

Table S1. Calculated electronic energies (including nuclear repulsion) in hartrees and vibrational zero-point energies in kcal/mol of the stationary points

	MP2/6-31G*		MP2/ADZP		MP2/ aug-cc-pVDZ	MP2/ aug-cc-pVTZ
	Energy	ZPE	Energy	ZPE	Energy	Energy
C ₂ H ₅ Cl	-538.52890	43.0	-538.59126	42.4	-538.61689	-538.75788
OF ⁻	-174.53407	1.3	-174.56500	1.2	-174.59780	-174.74039
OF ⁻ (H ₂ O)	-250.78039	16.6	-250.84617	16.3	-250.89501	-251.10623
C ₂ H ₄	-78.29118	32.5	-78.31530	32.2	-78.32892	-78.40453
HOF	-175.10665	8.6	-175.14893	8.7	-175.18043	-175.32671
HOF(H ₂ O)	-251.33273	24.4	-251.40823	24.4	-251.45456	-251.66865
Cl ⁻	-459.67115	0.0	-459.70382	0.0	-459.72276	-459.78079
E2 TS (not solvated)	-713.05823	40.9	-713.15874	40.5	-713.22371	N/A
E2 TS	-789.28877	56.2	-789.42373	56.0	-789.50482	N/A
Reactant-side Complex	-789.32986	N/A ^a	-789.45656	59.4	N/A	N/A

^aN/A = not available

Table S2. Cartesian coordinates (in Å) of C₂H₅Cl at PM3-SRP level

Atom	X	Y	Z
Cl	0.0000	0.0000	0.0000
C	1.7757	0.0000	0.0000
C	2.2764	1.3799	0.0000
H	3.3616	1.4228	0.0027
H	1.9446	1.9419	0.8685
H	1.9490	1.9401	-0.8713
H	2.1038	-0.5670	0.8698
H	2.1037	-0.5668	-0.8699

Table S3. Cartesian coordinates (in Å) of C₂H₅Cl at MP2/6-31+G* level

Atom	X	Y	Z
C	1.601751	-0.355780	0.000000
C	0.473339	0.656701	0.000000
H	1.554748	-0.992683	-0.886627
H	2.562467	0.170489	-0.000100
H	1.554865	-0.992559	0.886724
H	0.506471	1.291083	0.887114
H	0.506480	1.291088	-0.887108
Cl	-1.125622	-0.151350	0.000000

Table S4. Cartesian coordinates (in Å) of C₂H₅Cl at MP2/ADZP level

Atom	X	Y	Z
C	0.477282	0.658899	0.000000
Cl	-1.129746	-0.151874	0.000000
H	0.504986	1.299695	-0.893998
H	0.504985	1.299695	0.893999
H	1.606880	-0.357443	0.000000
H	1.557553	-0.998751	-0.893780
H	1.557552	-0.998751	0.893780
H	2.575635	0.171234	0.000002

Table S5. Cartesian coordinates (in Å) of C₂H₅Cl at MP2/aug-cc-pVDZ level

Atom	X	Y	Z
C	-0.484072	0.664813	0.000000
Cl	1.131693	-0.151970	0.000000
H	-0.504958	1.299287	0.896009
H	-0.504958	1.299287	-0.896009
C	-1.607309	-0.360846	-0.000001
H	-1.550837	-0.999648	0.893328
H	-1.550825	-0.999657	-0.893321
H	-2.578921	0.160427	-0.000004

Table S6. Cartesian coordinates (in Å) of C₂H₅Cl at MP2/aug-cc-pVTZ level

Atom	X	Y	Z
C	1.501994	0.643399	0.000000
C	0.000000	1.813220	0.000000
H	1.980748	1.623331	0.000000
H	1.826623	0.097162	0.883046
H	1.826623	0.097162	-0.883046
Cl	-0.820434	-0.778394	0.000000
H	-0.349290	1.337669	0.884864
H	-0.349290	1.337669	-0.884864

Table S7. Bond lengths (in Å) of OF⁻ at various levels of theory

Levels	Bond Lengths
PM3-SRP	1.4036
MP2/6-31+G*	1.5058
MP2/ADZP	1.5011
MP2/aug-cc-pVDZ	1.4996
MP2/aug-cc-pVTZ	1.4786

Table S8. Cartesian coordinates (in Å) of OF⁻(H₂O) at PM3-SRP level

Atom	X	Y	Z
O	-0.4966	-0.8791	0.0011
F	0.9055	-0.8791	0.0011
H	-0.7868	0.8059	0.0011
O	-0.5539	1.7594	-0.0019
H	0.3960	1.7892	-0.0091

Table S9. Cartesian coordinates (in Å) of OF⁻(H₂O) at MP2/6-31+G* level

Atom	X	Y	Z
O	0.764816	0.813161	-0.000032
F	1.168721	-0.628818	0.000017
H	-0.857883	0.400680	0.000264
O	-1.780232	-0.034082	0.000005
H	-1.537273	-0.973943	-0.000201

