652	0.748
	0.9	0.776	0.782	0.767	0.769	0.750	0.782	0.812	0.736	0.749	0.644	0.789	0.848	0.697	0.723	0.495
	1	0.837	0.848	0.843	0.840	0.859	0.798	0.852	0.825	0.809	0.904	0.747	0.857	0.802	0.769	0.957
	1.1	0.929	0.930	0.915	0.925	0.921	0.971	0.976	0.903	0.953	0.934	1.021	1.031	0.888	0.988	0.950
	1.2	0.984	0.969	0.983	0.969	1.003	0.972	0.897	0.967	0.894	1.067	0.957	0.799	0.948	0.791	1.142
	1.3	1.033	1.056	1.065	1.051	1.050	0.944	1.066	1.110	1.041	1.035	0.820	1.079	1.164	1.027	1.016
	1.4	1.140	1.139	1.146	1.114	1.111	1.218	1.217	1.247	1.095	1.080	1.308	1.307	1.361	1.070	1.040
	1.5	1.184	1.176	1.197	1.185	1.180	1.188	1.149	1.250	1.195	1.171	1.194	1.113	1.314	1.206	1.159
	1.6	1.258	1.249	1.242	1.254	1.246	1.310	1.267	1.233	1.291	1.254	1.370	1.289	1.221	1.336	1.262
	1.7	1.320	1.338	1.310	1.318	1.322	1.375	1.460	1.329	1.369	1.388	1.441	1.595	1.352	1.429	1.465
	1.8	1.356	1.374	1.361	1.371	1.359	1.322	1.412	1.348	1.397	1.336	1.278	1.458	1.331	1.429	1.307
	1.9	1.434	1.441	1.437	1.424	1.428	1.480	1.510	1.491	1.431	1.448	1.535	1.591	1.556	1.439	1.473
	2	1.475	1.481	1.466	1.482	1.471	1.458	1.488	1.411	1.496	1.436	1.436	1.498	1.337	1.512	1.391
	2.1	1.548	1.553	1.539	1.537	1.540	1.602	1.625	1.558	1.548	1.560	1.665	1.708	1.582	1.561	1.584
	2.2	1.591	1.572	1.595	1.592	1.593	1.598	1.501	1.619	1.606	1.609	1.608	1.405	1.649	1.623	1.629
	2.3	1.634	1.655	1.645	1.634	1.619	1.602	1.708	1.655	1.603	1.520	1.561	1.769	1.669	1.562	1.382
	2.4	1.693	1.711	1.707	1.706	1.705	1.688	1.778	1.755	1.750	1.748	1.683	1.855	1.813	1.802	1.800
	2.5	1.751	1.730	1.746	1.758	1.734	1.773	1.666	1.750	1.808	1.687	1.801	1.580	1.755	1.868	1.624
	2.6	1.787	1.801	1.799	1.807	1.812	1.749	1.822	1.810	1.851	1.876	1.700	1.847	1.824	1.903	1.950
	2.7	1.830	1.849	1.825	1.832	1.838	1.770	1.864	1.738	1.779	1.810	1.689	1.882	1.619	1.709	1.774
	2.8	1.907	1.903	1.887	1.901	1.910	1.957	1.938	1.860	1.931	1.972	2.018	1.980	1.825	1.968	2.045
	2.9	1.934	1.938	1.953	1.934	1.954	1.903	1.926	1.998	1.904	2.002	1.864	1.911	2.053	1.866	2.059
	3	1.982	2.009	2.005	2.005	2.004	1.955	2.089	2.068	2.069	2.066	1.921	2.181	2.143	2.144	2.139
	3.1	2.029	2.024	2.038	2.045	2.025	2.009	1.984	2.051	2.088	1.988	1.983	1.930	2.068	2.139	1.939
	3.2	2.091	2.093	2.071	2.088	2.084	2.136	2.145	2.037	2.123	2.101	2.189	2.207	1.993	2.164	2.122
	3.3	2.113	2.136	2.117	2.130	2.130	2.068	2.183	2.088	2.150	2.152	2.008	2.238	2.050	2.176	2.179
	3.4	2.171	2.167	2.174	2.171	2.168	2.181	2.163	2.195	2.183	2.166	2.193	2.158	2.221	2.196	2.164
	3.5	2.214	2.221	2.204	2.199	2.211	2.220	2.257	2.171	2.145	2.210	2.229	2.301	2.129	2.072	2.207
	3.6	2.265	2.245	2.247	2.280	2.260	2.304	2.207	2.216	2.374	2.282	2.352	2.157	2.175	2.481	2.308
	3.7	2.289	2.307	2.300	2.280	2.296	2.258	2.349	2.312	2.207	2.293	2.217	2.398	2.327	2.109	2.288
	3.8	2.343	2.337	2.339	2.321	2.352	2.359	2.332	2.339	2.249	2.406	2.379	2.326	2.340	2.151	2.469
	3.9	2.382	2.382	2.379	2.371	2.400	2.389	2.389	2.376	2.334	2.476	2.399	2.399	2.372	2.285	2.564
	4	2.431	2.420	2.408	2.417	2.401	2.471	2.418	2.355	2.404	2.321	2.519	2.415	2.286	2.387	2.211
	4.1	2.453	2.471	2.463	2.461	2.457	2.425	2.513	2.473	2.462	2.441	2.388	2.563	2.486	2.463	2.422
	4.2	2.483	2.505	2.499	2.496	2.502	2.414	2.527	2.497	2.480	2.511	2.321	2.553	2.493	2.459	2.522
	4.3	2.534	2.563	2.539	2.527	2.537	2.513	2.654	2.536	2.478	2.531	2.487	2.757	2.533	2.414	2.523
	4.4	2.566	2.571	2.570	2.571	2.577	2.516	2.542	2.539	2.542	2.575	2.450	2.505	2.499	2.506	2.573
	4.5	2.620	2.601	2.600	2.624	2.617	2.636	2.537	2.532	2.655	2.623	2.656	2.450	2.440	2.693	2.630
	4.6	2.655	2.637	2.661	2.635	2.674	2.660	2.567	2.688	2.555	2.749	2.667	2.472	2.720	2.445	2.836
	4.7	2.692	2.686	2.685	2.692	2.691	2.694	2.666	2.661	2.696	2.691	2.697	2.641	2.630	2.701	2.691
	4.8	2.728	2.738	2.702	2.728	2.723	2.727	2.776	2.592	2.727	2.702	2.727	2.821	2.434	2.725	2.675
	4.9	2.778	2.757	2.758	2.765	2.763	2.827	2.726	2.728	2.765	2.755	2.885	2.686	2.690	2.764	2.745
5	2.797	2.796	2.813	2.792	2.786	2.778	2.774	2.860	2.753	2.725	2.755	2.746	2.915	2.702	2.643	

Table S.4.8 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E6 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-5 kbar:

Generator Equation	Error Level	1%					5%					10%				
	P (kbar)	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E6	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.1	0.111	0.105	0.094	0.099	0.108	0.159	0.131	0.075	0.101	0.144	0.215	0.161	0.050	0.104	0.188
	0.2	0.200	0.193	0.186	0.208	0.190	0.225	0.187	0.153	0.261	0.175	0.256	0.180	0.110	0.323	0.156
	0.3	0.287	0.285	0.286	0.289	0.277	0.291	0.280	0.287	0.302	0.241	0.296	0.274	0.289	0.318	0.194
	0.4	0.387	0.363	0.352	0.388	0.389	0.436	0.317	0.259	0.443	0.446	0.495	0.256	0.128	0.507	0.513
	0.5	0.462	0.446	0.465	0.467	0.429	0.472	0.391	0.487	0.494	0.295	0.485	0.318	0.514	0.527	0.098
	0.6	0.541	0.556	0.543	0.542	0.561	0.535	0.608	0.547	0.541	0.631	0.528	0.670	0.551	0.541	0.713
	0.7	0.631	0.622	0.628	0.618	0.609	0.665	0.620	0.649	0.600	0.551	0.705	0.618	0.675	0.576	0.475
	0.8	0.695	0.690	0.702	0.695	0.705	0.677	0.650	0.708	0.677	0.724	0.654	0.598	0.716	0.653	0.748
	0.9	0.777	0.783	0.768	0.770	0.751	0.783	0.813	0.737	0.750	0.645	0.790	0.849	0.698	0.724	0.496
	1	0.839	0.849	0.844	0.841	0.860	0.799	0.853	0.826	0.810	0.905	0.748	0.858	0.803	0.770	0.958
	1.1	0.930	0.931	0.916	0.926	0.923	0.972	0.978	0.905	0.955	0.935	1.022	1.033	0.889	0.989	0.951
	1.2	0.985	0.971	0.985	0.970	1.005	0.974	0.899	0.969	0.895	1.069	0.959	0.800	0.949	0.793	1.143
	1.3	1.035	1.058	1.067	1.053	1.052	0.945	1.068	1.112	1.042	1.037	0.822	1.080	1.166	1.029	1.017
	1.4	1.142	1.142	1.148	1.116	1.113	1.220	1.219	1.250	1.097	1.082	1.310	1.309	1.363	1.072	1.042
	1.5	1.186	1.178	1.199	1.187	1.183	1.190	1.151	1.253	1.197	1.173	1.196	1.116	1.316	1.209	1.161
	1.6	1.260	1.252	1.245	1.257	1.249	1.312	1.270	1.236	1.294	1.256	1.373	1.292	1.224	1.339	1.265
	1.7	1.322	1.341	1.313	1.321	1.325	1.378	1.463	1.332	1.372	1.391	1.444	1.597	1.355	1.432	1.468
	1.8	1.359	1.377	1.364	1.374	1.362	1.325	1.415	1.351	1.400	1.339	1.281	1.460	1.333	1.431	1.310
	1.9	1.437	1.443	1.439	1.427	1.430	1.483	1.513	1.494	1.434	1.451	1.538	1.594	1.558	1.442	1.476
	2	1.478	1.484	1.469	1.485	1.473	1.461	1.491	1.413	1.498	1.439	1.439	1.501	1.340	1.515	1.394
	2.1	1.551	1.556	1.542	1.540	1.542	1.605	1.628	1.561	1.551	1.562	1.668	1.710	1.584	1.564	1.587
	2.2	1.593	1.575	1.598	1.595	1.596	1.601	1.504	1.622	1.609	1.612	1.611	1.407	1.651	1.626	1.632
	2.3	1.637	1.658	1.647	1.637	1.621	1.605	1.710	1.658	1.605	1.523	1.564	1.772	1.671	1.564	1.384
	2.4	1.695	1.714	1.709	1.708	1.708	1.691	1.780	1.758	1.752	1.751	1.685	1.857	1.815	1.805	1.802
	2.5	1.753	1.732	1.748	1.760	1.736	1.776	1.668	1.752	1.811	1.689	1.803	1.582	1.757	1.870	1.626
	2.6	1.788	1.803	1.800	1.809	1.814	1.751	1.824	1.812	1.852	1.878	1.702	1.849	1.826	1.905	1.952
	2.7	1.832	1.850	1.826	1.834	1.840	1.771	1.865	1.740	1.780	1.812	1.690	1.883	1.620	1.710	1.776
	2.8	1.908	1.903	1.888	1.902	1.911	1.958	1.939	1.861	1.932	1.973	2.018	1.981	1.826	1.969	2.046
	2.9	1.934	1.938	1.953	1.934	1.954	1.904	1.926	1.999	1.904	2.002	1.864	1.911	2.053	1.866	2.059
	3	1.981	2.009	2.004	2.005	2.004	1.955	2.089	2.068	2.069	2.066	1.921	2.181	2.142	2.144	2.139
	3.1	2.028	2.023	2.037	2.044	2.024	2.008	1.983	2.050	2.087	1.987	1.982	1.929	2.067	2.138	1.938
	3.2	2.089	2.091	2.070	2.087	2.082	2.134	2.144	2.036	2.121	2.099	2.187	2.205	1.991	2.162	2.120
	3.3	2.111	2.134	2.114	2.127	2.127	2.065	2.180	2.085	2.148	2.149	2.006	2.235	2.047	2.173	2.176
	3.4	2.167	2.164	2.170	2.168	2.164	2.177	2.159	2.191	2.179	2.162	2.189	2.154	2.217	2.193	2.160
	3.5	2.209	2.216	2.199	2.194	2.207	2.216	2.253	2.167	2.140	2.205	2.224	2.296	2.124	2.068	2.203
	3.6	2.259	2.239	2.241	2.274	2.254	2.299	2.201	2.210	2.368	2.276	2.346	2.151	2.169	2.475	2.302
	3.7	2.282	2.300	2.293	2.272	2.289	2.250	2.342	2.305	2.200	2.286	2.209	2.391	2.320	2.101	2.281
	3.8	2.334	2.329	2.330	2.313	2.344	2.351	2.324	2.331	2.241	2.398	2.370	2.318	2.332	2.143	2.461
	3.9	2.372	2.372	2.369	2.361	2.390	2.380	2.379	2.366	2.324	2.466	2.389	2.389	2.362	2.275	2.555
	4	2.419	2.408	2.396	2.406	2.390	2.460	2.406	2.344	2.392	2.310	2.508	2.404	2.275	2.375	2.200
	4.1	2.440	2.458	2.450	2.448	2.444	2.412	2.500	2.461	2.449	2.428	2.375	2.551	2.473	2.451	2.409
	4.2	2.469	2.491	2.485	2.481	2.488	2.400	2.512	2.482	2.465	2.496	2.306	2.538	2.479	2.444	2.507
	4.3	2.518	2.547	2.522	2.511	2.521	2.497	2.638	2.520	2.462	2.515	2.470	2.741	2.517	2.398	2.506
	4.4	2.547	2.552	2.552	2.552	2.559	2.497	2.524	2.521	2.524	2.557	2.431	2.486	2.481	2.487	2.554
	4.5	2.600	2.580	2.580	2.604	2.597	2.616	2.516	2.512	2.635	2.603	2.635	2.430	2.420	2.673	2.610
	4.6	2.633	2.615	2.638	2.613	2.651	2.638	2.545	2.665	2.533	2.727	2.644	2.450	2.698	2.423	2.814
	4.7	2.667	2.662	2.661	2.668	2.667	2.669	2.642	2.637	2.672	2.666	2.672	2.616	2.606	2.677	2.666
	4.8	2.701	2.711	2.676	2.701	2.696	2.701	2.749	2.565	2.700	2.675	2.700	2.794	2.408	2.698	2.649
	4.9	2.749	2.728	2.729	2.736	2.734	2.798	2.697	2.699	2.735	2.726	2.856	2.657	2.661	2.735	2.716
5	2.765	2.764	2.782	2.760	2.755	2.747	2.742	2.828	2.721	2.694	2.724	2.714	2.883	2.670	2.611	

Table S.4.9 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E7 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-5 kbar:

Generator Equation	Error Level	1%					5%					10%				
	P (kbar)	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.1	0.111	0.105	0.094	0.099	0.108	0.159	0.131	0.075	0.101	0.144	0.215	0.161	0.050	0.104	0.188
	0.2	0.200	0.193	0.186	0.208	0.190	0.225	0.187	0.153	0.260	0.175	0.256	0.180	0.110	0.323	0.156
	0.3	0.287	0.284	0.286	0.289	0.277	0.291	0.280	0.287	0.302	0.241	0.296	0.274	0.289	0.318	0.194
	0.4	0.387	0.363	0.352	0.388	0.389	0.436	0.317	0.258	0.443	0.446	0.494	0.256	0.128	0.507	0.513
	0.5	0.462	0.446	0.465	0.466	0.428	0.472	0.391	0.487	0.493	0.295	0.484	0.318	0.513	0.526	0.097
	0.6	0.540	0.555	0.543	0.542	0.560	0.535	0.608	0.546	0.541	0.631	0.528	0.670	0.551	0.540	0.712
	0.7	0.630	0.621	0.627	0.617	0.608	0.664	0.619	0.648	0.599	0.550	0.705	0.617	0.675	0.575	0.474
	0.8	0.694	0.689	0.700	0.694	0.704	0.676	0.649	0.707	0.675	0.723	0.653	0.597	0.715	0.652	0.747
	0.9	0.775	0.781	0.766	0.769	0.749	0.781	0.811	0.736	0.749	0.644	0.788	0.848	0.696	0.723	0.494
	1	0.837	0.847	0.842	0.839	0.858	0.797	0.851	0.824	0.808	0.903	0.746	0.856	0.801	0.768	0.956
	1.1	0.927	0.929	0.914	0.924	0.920	0.969	0.975	0.902	0.952	0.933	1.019	1.030	0.887	0.986	0.949
	1.2	0.982	0.968	0.981	0.967	1.002	0.971	0.896	0.966	0.892	1.066	0.956	0.797	0.946	0.790	1.140
	1.3	1.031	1.054	1.063	1.049	1.048	0.942	1.064	1.108	1.039	1.033	0.818	1.076	1.162	1.025	1.014
	1.4	1.137	1.137	1.143	1.112	1.109	1.215	1.215	1.245	1.092	1.078	1.305	1.304	1.359	1.067	1.037
	1.5	1.180	1.173	1.193	1.182	1.177	1.185	1.145	1.247	1.191	1.168	1.190	1.110	1.311	1.203	1.156
	1.6	1.254	1.245	1.238	1.250	1.242	1.305	1.263	1.229	1.287	1.249	1.366	1.285	1.217	1.332	1.258
	1.7	1.315	1.333	1.305	1.313	1.318	1.370	1.455	1.324	1.364	1.383	1.436	1.590	1.347	1.424	1.460
	1.8	1.350	1.368	1.355	1.365	1.353	1.316	1.406	1.342	1.391	1.330	1.272	1.452	1.325	1.423	1.301
	1.9	1.427	1.434	1.429	1.417	1.421	1.473	1.503	1.484	1.424	1.441	1.528	1.584	1.548	1.432	1.466
	2	1.467	1.473	1.457	1.474	1.462	1.449	1.480	1.402	1.487	1.428	1.428	1.490	1.329	1.504	1.383
	2.1	1.539	1.544	1.530	1.528	1.530	1.592	1.615	1.549	1.538	1.550	1.655	1.698	1.572	1.552	1.574
	2.2	1.580	1.561	1.584	1.581	1.582	1.587	1.490	1.608	1.595	1.598	1.597	1.393	1.638	1.612	1.618
	2.3	1.622	1.643	1.632	1.622	1.606	1.590	1.695	1.643	1.590	1.508	1.548	1.757	1.656	1.549	1.369
	2.4	1.679	1.697	1.692	1.691	1.691	1.674	1.763	1.741	1.735	1.734	1.668	1.840	1.798	1.788	1.786
	2.5	1.735	1.714	1.730	1.742	1.718	1.757	1.650	1.734	1.792	1.670	1.784	1.564	1.738	1.851	1.608
	2.6	1.768	1.783	1.780	1.789	1.794	1.731	1.804	1.792	1.832	1.858	1.682	1.829	1.806	1.884	1.932
	2.7	1.810	1.828	1.804	1.812	1.818	1.750	1.843	1.718	1.759	1.790	1.668	1.861	1.599	1.688	1.754
	2.8	1.884	1.880	1.864	1.879	1.887	1.935	1.915	1.837	1.909	1.950	1.995	1.958	1.803	1.945	2.023
	2.9	1.909	1.913	1.928	1.909	1.929	1.878	1.901	1.973	1.879	1.977	1.839	1.886	2.028	1.841	2.034
	3	1.954	1.982	1.977	1.977	1.977	1.927	2.062	2.041	2.042	2.039	1.893	2.154	2.115	2.117	2.111
	3.1	1.999	1.994	2.007	2.015	1.995	1.979	1.953	2.021	2.058	1.958	1.952	1.900	2.038	2.109	1.909
	3.2	2.058	2.060	2.038	2.055	2.051	2.103	2.112	2.004	2.090	2.068	2.156	2.174	1.960	2.131	2.089
	3.3	2.077	2.100	2.081	2.094	2.094	2.032	2.147	2.052	2.114	2.116	1.972	2.202	2.014	2.140	2.143
	3.4	2.132	2.128	2.135	2.132	2.129	2.142	2.124	2.156	2.143	2.127	2.154	2.119	2.182	2.157	2.124
	3.5	2.171	2.179	2.161	2.156	2.169	2.178	2.215	2.129	2.102	2.167	2.186	2.259	2.087	2.030	2.165
	3.6	2.219	2.199	2.201	2.234	2.214	2.259	2.161	2.170	2.328	2.236	2.306	2.111	2.129	2.435	2.262
	3.7	2.240	2.258	2.251	2.230	2.247	2.208	2.299	2.263	2.158	2.243	2.167	2.349	2.278	2.059	2.239
	3.8	2.290	2.284	2.286	2.268	2.299	2.306	2.279	2.286	2.196	2.353	2.326	2.273	2.287	2.098	2.416
	3.9	2.325	2.325	2.322	2.314	2.343	2.332	2.332	2.319	2.277	2.419	2.342	2.342	2.315	2.228	2.508
	4	2.370	2.359	2.347	2.356	2.340	2.410	2.357	2.295	2.343	2.260	2.458	2.354	2.225	2.326	2.151
	4.1	2.388	2.406	2.398	2.396	2.392	2.360	2.448	2.409	2.397	2.376	2.323	2.498	2.421	2.399	2.357
	4.2	2.414	2.436	2.430	2.427	2.433	2.345	2.457	2.427	2.410	2.442	2.252	2.483	2.424	2.390	2.453
	4.3	2.460	2.490	2.465	2.454	2.464	2.440	2.581	2.463	2.405	2.457	2.413	2.684	2.460	2.340	2.449
	4.4	2.488	2.493	2.492	2.493	2.499	2.438	2.464	2.461	2.464	2.497	2.371	2.427	2.421	2.427	2.494
	4.5	2.537	2.518	2.517	2.541	2.535	2.553	2.454	2.449	2.573	2.540	2.573	2.368	2.358	2.611	2.547
	4.6	2.568	2.550	2.573	2.547	2.586	2.573	2.480	2.600	2.467	2.662	2.579	2.385	2.633	2.358	2.749
	4.7	2.599	2.594	2.593	2.600	2.599	2.601	2.574	2.569	2.604	2.598	2.604	2.548	2.538	2.609	2.598
	4.8	2.631	2.640	2.605	2.630	2.626	2.630	2.678	2.494	2.629	2.605	2.629	2.723	2.337	2.627	2.578
	4.9	2.675	2.655	2.655	2.662	2.660	2.724	2.623	2.626	2.662	2.652	2.782	2.583	2.588	2.661	2.642
	5	2.689	2.688	2.705	2.684	2.678	2.670	2.666	2.752	2.644	2.617	2.647	2.638	2.807	2.593	2.534

E7

Table S.4.10 Simulated kinetic data, $\ln(k/k_0)$, generated using equation **E8** with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-5 kbar:

Generator Equation	Error Level	1%					5%					10%					
E8	P (kbar)	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	
	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.1	0.111	0.105	0.094	0.099	0.108	0.159	0.131	0.075	0.101	0.145	0.215	0.162	0.050	0.104	0.188	
	0.2	0.201	0.193	0.186	0.208	0.191	0.226	0.188	0.153	0.261	0.176	0.256	0.181	0.110	0.323	0.156	
	0.3	0.288	0.286	0.287	0.290	0.278	0.292	0.281	0.288	0.303	0.242	0.297	0.275	0.290	0.319	0.195	
	0.4	0.389	0.365	0.354	0.390	0.391	0.438	0.319	0.260	0.445	0.448	0.496	0.258	0.129	0.509	0.515	
	0.5	0.465	0.449	0.468	0.469	0.431	0.475	0.394	0.489	0.496	0.297	0.487	0.320	0.516	0.529	0.100	
	0.6	0.544	0.559	0.546	0.545	0.564	0.539	0.612	0.550	0.545	0.634	0.532	0.673	0.555	0.544	0.716	
	0.7	0.635	0.626	0.632	0.622	0.612	0.669	0.624	0.653	0.604	0.555	0.709	0.622	0.679	0.580	0.478	
	0.8	0.700	0.695	0.706	0.700	0.710	0.682	0.655	0.713	0.681	0.729	0.659	0.603	0.720	0.657	0.753	
	0.9	0.782	0.788	0.773	0.776	0.756	0.788	0.818	0.743	0.756	0.651	0.795	0.855	0.703	0.730	0.501	
	1	0.845	0.855	0.850	0.847	0.866	0.805	0.859	0.832	0.816	0.911	0.754	0.865	0.809	0.776	0.964	
	1.1	0.937	0.938	0.923	0.933	0.929	0.979	0.984	0.911	0.961	0.942	1.029	1.039	0.896	0.996	0.958	
	1.2	0.993	0.978	0.992	0.978	1.012	0.981	0.906	0.976	0.902	1.076	0.966	0.808	0.957	0.800	1.150	
	1.3	1.042	1.066	1.075	1.060	1.059	0.953	1.076	1.120	1.050	1.044	0.829	1.088	1.173	1.037	1.025	
	1.4	1.149	1.149	1.156	1.124	1.121	1.228	1.227	1.257	1.104	1.090	1.318	1.316	1.371	1.079	1.050	
	1.5	1.194	1.186	1.206	1.195	1.190	1.198	1.158	1.260	1.204	1.181	1.204	1.123	1.324	1.216	1.169	
	1.6	1.268	1.259	1.252	1.264	1.256	1.319	1.277	1.243	1.301	1.263	1.380	1.299	1.231	1.346	1.272	
	1.7	1.329	1.348	1.320	1.328	1.332	1.385	1.470	1.339	1.379	1.398	1.450	1.604	1.362	1.439	1.475	
	1.8	1.365	1.383	1.370	1.380	1.368	1.331	1.421	1.357	1.406	1.345	1.287	1.467	1.340	1.438	1.316	
	1.9	1.443	1.449	1.445	1.432	1.436	1.489	1.519	1.500	1.439	1.456	1.544	1.599	1.564	1.448	1.481	
	2	1.482	1.488	1.473	1.490	1.478	1.465	1.496	1.418	1.503	1.443	1.443	1.505	1.344	1.519	1.398	
	2.1	1.554	1.559	1.545	1.543	1.546	1.608	1.631	1.564	1.554	1.566	1.671	1.714	1.588	1.567	1.590	
	2.2	1.595	1.576	1.599	1.597	1.597	1.603	1.505	1.624	1.611	1.614	1.613	1.409	1.653	1.628	1.634	
	2.3	1.637	1.658	1.647	1.637	1.621	1.605	1.710	1.658	1.605	1.523	1.564	1.772	1.671	1.564	1.384	
	2.4	1.693	1.712	1.707	1.706	1.706	1.689	1.778	1.756	1.750	1.749	1.683	1.855	1.813	1.803	1.800	
	2.5	1.749	1.728	1.744	1.756	1.732	1.771	1.664	1.748	1.806	1.685	1.799	1.578	1.753	1.866	1.622	
	2.6	1.782	1.796	1.794	1.802	1.807	1.744	1.817	1.805	1.846	1.871	1.696	1.842	1.819	1.898	1.945	
	2.7	1.822	1.841	1.816	1.824	1.830	1.762	1.856	1.730	1.771	1.802	1.681	1.874	1.611	1.701	1.766	
	2.8	1.895	1.891	1.875	1.890	1.898	1.946	1.926	1.848	1.920	1.961	2.006	1.969	1.814	1.956	2.034	
	2.9	1.918	1.923	1.937	1.918	1.938	1.888	1.911	1.983	1.889	1.986	1.849	1.895	2.037	1.850	2.043	
3	1.962	1.989	1.985	1.985	1.985	1.935	2.070	2.049	2.050	2.047	1.901	2.162	2.123	2.125	2.119		
3.1	2.005	2.000	2.013	2.021	2.001	1.985	1.959	2.027	2.064	1.964	1.959	1.906	2.044	2.115	1.915		
3.2	2.062	2.064	2.042	2.059	2.055	2.107	2.116	2.008	2.093	2.072	2.160	2.178	1.964	2.135	2.093		
3.3	2.079	2.102	2.083	2.095	2.095	2.034	2.148	2.053	2.116	2.118	1.974	2.204	2.015	2.141	2.145		
3.4	2.131	2.127	2.134	2.131	2.128	2.141	2.123	2.155	2.142	2.126	2.153	2.118	2.181	2.156	2.123		
3.5	2.167	2.175	2.158	2.153	2.165	2.174	2.211	2.125	2.098	2.163	2.182	2.255	2.083	2.026	2.161		
3.6	2.212	2.193	2.194	2.227	2.208	2.252	2.154	2.163	2.322	2.229	2.299	2.105	2.122	2.428	2.256		
3.7	2.230	2.248	2.241	2.220	2.237	2.198	2.289	2.253	2.148	2.233	2.157	2.339	2.268	2.049	2.229		
3.8	2.276	2.271	2.272	2.255	2.286	2.292	2.266	2.273	2.183	2.339	2.312	2.260	2.273	2.085	2.403		
3.9	2.308	2.307	2.305	2.297	2.326	2.315	2.315	2.302	2.259	2.402	2.325	2.324	2.298	2.211	2.490		
4	2.349	2.338	2.326	2.335	2.319	2.389	2.336	2.273	2.322	2.239	2.437	2.333	2.204	2.305	2.129		
4.1	2.363	2.381	2.373	2.370	2.366	2.335	2.423	2.383	2.372	2.351	2.298	2.473	2.396	2.373	2.331		
4.2	2.384	2.406	2.400	2.397	2.403	2.315	2.428	2.398	2.381	2.412	2.222	2.454	2.394	2.360	2.423		
4.3	2.426	2.455	2.430	2.419	2.429	2.405	2.546	2.428	2.370	2.423	2.379	2.649	2.425	2.306	2.415		
4.4	2.448	2.453	2.453	2.453	2.460	2.398	2.424	2.422	2.425	2.458	2.332	2.387	2.382	2.388	2.455		
4.5	2.493	2.473	2.472	2.497	2.490	2.509	2.409	2.405	2.528	2.496	2.528	2.323	2.313	2.566	2.503		
4.6	2.518	2.500	2.523	2.497	2.536	2.523	2.430	2.550	2.417	2.612	2.529	2.335	2.583	2.308	2.699		
4.7	2.544	2.538	2.537	2.544	2.543	2.546	2.518	2.513	2.548	2.543	2.548	2.493	2.482	2.553	2.542		
4.8	2.569	2.579	2.543	2.569	2.564	2.568	2.617	2.433	2.568	2.543	2.567	2.662	2.275	2.566	2.516		
4.9	2.607	2.587	2.587	2.594	2.592	2.656	2.556	2.558	2.594	2.584	2.714	2.515	2.520	2.594	2.574		
5	2.614	2.614	2.631	2.609	2.604	2.596	2.592	2.677	2.570	2.543	2.573	2.564	2.733	2.519	2.460		

Table S.4.11 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E4 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-10 kbar:

Generator Equation	Error Level	1% Error					5% Error					10% Error				
E4	P (kbar)	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
	0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.2	0.186	0.181	0.191	0.204	0.186	0.154	0.128	0.181	0.242	0.155	0.113	0.057	0.168	0.288	0.115
	0.4	0.368	0.365	0.381	0.394	0.390	0.344	0.331	0.413	0.473	0.454	0.315	0.287	0.451	0.564	0.528
	0.6	0.534	0.537	0.535	0.542	0.557	0.510	0.525	0.516	0.550	0.619	0.479	0.510	0.491	0.560	0.693
	0.8	0.688	0.700	0.708	0.694	0.698	0.655	0.720	0.754	0.687	0.707	0.613	0.744	0.810	0.679	0.719
	1.0	0.846	0.849	0.821	0.840	0.843	0.869	0.880	0.740	0.839	0.854	0.897	0.919	0.629	0.838	0.868
	1.2	0.977	0.996	0.981	0.966	0.965	0.981	1.075	0.999	0.927	0.919	0.986	1.164	1.022	0.875	0.859
	1.4	1.109	1.083	1.118	1.112	1.096	1.131	0.998	1.177	1.148	1.065	1.159	0.880	1.246	1.191	1.026
	1.6	1.232	1.218	1.213	1.198	1.217	1.269	1.198	1.174	1.094	1.195	1.314	1.174	1.124	0.947	1.167
	1.8	1.331	1.332	1.341	1.332	1.326	1.318	1.323	1.364	1.323	1.292	1.301	1.311	1.392	1.312	1.247
	2.0	1.431	1.437	1.434	1.433	1.434	1.391	1.423	1.405	1.399	1.410	1.338	1.405	1.367	1.356	1.377
	2.2	1.551	1.538	1.542	1.538	1.539	1.594	1.527	1.545	1.527	1.534	1.644	1.513	1.550	1.514	1.526
	2.4	1.620	1.643	1.615	1.633	1.629	1.555	1.675	1.531	1.624	1.603	1.468	1.713	1.415	1.612	1.570
	2.6	1.726	1.725	1.735	1.722	1.713	1.728	1.727	1.775	1.711	1.662	1.731	1.728	1.822	1.697	1.595
	2.8	1.814	1.816	1.800	1.804	1.806	1.830	1.841	1.759	1.781	1.791	1.850	1.872	1.704	1.751	1.771
	3.0	1.876	1.891	1.898	1.892	1.896	1.815	1.891	1.928	1.898	1.916	1.734	1.891	1.963	1.905	1.941
	3.2	1.974	1.951	1.973	1.976	1.969	1.998	1.880	1.996	2.008	1.973	2.027	1.785	2.024	2.046	1.978
	3.4	2.041	2.045	2.034	2.037	2.045	2.040	2.063	2.003	2.019	2.060	2.038	2.085	1.965	1.998	2.079
	3.6	2.104	2.111	2.122	2.079	2.114	2.078	2.112	2.164	1.939	2.129	2.044	2.113	2.215	1.733	2.146
	3.8	2.180	2.187	2.185	2.187	2.181	2.190	2.225	2.214	2.224	2.195	2.203	2.270	2.249	2.269	2.212
4.0	2.246	2.248	2.213	2.249	2.238	2.265	2.276	2.094	2.280	2.226	2.288	2.309	1.920	2.318	2.211	
4.2	2.299	2.292	2.324	2.279	2.303	2.288	2.251	2.406	2.183	2.309	2.274	2.197	2.500	2.049	2.315	
4.4	2.342	2.368	2.369	2.353	2.362	2.266	2.399	2.404	2.324	2.369	2.161	2.437	2.445	2.287	2.378	
4.6	2.414	2.420	2.428	2.412	2.421	2.408	2.437	2.474	2.394	2.440	2.399	2.457	2.528	2.372	2.463	
4.8	2.482	2.483	2.452	2.466	2.486	2.532	2.533	2.378	2.452	2.548	2.590	2.592	2.276	2.434	2.621	
5.0	2.505	2.514	2.524	2.512	2.525	2.437	2.485	2.536	2.473	2.538	2.345	2.447	2.550	2.422	2.555	
5.2	2.580	2.580	2.570	2.559	2.585	2.618	2.619	2.568	2.513	2.640	2.662	2.665	2.565	2.453	2.704	
5.4	2.620	2.628	2.629	2.617	2.616	2.628	2.668	2.671	2.613	2.610	2.637	2.715	2.720	2.608	2.601	
5.6	2.656	2.662	2.660	2.674	2.670	2.623	2.654	2.645	2.712	2.694	2.580	2.644	2.625	2.759	2.723	
5.8	2.718	2.710	2.715	2.714	2.709	2.759	2.720	2.742	2.737	2.712	2.807	2.732	2.775	2.765	2.716	
6.0	2.746	2.739	2.743	2.746	2.759	2.731	2.694	2.714	2.729	2.792	2.711	2.634	2.677	2.708	2.832	
6.2	2.808	2.808	2.817	2.812	2.777	2.872	2.875	2.913	2.893	2.719	2.946	2.952	3.021	2.985	2.642	
6.4	2.825	2.818	2.824	2.829	2.829	2.804	2.766	2.794	2.823	2.822	2.777	2.696	2.757	2.816	2.813	
6.6	2.883	2.877	2.866	2.861	2.871	2.937	2.910	2.855	2.827	2.878	3.001	2.950	2.842	2.783	2.886	
6.8	2.895	2.901	2.921	2.896	2.902	2.850	2.884	2.981	2.855	2.887	2.791	2.862	3.051	2.802	2.867	
7.0	2.942	2.951	2.938	2.960	2.935	2.945	2.988	2.923	3.032	2.910	2.948	3.033	2.904	3.115	2.877	
7.2	2.989	2.970	2.979	2.965	2.976	3.040	2.945	2.990	2.923	2.977	3.101	2.914	3.005	2.868	2.979	
7.4	3.013	3.003	3.021	3.003	3.005	3.026	2.977	3.066	2.978	2.990	3.044	2.944	3.119	2.947	2.971	
7.6	3.050	3.025	3.035	3.045	3.046	3.082	2.957	3.009	3.059	3.065	3.122	2.864	2.975	3.077	3.088	
7.8	3.083	3.068	3.078	3.073	3.059	3.124	3.051	3.098	3.073	3.003	3.172	3.028	3.123	3.073	2.929	
8.0	3.112	3.099	3.110	3.097	3.091	3.149	3.083	3.138	3.074	3.040	3.192	3.062	3.172	3.045	2.974	
8.2	3.139	3.139	3.135	3.130	3.124	3.167	3.166	3.145	3.120	3.091	3.201	3.198	3.158	3.108	3.048	
8.4	3.150	3.167	3.166	3.152	3.182	3.106	3.194	3.184	3.114	3.263	3.049	3.226	3.208	3.065	3.356	
8.6	3.193	3.190	3.176	3.193	3.194	3.212	3.195	3.124	3.212	3.217	3.236	3.201	3.056	3.234	3.246	
8.8	3.220	3.227	3.229	3.217	3.217	3.240	3.274	3.284	3.224	3.226	3.264	3.330	3.349	3.233	3.237	
9.0	3.232	3.250	3.247	3.243	3.224	3.193	3.282	3.268	3.250	3.149	3.141	3.321	3.294	3.258	3.047	
9.2	3.270	3.270	3.260	3.276	3.260	3.285	3.281	3.234	3.310	3.235	3.302	3.294	3.200	3.351	3.202	
9.4	3.300	3.279	3.277	3.302	3.289	3.334	3.226	3.215	3.345	3.280	3.375	3.157	3.132	3.396	3.268	
9.6	3.304	3.309	3.309	3.305	3.312	3.256	3.282	3.285	3.261	3.296	3.193	3.248	3.253	3.203	3.277	
9.8	3.341	3.325	3.341	3.318	3.344	3.350	3.270	3.348	3.231	3.364	3.361	3.197	3.357	3.110	3.389	
10.0	3.373	3.367	3.372	3.367	3.368	3.417	3.389	3.413	3.389	3.395	3.470	3.415	3.461	3.416	3.427	

Table S.4.12 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E5 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-10 kbar:

Generator Equation	Error Level	1% Error					5% Error					10% Error					
		P (kbar)	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E5	0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.2	0.186	0.181	0.191	0.204	0.186	0.155	0.128	0.181	0.242	0.155	0.113	0.057	0.168	0.288	0.115	
	0.4	0.368	0.366	0.382	0.395	0.391	0.345	0.332	0.413	0.474	0.454	0.315	0.288	0.451	0.564	0.528	
	0.6	0.536	0.539	0.537	0.544	0.558	0.512	0.527	0.518	0.552	0.621	0.481	0.512	0.493	0.561	0.695	
	0.8	0.691	0.704	0.711	0.698	0.702	0.659	0.724	0.758	0.691	0.711	0.617	0.748	0.813	0.683	0.723	
	1.0	0.853	0.855	0.828	0.847	0.850	0.876	0.887	0.747	0.846	0.861	0.904	0.926	0.636	0.845	0.874	
	1.2	0.988	1.007	0.991	0.977	0.976	0.992	1.085	1.010	0.937	0.930	0.997	1.175	1.033	0.886	0.870	
	1.4	1.125	1.099	1.134	1.128	1.112	1.147	1.014	1.193	1.164	1.081	1.175	0.896	1.262	1.207	1.042	
	1.6	1.254	1.240	1.235	1.220	1.239	1.291	1.221	1.197	1.116	1.218	1.336	1.196	1.146	0.969	1.190	
	1.8	1.361	1.362	1.370	1.362	1.356	1.348	1.353	1.393	1.353	1.322	1.331	1.341	1.421	1.342	1.277	
	2.0	1.469	1.475	1.472	1.471	1.473	1.429	1.461	1.443	1.438	1.448	1.377	1.443	1.406	1.395	1.416	
	2.2	1.600	1.586	1.590	1.586	1.587	1.642	1.575	1.593	1.575	1.582	1.692	1.561	1.598	1.562	1.575	
	2.4	1.679	1.702	1.674	1.692	1.688	1.614	1.734	1.590	1.682	1.662	1.527	1.772	1.474	1.671	1.628	
	2.6	1.796	1.796	1.806	1.793	1.783	1.799	1.797	1.845	1.782	1.733	1.801	1.799	1.893	1.768	1.665	
	2.8	1.898	1.900	1.883	1.888	1.890	1.914	1.925	1.842	1.864	1.874	1.934	1.955	1.788	1.834	1.854	
	3.0	1.973	1.988	1.996	1.989	1.993	1.913	1.988	2.025	1.995	2.013	1.831	1.988	2.060	2.002	2.038	
	3.2	2.086	2.063	2.085	2.088	2.081	2.110	1.992	2.108	2.120	2.085	2.139	1.896	2.136	2.158	2.090	
	3.4	2.168	2.173	2.161	2.164	2.172	2.167	2.191	2.131	2.147	2.188	2.166	2.213	2.092	2.125	2.207	
	3.6	2.248	2.255	2.266	2.223	2.258	2.222	2.256	2.308	2.083	2.273	2.188	2.257	2.359	1.877	2.290	
	3.8	2.341	2.348	2.346	2.348	2.342	2.351	2.386	2.375	2.386	2.356	2.364	2.432	2.410	2.431	2.373	
	4.0	2.425	2.427	2.392	2.428	2.417	2.444	2.455	2.273	2.460	2.405	2.467	2.489	2.100	2.497	2.390	
	4.2	2.497	2.490	2.522	2.477	2.501	2.486	2.449	2.604	2.382	2.507	2.472	2.395	2.698	2.247	2.513	
	4.4	2.560	2.586	2.587	2.571	2.580	2.483	2.617	2.621	2.542	2.587	2.379	2.655	2.663	2.504	2.596	
	4.6	2.652	2.658	2.666	2.650	2.659	2.645	2.674	2.712	2.632	2.678	2.637	2.694	2.766	2.610	2.701	
	4.8	2.741	2.741	2.711	2.725	2.744	2.790	2.791	2.636	2.710	2.807	2.849	2.851	2.535	2.692	2.879	
	5.0	2.785	2.794	2.804	2.792	2.805	2.717	2.765	2.816	2.753	2.818	2.625	2.727	2.830	2.702	2.835	
	5.2	2.882	2.883	2.872	2.862	2.887	2.920	2.921	2.870	2.816	2.942	2.965	2.968	2.867	2.755	3.006	
	5.4	2.945	2.953	2.954	2.942	2.941	2.953	2.993	2.995	2.938	2.934	2.962	3.040	3.045	2.933	2.926	
	5.6	3.004	3.010	3.008	3.022	3.018	2.971	3.002	2.993	3.060	3.042	2.928	2.992	2.973	3.107	3.071	
	5.8	3.090	3.082	3.087	3.086	3.080	3.130	3.092	3.114	3.109	3.084	3.179	3.104	3.147	3.137	3.088	
6.0	3.142	3.135	3.139	3.142	3.155	3.127	3.090	3.110	3.125	3.188	3.107	3.030	3.073	3.104	3.228		
6.2	3.229	3.229	3.237	3.233	3.198	3.292	3.296	3.333	3.314	3.140	3.367	3.373	3.442	3.406	3.062		
6.4	3.271	3.264	3.270	3.275	3.275	3.250	3.212	3.240	3.269	3.268	3.223	3.142	3.203	3.262	3.259		
6.6	3.354	3.349	3.338	3.332	3.342	3.409	3.382	3.327	3.298	3.349	3.473	3.421	3.314	3.255	3.358		
6.8	3.392	3.399	3.419	3.393	3.399	3.348	3.382	3.479	3.353	3.384	3.289	3.360	3.549	3.300	3.365		
7.0	3.466	3.475	3.462	3.484	3.459	3.469	3.512	3.447	3.556	3.434	3.472	3.557	3.428	3.639	3.401		
7.2	3.540	3.521	3.530	3.516	3.527	3.591	3.496	3.541	3.474	3.528	3.652	3.465	3.556	3.419	3.530		
7.4	3.591	3.581	3.599	3.581	3.583	3.605	3.555	3.644	3.557	3.568	3.622	3.522	3.698	3.525	3.549		
7.6	3.655	3.631	3.641	3.651	3.652	3.688	3.562	3.614	3.665	3.671	3.728	3.470	3.581	3.683	3.694		
7.8	3.717	3.702	3.711	3.706	3.693	3.757	3.684	3.732	3.707	3.637	3.806	3.662	3.756	3.707	3.563		
8.0	3.774	3.761	3.772	3.759	3.753	3.811	3.745	3.800	3.736	3.702	3.854	3.724	3.834	3.706	3.636		
8.2	3.830	3.830	3.825	3.820	3.815	3.858	3.856	3.836	3.811	3.781	3.891	3.888	3.849	3.799	3.738		
8.4	3.870	3.887	3.885	3.871	3.901	3.826	3.913	3.904	3.834	3.982	3.768	3.945	3.927	3.785	4.075		
8.6	3.942	3.938	3.925	3.942	3.943	3.961	3.943	3.873	3.960	3.966	3.984	3.949	3.805	3.983	3.994		
8.8	3.998	4.005	4.008	3.995	3.996	4.018	4.052	4.062	4.002	4.004	4.042	4.108	4.127	4.011	4.015		
9.0	4.040	4.058	4.055	4.051	4.031	4.001	4.090	4.076	4.057	3.957	3.949	4.129	4.102	4.065	3.855		
9.2	4.108	4.107	4.098	4.113	4.098	4.123	4.119	4.072	4.148	4.073	4.140	4.132	4.038	4.189	4.039		
9.4	4.168	4.147	4.145	4.171	4.157	4.202	4.095	4.083	4.213	4.148	4.243	4.025	4.001	4.264	4.137		
9.6	4.202	4.208	4.208	4.203	4.210	4.155	4.181	4.183	4.160	4.195	4.091	4.146	4.152	4.102	4.176		
9.8	4.270	4.255	4.270	4.247	4.273	4.279	4.200	4.277	4.160	4.293	4.290	4.126	4.287	4.039	4.318		
10.0	4.333	4.327	4.332	4.327	4.329	4.377	4.349	4.373	4.349	4.355	4.430	4.376	4.422	4.376	4.387		

Table S.4.13 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E6 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-10 kbar:

Generator Equation	Error Level	1% Error					5% Error					10% Error				
		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E6	P (kbar)															
	0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.2	0.186	0.181	0.191	0.204	0.186	0.155	0.128	0.181	0.242	0.155	0.114	0.057	0.168	0.288	0.115
	0.4	0.368	0.366	0.382	0.395	0.391	0.345	0.332	0.414	0.474	0.454	0.315	0.288	0.451	0.565	0.528
	0.6	0.536	0.539	0.537	0.544	0.559	0.512	0.527	0.518	0.552	0.622	0.481	0.512	0.493	0.562	0.695
	0.8	0.692	0.705	0.712	0.698	0.702	0.660	0.724	0.759	0.692	0.712	0.618	0.748	0.814	0.684	0.724
	1.0	0.854	0.856	0.829	0.848	0.851	0.877	0.888	0.748	0.847	0.862	0.905	0.927	0.637	0.846	0.876
	1.2	0.989	1.009	0.993	0.979	0.977	0.993	1.087	1.012	0.939	0.932	0.998	1.177	1.034	0.887	0.872
	1.4	1.127	1.101	1.136	1.130	1.114	1.149	1.016	1.195	1.166	1.083	1.177	0.899	1.264	1.210	1.044
	1.6	1.257	1.242	1.238	1.223	1.242	1.294	1.223	1.199	1.119	1.220	1.339	1.199	1.149	0.972	1.192
	1.8	1.364	1.365	1.373	1.365	1.359	1.351	1.356	1.396	1.356	1.324	1.334	1.344	1.424	1.345	1.279
	2.0	1.472	1.478	1.475	1.474	1.476	1.432	1.464	1.446	1.441	1.451	1.379	1.446	1.409	1.398	1.419
	2.2	1.602	1.589	1.592	1.589	1.590	1.644	1.578	1.596	1.578	1.584	1.695	1.564	1.600	1.565	1.577
	2.4	1.681	1.705	1.677	1.694	1.690	1.616	1.736	1.592	1.685	1.664	1.529	1.774	1.476	1.673	1.631
	2.6	1.798	1.798	1.808	1.795	1.785	1.800	1.799	1.847	1.784	1.734	1.803	1.801	1.895	1.770	1.667
	2.8	1.898	1.901	1.884	1.889	1.891	1.915	1.926	1.843	1.865	1.875	1.934	1.956	1.789	1.835	1.855
	3.0	1.973	1.988	1.995	1.989	1.993	1.912	1.988	2.024	1.995	2.013	1.831	1.988	2.060	2.002	2.038
	3.2	2.084	2.061	2.084	2.086	2.079	2.108	1.990	2.106	2.118	2.083	2.137	1.895	2.134	2.156	2.088
	3.4	2.164	2.169	2.157	2.161	2.169	2.163	2.187	2.127	2.143	2.184	2.162	2.209	2.089	2.121	2.203
	3.6	2.242	2.249	2.260	2.217	2.252	2.216	2.250	2.302	2.078	2.267	2.182	2.251	2.353	1.871	2.285
	3.8	2.333	2.340	2.338	2.340	2.334	2.343	2.378	2.366	2.377	2.348	2.356	2.423	2.402	2.422	2.365
	4.0	2.414	2.416	2.381	2.417	2.406	2.433	2.444	2.261	2.448	2.394	2.456	2.477	2.088	2.486	2.379
	4.2	2.483	2.475	2.507	2.463	2.487	2.471	2.434	2.589	2.367	2.492	2.457	2.380	2.684	2.233	2.499
	4.4	2.541	2.567	2.568	2.552	2.561	2.465	2.599	2.603	2.524	2.569	2.360	2.636	2.645	2.486	2.578
	4.6	2.630	2.636	2.643	2.627	2.636	2.623	2.652	2.689	2.610	2.655	2.614	2.672	2.744	2.588	2.679
	4.8	2.714	2.715	2.684	2.698	2.718	2.764	2.765	2.610	2.684	2.780	2.822	2.824	2.508	2.666	2.853
	5.0	2.753	2.763	2.773	2.760	2.773	2.685	2.733	2.784	2.721	2.787	2.593	2.695	2.798	2.671	2.803
	5.2	2.846	2.846	2.835	2.825	2.850	2.883	2.885	2.833	2.779	2.905	2.928	2.931	2.830	2.718	2.970
	5.4	2.903	2.911	2.911	2.900	2.899	2.910	2.951	2.953	2.896	2.892	2.920	2.998	3.003	2.891	2.884
	5.6	2.956	2.962	2.960	2.974	2.970	2.923	2.954	2.944	3.012	2.994	2.880	2.944	2.925	3.059	3.023
5.8	3.036	3.028	3.032	3.031	3.026	3.076	3.037	3.059	3.054	3.029	3.124	3.049	3.093	3.083	3.033	
6.0	3.081	3.074	3.078	3.081	3.094	3.066	3.029	3.049	3.064	3.127	3.046	2.969	3.012	3.043	3.167	
6.2	3.161	3.161	3.169	3.165	3.130	3.224	3.227	3.265	3.246	3.072	3.299	3.305	3.374	3.338	2.994	
6.4	3.196	3.189	3.194	3.200	3.199	3.175	3.136	3.165	3.194	3.193	3.148	3.067	3.127	3.187	3.184	
6.6	3.271	3.266	3.255	3.249	3.259	3.326	3.298	3.244	3.215	3.266	3.390	3.338	3.230	3.172	3.275	
6.8	3.301	3.308	3.328	3.302	3.308	3.256	3.291	3.387	3.261	3.293	3.197	3.269	3.458	3.208	3.273	
7.0	3.366	3.375	3.362	3.384	3.359	3.369	3.413	3.347	3.456	3.334	3.372	3.458	3.329	3.539	3.302	
7.2	3.431	3.412	3.421	3.408	3.419	3.483	3.388	3.433	3.366	3.420	3.543	3.356	3.447	3.311	3.421	
7.4	3.473	3.463	3.481	3.464	3.466	3.487	3.438	3.526	3.439	3.451	3.504	3.405	3.580	3.407	3.431	
7.6	3.528	3.504	3.514	3.524	3.525	3.561	3.435	3.487	3.538	3.544	3.601	3.343	3.454	3.556	3.567	
7.8	3.580	3.565	3.575	3.570	3.556	3.621	3.548	3.595	3.570	3.500	3.669	3.525	3.620	3.570	3.426	
8.0	3.627	3.614	3.625	3.612	3.606	3.664	3.598	3.653	3.589	3.556	3.707	3.577	3.687	3.560	3.489	
8.2	3.673	3.672	3.668	3.663	3.657	3.700	3.699	3.679	3.654	3.624	3.734	3.731	3.692	3.641	3.581	
8.4	3.702	3.719	3.717	3.703	3.734	3.658	3.745	3.736	3.666	3.814	3.600	3.778	3.759	3.617	3.907	
8.6	3.763	3.759	3.746	3.763	3.764	3.782	3.764	3.694	3.781	3.787	3.805	3.770	3.626	3.804	3.815	
8.8	3.808	3.815	3.817	3.805	3.805	3.828	3.862	3.872	3.812	3.814	3.851	3.917	3.937	3.821	3.825	
9.0	3.838	3.856	3.853	3.849	3.830	3.799	3.888	3.874	3.855	3.755	3.747	3.927	3.900	3.864	3.653	
9.2	3.894	3.894	3.884	3.900	3.884	3.909	3.905	3.858	3.934	3.859	3.926	3.918	3.824	3.975	3.826	
9.4	3.942	3.921	3.919	3.944	3.931	3.976	3.868	3.857	3.987	3.922	4.017	3.799	3.775	4.038	3.911	
9.6	3.964	3.969	3.969	3.965	3.972	3.916	3.942	3.945	3.921	3.956	3.853	3.908	3.913	3.864	3.937	
9.8	4.019	4.004	4.019	3.996	4.022	4.028	3.948	4.026	3.909	4.042	4.039	3.875	4.035	3.788	4.067	
10.0	4.069	4.063	4.068	4.063	4.064	4.113	4.085	4.109	4.085	4.091	4.166	4.112	4.157	4.112	4.123	

Table S.4.14 Simulated kinetic data, $\ln(k/k_0)$, generated using equation E7 with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-10 kbar:

Generator Equation	Error Level	1% Error					5% Error					10% Error				
		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E7	P (kbar)															
	0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.2	0.186	0.181	0.191	0.204	0.186	0.155	0.128	0.181	0.242	0.155	0.113	0.057	0.168	0.288	0.115
	0.4	0.368	0.366	0.382	0.395	0.391	0.345	0.332	0.413	0.474	0.454	0.315	0.288	0.451	0.564	0.528
	0.6	0.536	0.539	0.537	0.544	0.558	0.512	0.527	0.517	0.552	0.621	0.481	0.511	0.492	0.561	0.694
	0.8	0.691	0.704	0.711	0.697	0.701	0.658	0.723	0.758	0.691	0.711	0.616	0.747	0.813	0.683	0.722
	1.0	0.852	0.854	0.827	0.846	0.849	0.875	0.886	0.746	0.845	0.860	0.903	0.925	0.635	0.844	0.874
	1.2	0.986	1.006	0.990	0.975	0.974	0.990	1.084	1.008	0.936	0.928	0.995	1.174	1.031	0.884	0.868
	1.4	1.122	1.096	1.132	1.126	1.109	1.145	1.011	1.190	1.162	1.079	1.172	0.894	1.259	1.205	1.039
	1.6	1.250	1.236	1.231	1.216	1.235	1.287	1.217	1.193	1.112	1.214	1.332	1.192	1.142	0.965	1.186
	1.8	1.355	1.356	1.364	1.356	1.350	1.342	1.347	1.387	1.347	1.316	1.325	1.335	1.415	1.336	1.271
	2.0	1.461	1.467	1.464	1.463	1.465	1.421	1.453	1.435	1.430	1.440	1.368	1.435	1.398	1.387	1.408
	2.2	1.589	1.575	1.579	1.575	1.576	1.631	1.564	1.582	1.564	1.571	1.681	1.550	1.587	1.551	1.564
	2.4	1.664	1.688	1.660	1.677	1.673	1.600	1.719	1.576	1.668	1.647	1.512	1.758	1.459	1.656	1.614
	2.6	1.778	1.778	1.788	1.775	1.765	1.780	1.779	1.827	1.764	1.714	1.783	1.781	1.875	1.750	1.647
	2.8	1.875	1.877	1.861	1.865	1.867	1.891	1.902	1.819	1.842	1.851	1.911	1.932	1.765	1.812	1.832
	3.0	1.946	1.960	1.968	1.962	1.966	1.885	1.961	1.997	1.967	1.986	1.804	1.961	2.033	1.974	2.011
	3.2	2.053	2.030	2.052	2.055	2.048	2.076	1.959	2.075	2.086	2.051	2.105	1.863	2.103	2.125	2.056
	3.4	2.129	2.134	2.122	2.125	2.133	2.128	2.152	2.092	2.108	2.149	2.126	2.174	2.053	2.086	2.168
	3.6	2.202	2.209	2.220	2.177	2.212	2.176	2.210	2.262	2.038	2.227	2.142	2.211	2.313	1.831	2.245
	3.8	2.288	2.295	2.293	2.295	2.289	2.298	2.333	2.322	2.333	2.303	2.311	2.379	2.357	2.378	2.320
	4.0	2.364	2.366	2.332	2.367	2.356	2.383	2.394	2.212	2.399	2.344	2.407	2.428	2.039	2.437	2.329
	4.2	2.428	2.421	2.452	2.408	2.432	2.417	2.379	2.535	2.312	2.437	2.403	2.325	2.629	2.178	2.444
	4.4	2.481	2.508	2.509	2.493	2.501	2.405	2.539	2.543	2.464	2.509	2.301	2.577	2.585	2.426	2.518
	4.6	2.565	2.570	2.578	2.562	2.571	2.558	2.587	2.624	2.545	2.590	2.549	2.607	2.679	2.522	2.614
	4.8	2.643	2.644	2.613	2.627	2.647	2.693	2.694	2.539	2.613	2.709	2.751	2.753	2.437	2.595	2.782
	5.0	2.677	2.686	2.696	2.684	2.696	2.609	2.657	2.708	2.645	2.710	2.517	2.619	2.722	2.594	2.727
	5.2	2.763	2.763	2.753	2.742	2.768	2.801	2.802	2.751	2.696	2.823	2.845	2.848	2.748	2.636	2.887
	5.4	2.814	2.822	2.823	2.811	2.810	2.822	2.862	2.865	2.807	2.804	2.831	2.909	2.915	2.802	2.795
	5.6	2.861	2.867	2.865	2.879	2.875	2.828	2.859	2.850	2.917	2.899	2.785	2.849	2.830	2.964	2.928
5.8	2.934	2.926	2.931	2.930	2.925	2.975	2.936	2.958	2.953	2.928	3.023	2.948	2.991	2.982	2.932	
6.0	2.974	2.967	2.970	2.973	2.986	2.958	2.921	2.942	2.956	3.019	2.938	2.862	2.904	2.935	3.059	
6.2	3.046	3.047	3.055	3.051	3.016	3.110	3.113	3.151	3.131	2.957	3.184	3.190	3.259	3.224	2.880	
6.4	3.075	3.067	3.073	3.079	3.078	3.054	3.015	3.044	3.073	3.071	3.027	2.945	3.006	3.066	3.063	
6.6	3.143	3.138	3.127	3.121	3.131	3.198	3.170	3.116	3.087	3.138	3.262	3.210	3.102	3.044	3.147	
6.8	3.166	3.173	3.193	3.167	3.173	3.121	3.156	3.252	3.126	3.158	3.062	3.134	3.323	3.073	3.138	
7.0	3.224	3.233	3.220	3.242	3.217	3.227	3.271	3.205	3.314	3.192	3.230	3.315	3.187	3.397	3.160	
7.2	3.282	3.263	3.272	3.259	3.269	3.333	3.238	3.284	3.217	3.270	3.394	3.207	3.298	3.161	3.272	
7.4	3.316	3.307	3.325	3.307	3.309	3.330	3.281	3.370	3.282	3.294	3.348	3.248	3.423	3.251	3.275	
7.6	3.364	3.340	3.349	3.360	3.361	3.397	3.271	3.323	3.374	3.380	3.437	3.179	3.290	3.392	3.403	
7.8	3.408	3.393	3.403	3.398	3.384	3.449	3.376	3.423	3.398	3.329	3.498	3.354	3.448	3.399	3.255	
8.0	3.448	3.435	3.446	3.433	3.426	3.484	3.419	3.474	3.410	3.376	3.528	3.398	3.507	3.380	3.310	
8.2	3.486	3.485	3.481	3.476	3.470	3.513	3.512	3.492	3.467	3.437	3.547	3.544	3.505	3.454	3.394	
8.4	3.507	3.524	3.522	3.508	3.539	3.463	3.551	3.541	3.471	3.619	3.406	3.583	3.564	3.422	3.712	
8.6	3.560	3.557	3.543	3.560	3.561	3.579	3.561	3.491	3.578	3.584	3.602	3.568	3.423	3.601	3.612	
8.8	3.597	3.604	3.607	3.594	3.595	3.617	3.651	3.661	3.601	3.603	3.641	3.707	3.726	3.610	3.614	
9.0	3.619	3.637	3.634	3.630	3.611	3.580	3.669	3.655	3.637	3.536	3.528	3.708	3.681	3.645	3.435	
9.2	3.667	3.667	3.657	3.673	3.657	3.682	3.678	3.631	3.707	3.632	3.699	3.691	3.597	3.748	3.599	
9.4	3.707	3.686	3.683	3.709	3.696	3.741	3.633	3.622	3.752	3.687	3.781	3.564	3.539	3.803	3.675	
9.6	3.720	3.725	3.726	3.721	3.728	3.673	3.699	3.701	3.678	3.713	3.609	3.664	3.670	3.620	3.694	
9.8	3.767	3.752	3.767	3.744	3.770	3.776	3.696	3.774	3.657	3.790	3.787	3.623	3.783	3.536	3.815	
10.0	3.809	3.803	3.808	3.803	3.804	3.853	3.825	3.848	3.825	3.830	3.905	3.851	3.897	3.851	3.862	

Table S.4.15 Simulated kinetic data, $\ln(k/k_0)$, generated using equation **E8** with parameters $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ for different levels of errors and the pressure range of 0-10 kbar:

Generator Equation	Error Level	1% Error					5% Error					10% Error				
		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E8	P (kbar)															
	0.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	0.2	0.187	0.182	0.192	0.204	0.187	0.155	0.128	0.181	0.243	0.156	0.114	0.057	0.168	0.289	0.116
	0.4	0.370	0.368	0.384	0.397	0.392	0.347	0.334	0.415	0.476	0.456	0.317	0.290	0.453	0.566	0.530
	0.6	0.540	0.543	0.541	0.547	0.562	0.516	0.530	0.521	0.555	0.625	0.485	0.515	0.496	0.565	0.698
	0.8	0.697	0.710	0.717	0.703	0.707	0.664	0.729	0.763	0.697	0.717	0.622	0.753	0.819	0.689	0.728
	1.0	0.860	0.863	0.835	0.854	0.857	0.883	0.895	0.754	0.853	0.868	0.911	0.933	0.643	0.852	0.882
	1.2	0.997	1.016	1.000	0.986	0.984	1.001	1.094	1.019	0.946	0.939	1.006	1.184	1.041	0.894	0.879
	1.4	1.134	1.109	1.144	1.138	1.121	1.157	1.024	1.203	1.174	1.091	1.185	0.906	1.271	1.217	1.052
	1.6	1.264	1.250	1.245	1.230	1.249	1.301	1.231	1.207	1.126	1.227	1.346	1.206	1.156	0.979	1.200
	1.8	1.370	1.371	1.379	1.371	1.365	1.357	1.362	1.402	1.362	1.331	1.340	1.350	1.431	1.351	1.286
	2.0	1.477	1.483	1.479	1.478	1.480	1.437	1.469	1.451	1.445	1.455	1.384	1.450	1.413	1.402	1.423
	2.2	1.604	1.591	1.594	1.591	1.592	1.646	1.580	1.598	1.580	1.586	1.697	1.566	1.602	1.566	1.579
	2.4	1.679	1.703	1.675	1.692	1.688	1.614	1.734	1.590	1.683	1.662	1.527	1.773	1.474	1.671	1.629
	2.6	1.791	1.791	1.801	1.788	1.778	1.794	1.792	1.841	1.777	1.728	1.797	1.794	1.888	1.763	1.661
	2.8	1.886	1.888	1.872	1.876	1.878	1.902	1.913	1.830	1.853	1.863	1.922	1.943	1.776	1.823	1.843
	3.0	1.954	1.968	1.976	1.970	1.974	1.893	1.968	2.005	1.975	1.994	1.811	1.969	2.041	1.982	2.019
	3.2	2.057	2.034	2.056	2.059	2.051	2.080	1.963	2.079	2.090	2.055	2.109	1.867	2.107	2.129	2.060
	3.4	2.128	2.133	2.121	2.124	2.132	2.127	2.151	2.091	2.107	2.148	2.126	2.173	2.052	2.085	2.167
	3.6	2.196	2.202	2.213	2.170	2.206	2.169	2.203	2.255	2.031	2.220	2.135	2.204	2.306	1.824	2.238
	3.8	2.275	2.282	2.279	2.282	2.276	2.285	2.320	2.308	2.319	2.289	2.297	2.365	2.343	2.364	2.307
	4.0	2.343	2.345	2.310	2.346	2.335	2.362	2.373	2.191	2.378	2.323	2.385	2.407	2.018	2.415	2.308
	4.2	2.398	2.391	2.423	2.378	2.402	2.387	2.350	2.505	2.283	2.408	2.373	2.296	2.599	2.148	2.414
	4.4	2.442	2.468	2.469	2.453	2.462	2.366	2.499	2.504	2.424	2.469	2.261	2.537	2.545	2.387	2.478
	4.6	2.515	2.520	2.528	2.512	2.521	2.508	2.537	2.574	2.495	2.540	2.499	2.557	2.629	2.472	2.564
	4.8	2.582	2.582	2.551	2.566	2.585	2.631	2.632	2.477	2.551	2.648	2.690	2.692	2.376	2.533	2.720
	5.0	2.603	2.612	2.622	2.609	2.622	2.535	2.582	2.633	2.571	2.636	2.442	2.545	2.648	2.520	2.653
	5.2	2.675	2.676	2.665	2.655	2.680	2.713	2.714	2.663	2.609	2.735	2.758	2.761	2.660	2.548	2.800
	5.4	2.712	2.720	2.721	2.709	2.708	2.720	2.760	2.762	2.705	2.701	2.729	2.807	2.812	2.700	2.693
	5.6	2.743	2.749	2.747	2.761	2.757	2.710	2.741	2.732	2.800	2.781	2.668	2.731	2.712	2.846	2.811
5.8	2.800	2.792	2.797	2.796	2.791	2.841	2.802	2.824	2.819	2.794	2.889	2.814	2.857	2.848	2.798	
6.0	2.822	2.815	2.819	2.822	2.834	2.806	2.770	2.790	2.805	2.868	2.786	2.710	2.753	2.783	2.907	
6.2	2.876	2.877	2.885	2.881	2.846	2.940	2.943	2.981	2.961	2.787	3.015	3.020	3.089	3.054	2.710	
6.4	2.885	2.878	2.884	2.889	2.889	2.864	2.826	2.854	2.883	2.882	2.837	2.756	2.817	2.876	2.873	
6.6	2.934	2.928	2.917	2.911	2.921	2.988	2.961	2.906	2.878	2.928	3.052	3.000	2.893	2.834	2.937	
6.8	2.935	2.942	2.961	2.936	2.942	2.890	2.925	3.021	2.895	2.927	2.831	2.903	3.091	2.842	2.907	
7.0	2.971	2.980	2.967	2.989	2.964	2.974	3.017	2.952	3.061	2.939	2.977	3.062	2.933	3.144	2.906	
7.2	3.005	2.986	2.995	2.982	2.993	3.057	2.962	3.007	2.940	2.994	3.117	2.930	3.021	2.885	2.996	
7.4	3.016	3.006	3.024	3.006	3.008	3.030	2.980	3.069	2.982	2.993	3.047	2.947	3.123	2.950	2.974	
7.6	3.038	3.014	3.024	3.034	3.035	3.071	2.945	2.997	3.048	3.054	3.111	2.853	2.964	3.066	3.077	
7.8	3.056	3.042	3.051	3.046	3.032	3.097	3.024	3.071	3.046	2.977	3.146	3.002	3.096	3.047	2.903	
8.0	3.069	3.056	3.067	3.054	3.048	3.106	3.040	3.095	3.031	2.997	3.149	3.019	3.129	3.001	2.931	
8.2	3.079	3.079	3.074	3.069	3.064	3.106	3.105	3.085	3.060	3.030	3.140	3.137	3.098	3.048	2.987	
8.4	3.071	3.089	3.087	3.073	3.103	3.028	3.115	3.106	3.035	3.184	2.970	3.147	3.129	2.986	3.277	
8.6	3.095	3.091	3.078	3.095	3.096	3.114	3.096	3.026	3.113	3.119	3.137	3.102	2.958	3.136	3.147	
8.8	3.101	3.109	3.111	3.098	3.099	3.121	3.155	3.165	3.106	3.107	3.145	3.211	3.230	3.114	3.118	
9.0	3.092	3.109	3.107	3.103	3.083	3.052	3.142	3.128	3.109	3.009	3.001	3.181	3.154	3.117	2.907	
9.2	3.108	3.107	3.098	3.113	3.098	3.122	3.118	3.071	3.147	3.072	3.140	3.132	3.037	3.189	3.039	
9.4	3.114	3.093	3.091	3.116	3.103	3.148	3.040	3.029	3.159	3.094	3.189	2.971	2.946	3.210	3.082	
9.6	3.093	3.098	3.099	3.094	3.101	3.045	3.072	3.074	3.051	3.086	2.982	3.037	3.043	2.993	3.066	
9.8	3.105	3.090	3.105	3.082	3.108	3.114	3.034	3.112	2.995	3.128	3.125	2.961	3.121	2.874	3.153	
10.0	3.111	3.105	3.110	3.105	3.106	3.155	3.127	3.151	3.127	3.132	3.207	3.153	3.199	3.153	3.165	

S.3 Activation volumes (cm³/mol) obtained by fitting equations E1-E11 to kinetic data in Tables S.1.1-S.1.15.

Table S.5.1 Activation volumes (cm³/mol) obtained by fitting equations E1-E11 to kinetic data generated using equations E4-E8 with $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ over ² over pressure range of 0-1 kbar with 1% error.

		Fitted Equation														
		E1					E2					E3				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.4	-24.6	-24.3	-24.2	-24.7	-23.0	-22.9	-22.8	-22.7	-23.1	-24.2	-25.2	-23.7	-24.2	-25.4
E5		-24.4	-24.5	-24.2	-24.1	-24.6	-23.0	-22.9	-22.9	-22.7	-23.2	-24.2	-25.2	-23.7	-24.2	-25.4
E6		-24.4	-24.6	-24.3	-24.2	-24.6	-23.1	-23.1	-23.0	-22.9	-23.3	-24.2	-25.2	-23.7	-24.2	-25.4
E7		-24.4	-24.6	-24.2	-24.1	-24.6	-23.0	-22.9	-22.9	-22.8	-23.2	-24.2	-25.2	-23.7	-24.2	-25.4
E8		-24.5	-24.6	-24.3	-24.2	-24.7	-23.1	-23.1	-23.0	-22.9	-23.3	-24.2	-25.2	-23.7	-24.2	-25.4
		E4					E5					E6				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.8	-25.1	-24.6	-24.6	-25.1	-24.4	-25.4	-24.3	-24.2	-25.3	-25.0	-25.3	-24.8	-24.7	-25.2
E5		-24.7	-25.0	-24.5	-24.5	-25.0	-24.4	-25.4	-24.2	-24.3	-25.2	-24.8	-25.2	-24.6	-24.6	-25.1
E6		-24.7	-25.0	-24.5	-24.5	-25.0	-24.4	-25.4	-24.3	-24.2	-25.2	-24.8	-25.1	-24.6	-24.6	-25.1
E7		-24.7	-25.0	-24.5	-24.5	-25.0	-24.4	-25.4	-24.2	-24.2	-25.2	-24.8	-25.2	-24.7	-24.6	-25.1
E8		-24.8	-25.1	-24.6	-24.5	-25.0	-24.5	-25.4	-24.3	-24.2	-25.2	-24.9	-25.2	-24.7	-24.6	-25.1
		E7					E8					E9				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.4	-25.4	-24.3	-24.2	-25.3	-24.4	-25.5	-24.3	-24.2	-25.2	-24.4	-25.6	-24.3	-24.3	-25.2
E5		-24.4	-25.5	-24.2	-24.3	-25.2	-24.4	-25.7	-24.2	-24.3	-25.2	-24.4	-25.8	-24.2	-24.3	-25.2
E6		-24.4	-25.5	-24.3	-24.2	-25.2	-24.4	-25.6	-24.3	-24.2	-25.2	-24.4	-25.8	-24.3	-24.2	-25.2
E7		-24.4	-25.5	-24.2	-24.2	-25.2	-24.4	-25.6	-24.2	-24.3	-25.2	-24.4	-25.7	-24.2	-24.3	-25.2
E8		-24.5	-25.4	-24.3	-24.2	-25.2	-24.5	-25.5	-24.3	-24.2	-25.2	-24.5	-25.6	-24.3	-24.2	-25.2
		E10					E11									
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4		-24.2	-25.6	-23.7	-24.3	-25.4	-26.9	-27.5	-26.7	-26.7	-27.2					
E5		-24.2	-25.8	-23.7	-24.3	-25.4	-26.7	-27.3	-26.5	-26.5	-27.0					
E6		-24.2	-25.8	-23.7	-24.2	-25.4	-26.6	-27.2	-26.4	-26.4	-26.9					
E7		-24.2	-25.7	-23.7	-24.3	-25.4	-26.7	-27.3	-26.5	-26.5	-27.0					
E8		-24.2	-25.6	-23.7	-24.2	-25.4	-26.7	-27.3	-26.5	-26.5	-27.0					

Table S.5.2 Activation volumes (cm^3/mol) obtained by fitting equations **E1-E11** to kinetic data generated using equations **E4-E8** with $\Delta V_0^\ddagger = -25 \text{ cm}^3\text{mol}^{-1}$, $\Delta\beta_0^\ddagger = 10. \text{ cm}^3\text{mol}^{-1}\text{kbar}^{-1}$, $\Delta\xi_0^\ddagger = -7.5 \text{ cm}^3\text{mol}^{-1}\text{kbar}^{-2}$ over 2 over pressure range of 0-1 kbar with 5% error.

		Fitted Equation														
		E1					E2					E3				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.0	-24.8	-23.2	-22.9	-25.1	-23.0	-22.7	-22.3	-21.8	-23.8	-21.0	-26.2	-18.7	-21.5	-27.0
E5		-23.9	-24.7	-23.2	-22.8	-25.0	-23.0	-22.7	-22.3	-21.8	-23.8	-20.9	-26.2	-18.7	-21.4	-27.0
E6		-24.0	-24.8	-23.2	-22.8	-25.0	-23.1	-22.8	-22.5	-21.9	-23.9	-20.9	-26.2	-18.7	-21.4	-27.0
E7		-24.0	-24.7	-23.2	-22.8	-25.0	-23.0	-22.7	-22.3	-21.8	-23.8	-20.9	-26.2	-18.7	-21.4	-27.0
E8		-24.0	-24.8	-23.3	-22.9	-25.1	-23.1	-22.8	-22.5	-21.9	-23.9	-20.9	-26.2	-18.7	-21.4	-27.0
		E4					E5					E6				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.1	-25.7	-23.3	-23.0	-25.4	-24.0	-44.3	-23.2	-60.6	-25.8	-24.2	-26.1	-23.3	-23.1	-25.5
E5		-24.0	-25.5	-23.2	-22.9	-25.2	-23.9	-46.4	-23.2	-62.4	-25.8	-24.1	-25.9	-23.2	-23.0	-25.3
E6		-24.1	-25.5	-23.2	-22.9	-25.3	-24.0	-47.6	-23.2	-63.6	-25.7	-24.1	-25.8	-23.2	-23.0	-25.3
E7		-24.1	-25.6	-23.2	-23.0	-25.3	-24.0	-46.0	-23.2	-62.1	-25.8	-24.1	-25.9	-23.3	-23.0	-25.4
E8		-24.1	-25.6	-23.3	-23.0	-25.3	-24.0	-46.6	-23.3	-62.7	-25.8	-24.1	-25.9	-23.3	-23.1	-25.4
		E7					E8					E9				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-21.2	-48.4	-23.2	-69.4	-25.8	-21.2	-95.7	-23.2	-61.9	-25.7	-21.2	-91.8	-23.2	-59.7	-25.7
E5		-21.4	-50.2	-23.2	-73.2	-25.7	-21.4	-92.6	-23.2	-58.8	-25.6	-21.4	-88.9	-23.2	-56.8	-25.6
E6		-21.6	-51.1	-20.9	-76.2	-25.7	-21.6	-90.0	-23.2	-56.2	-25.6	-21.6	-86.4	-23.2	-54.3	-25.6
E7		-21.4	-49.9	-23.2	-72.5	-25.7	-21.4	-93.1	-23.2	-59.3	-25.6	-21.4	-89.3	-23.2	-57.3	-25.6
E8		-21.5	-50.3	-23.3	-74.0	-25.7	-21.5	-91.5	-23.3	-57.7	-25.7	-21.5	-87.8	-23.3	-55.8	-25.6
		E10					E11									
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4		-21.2	-56.6	-18.3	-20.1	-22.2	-25.8	-28.5	-24.8	-24.8	-27.1					
E5		-21.4	-57.2	-18.3	-20.3	-22.3	-25.5	-28.2	-24.6	-24.6	-26.9					
E6		-21.6	-57.5	-18.3	-20.5	-22.6	-25.4	-28.1	-24.5	-24.5	-26.8					
E7		-21.4	-57.1	-18.3	-20.3	-22.3	-25.6	-28.3	-24.6	-24.6	-26.9					
E8		-21.5	-57.2	-18.3	-20.5	-22.5	-25.6	-28.2	-24.6	-24.6	-26.9					

Table S.5.3 Activation volumes (cm^3/mol) obtained by fitting equations **E1-E11** to kinetic data generated using equations **E4-E8** with $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ over 2 over pressure range of 0-1 kbar with 10% error.

Fitted Equation															
	E1					E2					E3				
Generator Equation	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4	-23.5	-24.9	-22.0	-21.3	-25.4	-23.0	-22.3	-21.7	-20.7	-24.5	-16.6	-27.4	-12.0	-18.3	-29.0
E5	-23.4	-24.8	-21.9	-21.2	-25.3	-23.1	-22.3	-21.7	-20.7	-24.5	-16.6	-27.4	-12.0	-18.3	-29.0
E6	-23.5	-24.9	-21.9	-21.3	-25.4	-23.2	-22.5	-21.9	-20.8	-24.7	-16.6	-27.4	-12.0	-18.3	-29.0
E7	-23.4	-24.8	-21.9	-21.2	-25.4	-23.1	-22.3	-21.7	-20.7	-24.5	-16.6	-27.4	-12.0	-18.3	-29.0
E8	-23.5	-24.9	-22.0	-21.3	-25.4	-23.2	-22.5	-21.9	-20.8	-24.7	-16.6	-27.4	-12.0	-18.3	-29.0
	E4					E5					E6				
Generator Equation	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4	-23.5	-26.4	-21.9	-21.3	-25.6	-23.5	-84.4	-22.0	-112.7	-26.1	-23.4	-27.1	-21.9	-21.4	-25.6
E5	-23.4	-26.2	-21.8	-21.2	-25.5	-23.4	-85.8	-20.5	-114.4	-25.9	-23.4	-26.8	-21.8	-21.3	-25.5
E6	-23.4	-26.1	-21.9	-21.3	-25.5	-23.5	-86.7	-20.0	-115.5	-25.9	-23.4	-26.7	-21.8	-21.3	-25.5
E7	-23.4	-26.2	-21.8	-21.3	-25.5	-23.4	-85.6	-20.6	-114.1	-26.0	-23.4	-26.9	-21.8	-21.3	-25.5
E8	-23.5	-26.2	-21.9	-21.3	-25.5	-23.5	-86.0	-20.3	-114.7	-26.0	-23.4	-26.8	-21.9	-21.3	-25.6
	E7					E8					E9				
Generator Equation	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4	-21.7	-91.5	-20.3	-213.1	-26.0	-21.7	-114.0	-20.3	-51.3	-25.9	-21.7	-109.1	-20.3	-49.7	-25.9
E5	-21.8	-93.3	-20.5	-240.2	-25.9	-21.8	-110.9	-20.5	-48.2	-25.8	-21.8	-106.2	-20.5	-46.8	-23.8
E6	-22.1	-94.4	-20.7	-270.8	-24.0	-22.1	-108.3	-20.7	-45.6	-24.0	-22.1	-103.7	-20.7	-44.3	-24.0
E7	-21.8	-93.0	-20.4	-235.6	-25.9	-21.8	-111.4	-20.4	-48.7	-25.8	-21.8	-106.7	-20.4	-47.2	-23.7
E8	-22.0	-93.4	-20.6	-251.5	-23.9	-22.0	-109.8	-20.6	-47.1	-23.9	-22.0	-105.2	-20.6	-45.7	-23.9
	E10					E11									
Generator Equation	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4	-21.7	-91.7	-11.0	-19.5	-23.6	-24.3	-29.4	-22.5	-22.7	-26.7					
E5	-21.8	-92.1	-11.0	-19.6	-23.8	-24.1	-29.2	-22.2	-22.4	-26.5					
E6	-22.1	-92.3	-11.0	-19.9	-24.0	-24.0	-29.1	-22.1	-22.3	-26.4					
E7	-21.8	-92.0	-11.0	-19.6	-23.7	-24.1	-29.2	-22.3	-22.5	-26.5					
E8	-22.0	-92.1	-11.0	-19.8	-23.9	-24.1	-29.2	-22.3	-22.5	-26.5					

Table S.5.4 Activation volumes (cm^3/mol) obtained by fitting equations **E1-E11** to kinetic data generated using equations **E4-E8** with $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ over 2 over pressure range of 0-5 kbar with 1% error.

		Fitted Equation														
		E1					E2					E3				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-20.1	-20.4	-20.9	-20.2	-20.3	-16.6	-16.7	-16.9	-16.7	-16.7	-23.5	-23.7	-25.5	-23.5	-23.4
E5		-20.0	-20.3	-20.2	-20.1	-20.2	-17.1	-17.3	-17.2	-17.2	-17.2	-23.3	-23.5	-23.7	-23.2	-23.1
E6		-20.5	-20.8	-20.8	-20.7	-20.7	-17.5	-17.7	-17.7	-17.6	-17.7	-23.5	-23.7	-23.9	-23.4	-23.3
E7		-20.2	-20.5	-20.5	-20.4	-20.4	-17.0	-17.2	-17.2	-17.1	-17.2	-23.4	-23.6	-23.8	-23.3	-23.2
E8		-21.0	-21.2	-21.2	-21.1	-21.1	-17.3	-17.5	-17.4	-17.4	-17.5	-23.6	-23.8	-24.0	-23.6	-23.5
		E4					E5					E6				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.9	-25.5	-27.2	-25.1	-25.1	-25.0	-25.0	-27.3	-24.6	-24.7	-27.5	-28.3	-30.8	-27.8	-27.8
E5		-22.8	-23.3	-23.2	-23.0	-23.1	-25.0	-25.0	-25.5	-24.6	-24.6	-24.2	-24.8	-24.8	-24.5	-24.5
E6		-23.4	-23.9	-23.9	-23.7	-23.7	-24.7	-24.8	-25.2	-24.4	-24.4	-24.9	-25.5	-25.4	-25.1	-25.1
E7		-23.8	-24.3	-24.3	-24.1	-24.1	-24.7	-24.8	-25.2	-24.4	-24.4	-25.7	-26.3	-26.3	-25.9	-25.9
E8		-25.6	-26.2	-26.1	-25.9	-25.9	-24.5	-24.6	-25.0	-24.2	-24.2	-28.1	-28.8	-28.8	-28.4	-28.4
		E7					E8					E9				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-25.2	-25.3	-27.6	-24.8	-24.9	-26.0	-25.8	-28.2	-25.4	-25.4	-26.3	-26.1	-28.5	-25.7	-25.7
E5		-25.3	-25.3	-25.8	-24.8	-24.9	-26.4	-26.0	-26.8	-25.6	-25.6	-26.9	-26.4	-27.3	-26.0	-26.0
E6		-25.0	-25.0	-25.5	-24.6	-24.6	-25.6	-25.5	-26.1	-25.1	-25.1	-26.0	-25.7	-26.5	-25.3	-25.3
E7		-25.0	-25.0	-25.5	-24.6	-24.6	-25.7	-25.5	-26.2	-25.1	-25.1	-26.0	-25.8	-26.5	-25.4	-25.4
E8		-24.6	-24.7	-25.1	-24.3	-24.3	-25.0	-25.0	-25.5	-24.6	-24.6	-25.2	-25.1	-25.7	-24.7	-24.7
		E10					E11									
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4		-24.6	-24.8	-25.6	-24.0	-24.8	-26.1	-26.5	-27.6	-26.3	-26.3					
E5		-24.6	-24.7	-24.9	-23.9	-24.8	-24.9	-25.4	-25.3	-25.1	-25.2					
E6		-24.6	-24.7	-24.9	-23.9	-24.7	-25.6	-26.1	-26.0	-25.9	-25.9					
E7		-24.6	-24.7	-24.9	-23.9	-24.7	-25.7	-26.1	-26.1	-25.9	-25.9					
E8		-24.6	-24.7	-24.9	-23.9	-24.7	-27.1	-27.6	-27.5	-27.3	-27.4					

Table S.5.5 Activation volumes (cm^3/mol) obtained by fitting equations **E1-E11** to kinetic data generated using equations **E4-E8** with $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ over 2 over pressure range of 0-5 kbar with 5% error.

		Fitted Equation														
		E1					E2					E3				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-19.8	-21.2	-20.9	-20.5	-20.8	-16.3	-17.2	-16.9	-16.8	-17.0	-23.4	-24.4	-25.5	-23.3	-22.9
E5		-19.7	-21.1	-20.8	-20.4	-20.6	-16.8	-17.8	-17.5	-17.3	-17.6	-23.2	-24.1	-25.2	-23.0	-22.6
E6		-20.2	-21.7	-21.3	-20.9	-21.2	-17.3	-18.2	-17.9	-17.7	-18.0	-23.4	-24.3	-25.4	-23.2	-22.8
E7		-19.9	-21.4	-21.0	-20.6	-20.9	-16.8	-17.7	-17.4	-17.2	-17.5	-23.3	-24.2	-25.3	-23.1	-22.7
E8		-20.6	-22.1	-21.8	-21.3	-21.6	-17.1	-18.0	-17.7	-17.5	-17.8	-23.6	-24.5	-25.6	-23.4	-23.0
		E4					E5					E6				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.4	-27.3	-27.2	-25.6	-25.7	-24.9	-25.3	-27.3	-23.6	-23.4	-26.9	-30.6	-30.8	-28.4	-28.4
E5		-22.4	-24.9	-24.7	-23.5	-23.6	-24.8	-25.1	-27.3	-23.3	-23.2	-23.7	-26.7	-26.7	-25.0	-25.1
E6		-23.0	-25.5	-25.3	-24.1	-24.3	-24.6	-25.1	-27.1	-23.4	-23.2	-24.3	-27.4	-27.3	-25.6	-25.8
E7		-23.4	-26.0	-25.9	-24.5	-24.7	-24.6	-25.0	-27.1	-23.3	-23.2	-25.1	-28.4	-28.4	-26.5	-26.5
E8		-25.2	-27.9	-27.9	-26.4	-26.5	-24.4	-25.0	-26.8	-23.5	-23.2	-27.5	-31.1	-31.2	-29.0	-29.0
		E7					E8					E9				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-25.1	-25.4	-27.6	-23.6	-23.5	-25.8	-25.6	-28.2	-23.8	-23.7	-26.3	-25.7	-28.5	-23.9	-23.8
E5		-25.2	-25.2	-27.6	-23.4	-23.3	-26.3	-25.5	-28.2	-23.6	-23.5	-27.0	-25.6	-28.7	-23.7	-23.6
E6		-24.8	-25.1	-27.3	-23.4	-23.3	-25.5	-25.3	-27.8	-23.5	-23.4	-25.9	-25.4	-28.1	-23.6	-23.5
E7		-24.8	-25.1	-27.3	-23.4	-23.3	-25.6	-25.3	-27.9	-23.5	-23.4	-26.0	-25.4	-28.2	-23.6	-23.5
E8		-24.5	-25.1	-27.0	-23.5	-23.3	-24.8	-25.2	-27.3	-23.5	-23.3	-25.0	-25.2	-27.6	-23.5	-23.4
		E10					E11									
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4		-23.5	-24.7	-25.6	-23.3	-23.7	-25.6	-28.0	-27.6	-26.8	-27.0					
E5		-23.3	-24.5	-25.5	-23.0	-23.5	-24.4	-26.8	-26.4	-25.6	-25.9					
E6		-23.4	-24.6	-25.5	-23.2	-20.7	-25.1	-27.5	-27.1	-26.3	-26.6					
E7		-23.4	-24.5	-25.5	-23.1	-20.6	-25.2	-27.6	-27.2	-26.4	-26.6					
E8		-23.6	-16.0	-25.6	-22.6	-21.8	-26.6	-29.0	-28.6	-27.8	-28.1					

Table S.5.6 Activation volumes (cm^3/mol) obtained by fitting equations **E1-E11** to kinetic data generated using equations **E4-E8** with $\Delta V_0^\ddagger = -25 \text{ cm}^3\text{mol}^{-1}$, $\Delta\beta_0^\ddagger = 10. \text{ cm}^3\text{mol}^{-1}\text{kbar}^{-1}$, $\Delta\xi_0^\ddagger = -7.5 \text{ cm}^3\text{mol}^{-1}\text{kbar}^{-2}$ over 2 over pressure range of 0-5 kbar with 10% error.

		Fitted Equation														
		E1					E2					E3				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-19.3	-22.2	-21.6	-20.8	-21.4	-16.0	-17.8	-17.3	-16.9	-17.5	-23.3	-25.1	-27.3	-23.0	-22.2
E5		-19.2	-22.1	-21.5	-20.7	-21.3	-16.5	-18.3	-17.8	-17.4	-18.0	-23.0	-24.8	-27.0	-22.8	-21.9
E6		-19.8	-22.7	-22.1	-21.2	-21.8	-16.9	-18.8	-18.3	-17.8	-18.5	-23.2	-25.0	-27.2	-23.0	-22.1
E7		-19.5	-22.4	-21.8	-20.9	-21.5	-16.4	-18.3	-17.7	-17.3	-18.0	-23.1	-24.9	-27.1	-22.9	-22.0
E8		-20.2	-23.1	-22.5	-21.6	-22.2	-16.7	-18.6	-18.0	-17.6	-18.3	-23.4	-25.2	-27.4	-23.2	-22.3
		E4					E5					E6				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-23.7	-29.4	-29.6	-26.2	-26.4	-24.6	-25.6	-29.4	-22.8	-22.3	-26.1	-33.3	-34.3	-29.1	-29.1
E5		-21.7	-26.8	-26.6	-24.0	-24.4	-24.5	-25.3	-29.3	-22.5	-22.0	-23.0	-29.1	-29.4	-25.6	-25.8
E6		-22.4	-27.4	-27.3	-24.7	-25.0	-24.3	-25.4	-29.1	-22.7	-22.2	-23.6	-29.7	-30.0	-26.3	-26.5
E7		-22.7	-28.0	-28.0	-25.1	-25.4	-24.3	-25.4	-29.1	-22.6	-22.1	-24.3	-30.9	-31.4	-27.1	-27.3
E8		-24.5	-30.1	-30.2	-26.9	-27.2	-24.1	-25.5	-28.9	-22.9	-22.3	-26.7	-33.7	-34.6	-29.6	-29.7
		E7					E8					E9				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.8	-25.6	-29.6	-22.8	-22.3	-25.5	-25.7	-29.9	-22.8	-22.3	-26.0	-25.7	-30.3	-22.8	-22.3
E5		-24.8	-25.4	-29.5	-22.5	-22.0	-26.2	-25.4	-29.8	-22.5	-22.1	-27.4	-25.5	-30.3	-22.5	-22.1
E6		-24.5	-25.4	-29.3	-22.7	-22.2	-25.2	-25.4	-29.6	-22.7	-22.2	-25.7	-25.5	-29.9	-22.6	-22.2
E7		-24.5	-25.4	-29.3	-22.6	-22.1	-25.2	-25.4	-29.6	-22.6	-22.1	-25.8	-25.5	-30.0	-22.6	-22.1
E8		-24.2	-25.5	-29.1	-22.9	-22.3	-24.5	-25.5	-29.3	-22.9	-22.3	-24.7	-25.5	-29.5	-22.9	-22.3
		E10					E11									
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4		-23.3	-25.1	-27.3	-20.8	-14.6	-25.0	-29.7	-29.0	-27.3	-27.9					
E5		-23.0	-24.9	-27.1	-20.9	-14.7	-23.8	-28.5	-27.8	-26.2	-26.7					
E6		-23.2	-7.7	-27.3	-20.5	-15.1	-24.5	-29.2	-28.5	-26.9	-27.5					
E7		-23.1	-7.6	-27.2	-20.6	-15.0	-24.5	-29.3	-28.6	-26.9	-27.5					
E8		-23.4	-8.1	-27.5	-20.0	-16.0	-26.0	-30.7	-30.0	-28.4	-28.9					

Table S.5.7 Activation volumes (cm^3/mol) obtained by fitting equations **E1-E11** to kinetic data generated using equations **E4-E8** with $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta \beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta \xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ over 2 over pressure range of 0-10 kbar with 1% error.

		Fitted Equation														
		E1					E2					E3				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-15.5	-15.5	-15.6	-15.4	-15.5	-12.0	-12.0	-12.1	-11.9	-11.9	-20.6	-20.7	-20.4	-20.4	-20.6
E5		-16.0	-16.0	-16.0	-15.9	-16.0	-13.3	-13.3	-13.3	-13.3	-13.3	-20.3	-20.4	-20.3	-20.1	-20.3
E6		-16.8	-16.8	-16.8	-16.7	-16.8	-13.7	-13.7	-13.7	-13.6	-13.7	-20.9	-21.0	-20.9	-20.7	-20.9
E7		-16.3	-16.3	-16.3	-16.2	-16.2	-12.9	-12.9	-12.9	-12.9	-12.9	-20.7	-20.8	-20.6	-20.4	-20.7
E8		-17.3	-17.3	-17.3	-17.2	-17.3	-12.8	-12.8	-12.8	-12.8	-12.8	-21.4	-21.5	-21.4	-21.2	-21.4
		E4					E5					E6				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-25.0	-25.2	-25.1	-24.7	-25.0	-25.0	-25.1	-24.0	-24.5	-24.7	-32.4	-32.7	-32.3	-31.8	-32.3
E5		-19.7	-19.8	-19.7	-19.5	-19.7	-25.0	-25.1	-24.8	-24.4	-24.7	-21.8	-22.0	-21.9	-21.6	-21.8
E6		-21.9	-22.0	-21.9	-21.7	-21.9	-24.3	-24.4	-24.1	-23.7	-24.0	-25.0	-25.2	-25.0	-24.7	-25.0
E7		-23.0	-23.1	-23.0	-22.7	-23.0	-24.2	-24.3	-24.0	-23.7	-24.0	-27.6	-27.8	-27.6	-27.2	-27.5
E8		-32.5	-32.7	-32.5	-32.1	-32.4	-23.5	-23.6	-23.3	-23.1	-23.3	-45.5	-45.9	-45.5	-44.8	-45.4
		E7					E8					E9				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-26.0	-26.1	-24.8	-25.4	-25.7	-30.8	-30.9	-28.9	-30.2	-30.5	-33.1	-33.2	-30.4	-32.3	-32.7
E5		-26.2	-26.3	-25.9	-25.5	-25.8	-33.5	-33.4	-33.4	-34.2	-33.8	-39.8	-39.6	-39.4	-41.0	-40.0
E6		-25.0	-25.1	-24.8	-24.4	-24.7	-28.4	-28.5	-28.0	-27.6	-27.9	-29.7	-29.9	-29.3	-28.8	-29.2
E7		-25.0	-25.1	-24.8	-24.4	-24.7	-28.6	-28.8	-28.3	-27.9	-28.2	-30.1	-30.2	-29.7	-29.2	-29.6
E8		-23.8	-24.0	-23.7	-23.4	-23.7	-25.0	-25.1	-24.8	-24.4	-24.7	-25.5	-25.6	-25.2	-24.8	-25.2
		E10					E11									
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4		-25.5	-25.3	-25.0	-24.9	-24.4	-14.9	-15.0	-15.2	-14.7	-14.9					
E5		-25.6	-25.3	-25.2	-25.0	-24.5	-20.6	-20.7	-20.6	-20.5	-20.6					
E6		-25.4	-25.2	-25.0	-24.8	-24.3	-22.1	-22.2	-22.2	-22.0	-22.1					
E7		-25.4	-25.2	-25.0	-24.8	-24.3	-21.9	-22.0	-22.0	-21.8	-21.9					
E8		-24.8	-25.2	-25.1	-24.8	-24.3	-24.9	-25.0	-25.0	-24.8	-24.9					

Table S.5.8 Activation volumes (cm^3/mol) obtained by fitting equations **E1-E11** to kinetic data generated using equations **E4-E8** with $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta\beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta\xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ over 2 over pressure range of 0-10 kbar with 5% error.

		Fitted Equation														
		E1					E2					E3				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-15.6	-15.7	-15.6	-15.2	-15.5	-12.1	-12.1	-12.1	-11.8	-12.0	-20.5	-21.0	-20.4	-19.4	-20.6
E5		-16.1	-16.2	-16.1	-15.7	-16.0	-13.4	-13.4	-13.4	-13.2	-13.3	-20.2	-20.8	-20.1	-19.1	-20.3
E6		-16.9	-17.0	-16.9	-16.5	-16.8	-13.8	-13.8	-13.8	-13.6	-13.7	-20.8	-21.4	-20.7	-19.7	-20.9
E7		-16.3	-16.5	-16.4	-16.0	-16.3	-13.0	-13.0	-13.0	-12.8	-12.9	-20.5	-21.1	-20.4	-19.4	-20.6
E8		-17.4	-17.6	-17.4	-17.0	-17.3	-12.9	-13.0	-12.9	-12.7	-12.8	-21.3	-21.9	-21.2	-20.2	-21.4
		E4					E5					E6				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-25.0	-25.9	-25.1	-23.5	-24.8	-25.0	-25.5	-24.0	-22.4	-23.7	-32.3	-34.0	-32.3	-29.7	-31.9
E5		-19.7	-20.3	-19.8	-18.9	-19.7	-25.1	-25.5	-23.9	-22.2	-23.4	-21.9	-22.7	-22.0	-20.6	-21.7
E6		-21.9	-22.5	-22.0	-20.9	-21.8	-24.3	-24.8	-23.3	-21.8	-23.1	-25.0	-26.0	-25.1	-23.5	-24.8
E7		-23.0	-23.8	-23.1	-21.8	-22.9	-24.2	-24.7	-23.3	-21.7	-23.0	-27.6	-28.8	-27.6	-25.6	-27.3
E8		-32.5	-33.6	-32.4	-30.6	-32.1	-23.3	-24.0	-22.8	-21.4	-22.8	-45.4	-47.6	-45.3	-41.9	-44.9
		E7					E8					E9				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-26.1	-26.6	-24.8	-23.1	-24.4	-30.7	-31.2	-28.9	-26.7	-28.6	-32.8	-33.3	-30.4	-28.1	-30.3
E5		-26.4	-26.7	-24.8	-22.9	-24.3	-32.2	-32.3	-31.3	-109.1	-32.8	-36.9	-36.5	-34.3	-104.5	-35.9
E6		-25.0	-25.5	-23.9	-22.2	-23.6	-28.5	-28.9	-26.5	-24.1	-26.0	-29.6	-30.2	-27.4	-24.9	-27.0
E7		-25.1	-25.6	-23.9	-22.2	-23.6	-28.7	-29.2	-26.7	-24.4	-26.2	-30.0	-30.6	-27.7	-25.3	-27.4
E8		-23.7	-24.4	-23.1	-21.6	-23.0	-25.0	-25.6	-23.9	-22.2	-23.7	-25.5	-26.1	-24.3	-22.5	-24.1
		E10					E11									
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4		-27.1	-25.8	-25.0	-28.1	-21.3	-15.2	-15.6	-15.2	-14.0	-14.9					
E5		-27.2	-26.0	-25.4	>1·105	-21.0	-20.7	-21.0	-20.8	-20.1	-20.6					
E6		-26.9	-25.8	-25.3	-24.9	-21.1	-22.2	-22.6	-22.3	-21.6	-22.2					
E7		-27.0	-25.8	-25.3	-25.3	-21.0	-22.0	-22.4	-22.1	-21.4	-22.0					
E8		-25.5	-15.9	-24.3	-22.5	-21.4	-25.0	-25.4	-25.1	-24.4	-25.0					

Table S.5.9 Activation volumes (cm^3/mol) obtained by fitting equations **E1-E11** to kinetic data generated using equations **E4-E8** with $\Delta V_0^\ddagger = -25 \text{ cm}^3 \text{ mol}^{-1}$, $\Delta\beta_0^\ddagger = 10. \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-1}$, $\Delta\xi_0^\ddagger = -7.5 \text{ cm}^3 \text{ mol}^{-1} \text{ kbar}^{-2}$ over 2 over pressure range of 0-10 kbar with 10% error.

		Fitted Equation														
		E1					E2					E3				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-15.7	-16.0	-15.8	-15.0	-15.6	-12.2	-12.2	-12.2	-11.7	-12.0	-20.3	-21.4	-20.1	-18.1	-20.6
E5		-16.2	-16.5	-16.3	-15.5	-16.1	-13.5	-13.6	-13.5	-13.1	-13.3	-20.0	-21.2	-19.8	-17.8	-20.3
E6		-17.0	-17.3	-17.1	-16.3	-16.9	-13.9	-14.0	-13.9	-13.5	-13.7	-20.6	-21.8	-20.4	-18.4	-20.9
E7		-16.5	-16.8	-16.5	-15.7	-16.3	-13.1	-13.2	-13.1	-12.7	-12.9	-20.4	-21.5	-20.1	-18.1	-20.7
E8		-17.5	-17.8	-17.6	-16.8	-17.4	-13.0	-13.1	-13.0	-12.6	-12.8	-21.1	-22.3	-20.9	-18.9	-21.4
		E4					E5					E6				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-24.9	-26.9	-25.0	-22.1	-24.7	-25.0	-26.0	-23.0	-19.8	-22.6	-32.2	-35.7	-32.0	-27.1	-31.5
E5		-19.8	-20.9	-19.9	-18.1	-19.7	-25.2	-26.0	-22.7	-19.4	-22.2	-21.9	-23.6	-22.0	-19.5	-21.7
E6		-21.9	-23.2	-22.1	-20.0	-21.9	-24.2	-25.3	-22.3	-19.4	-22.2	-25.0	-27.0	-25.1	-22.1	-24.7
E7		-23.0	-24.6	-23.1	-20.7	-22.9	-24.2	-25.2	-22.3	-19.3	-22.1	-27.5	-30.1	-27.5	-23.8	-27.1
E8		-32.4	-34.7	-32.2	-28.7	-31.9	-23.2	-24.4	-22.1	-19.5	-22.2	-45.1	-49.7	-44.8	-38.3	-44.3
		E7					E8					E9				
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5
E4		-26.2	-27.1	-23.6	-20.2	-23.1	-30.7	-31.4	-26.6	-21.8	-25.8	-32.4	-33.3	-27.7	-22.5	-27.2
E5		-26.6	-27.3	-23.4	-19.8	-22.8	-31.3	-31.8	-28.2	-103.2	-29.7	-34.9	-34.8	-29.5	-23.8	-30.4
E6		-25.1	-26.1	-22.8	-19.6	-22.5	-28.5	-29.4	-24.5	-20.2	-23.7	-29.5	-30.5	-25.1	-20.5	-24.5
E7		-25.1	-26.1	-22.8	-19.5	-22.5	-28.8	-29.7	-24.7	-20.3	-23.9	-29.8	-30.9	-25.4	-20.7	-24.8
E8		-23.6	-24.9	-22.3	-19.6	-22.4	-25.0	-26.2	-22.9	-19.8	-22.7	-25.4	-26.7	-23.1	-19.9	-23.0
		E10					E11									
Generator Equation		Set1	Set2	Set3	Set4	Set5	Set1	Set2	Set3	Set4	Set5					
E4		-28.5	-26.4	-26.2	-22.5	-20.6	-15.4	-16.4	-15.4	-13.1	-15.0					
E5		-28.5	-26.6	-28.2	-23.8	-20.4	-20.8	-21.5	-21.0	-19.6	-20.7					
E6		-27.9	-26.5	-25.1	-20.5	-21.0	-22.3	-23.0	-22.5	-21.1	-22.2					
E7		-28.0	-26.5	-25.4	-20.7	-20.7	-22.1	-22.8	-22.3	-20.9	-22.0					
E8		-25.4	99.4	-23.1	-19.9	-21.5	-25.2	-25.8	-25.3	-23.9	-25.0					