Table S10. Cartesian coordinates (in Å) of OF⁻(H₂O) at MP2/ADZP level

Atom	X	Y	Z
O	0.670050	0.796560	0.000011
F	1.243223	-0.576892	-0.000007
H	-0.824520	0.343311	-0.000058
O	-1.773118	-0.065140	-0.000007
H	-1.539947	-1.002652	0.000089

Table S11. Cartesian coordinates (in Å) of OF⁻(H₂O) at MP2/aug-cc-pVDZ level

Atom	X	Y	Z
O	0.681881	0.798118	0.000014
F	1.231382	-0.584097	-0.000008
H	-0.813156	0.334325	-0.000092
O	-1.768802	-0.057476	-0.000007
H	-1.573920	-1.002593	0.000107

Table S12. Cartesian coordinates (in Å) of OF⁻(H₂O) at MP2/aug-cc-pVTZ level

Atom	X	Y	Z
O	-0.663994	0.782961	0.000030
F	-1.238546	-0.567491	-0.000021
H	0.797895	0.325482	-0.000060
O	1.760243	-0.059814	-0.000035
H	1.579023	-1.003235	0.000294

Table S13. Cartesian coordinates (in Å) of C₂H₄ at PM3-SRP level

Atom	X	Y	Z
C	0.0000	0.0000	0.0000
C	1.2980	0.0000	0.0000
H	1.9014	0.8847	0.0000
H	1.9014	-0.8847	0.0000
H	-0.6034	-0.8847	-0.0001
H	-0.6034	0.8847	0.0000

Table S14. Cartesian coordinates (in Å) of C₂H₄ at MP2/6-31+G* level

Atom	X	Y	Z
C	0.000000	0.000000	0.670068
C	0.000000	0.000000	-0.670068
H	0.000000	0.925032	1.238676
H	0.000000	-0.925032	1.238676
H	0.000000	-0.925032	-1.238676
H	0.000000	0.925032	-1.238676

Table S15. Cartesian coordinates (in Å) of C₂H₄ at MP2/ADZP level

Atom	X	Y	Z
C	0.000000	0.000000	0.672699
C	0.000000	0.000000	-0.672699
H	0.000000	0.934592	1.243019
H	0.000000	-0.934592	1.243019
H	0.000000	-0.934592	-1.243019
H	0.000000	0.934592	-1.243019

Table S16. Cartesian coordinates (in Å) of C₂H₄ at MP2/aug-cc-pVDZ level

Atom	X	Y	Z
C	0.000000	0.000000	-0.674542
C	0.000000	0.000000	0.674542
H	0.933538	0.000000	-1.243455
H	-0.933538	0.000000	-1.243455
H	0.933538	0.000000	1.243455
H	-0.933538	0.000000	1.243455

Table S17. Cartesian coordinates (in Å) of C₂H₄ at MP2/aug-cc-pVTZ level

Atom	X	Y	Z
C	0.000000	0.000000	0.666627
C	0.000000	0.000000	-0.666627
H	0.000000	0.923365	1.228619
H	0.000000	-0.923365	1.228619
H	0.000000	-0.923365	-1.228619
H	0.000000	0.923365	-1.228619

Table S18. Cartesian coordinates (in Å) of HOF at PM3-SRP level

Atom	X	Y	Z
F	0.0000	0.0000	0.0000
O	1.3956	0.0000	0.0000
H	1.5337	0.9361	0.0000

Table S19. Cartesian coordinates (in Å) of HOF at MP2/6-31+G* level

Atom	X	Y	Z
O	0.054076	0.720138	0.000000
F	0.054076	-0.734018	0.000000
H	-0.919297	0.845058	0.000000

Table S20. Cartesian coordinates (in Å) of HOF at MP2/ADZP level

Atom	X	Y	Z
O	0.053757	0.715351	0.000000
F	0.053757	-0.729517	0.000000
H	-0.913861	0.842843	0.000000

Table S21. Cartesian coordinates (in Å) of HOF at MP2/aug-cc-pVDZ level

Atom	X	Y	Z
O	0.053703	0.716126	0.000000
F	0.053703	-0.730227	0.000000
H	-0.912943	0.843030	0.000000

Table S22. Cartesian coordinates (in Å) of HOF at MP2/aug-cc-pVTZ level

Atom	X	Y	Z
O	0.053385	0.706793	0.000000
F	0.053385	-0.721603	0.000000
H	-0.907551	0.840079	0.000000

Table S23. Cartesian coordinates (in Å) of HOF(H₂O) at PM3-SRP level

Atom	X	Y	Z
F	0.0000	0.0000	0.0000
O	1.3988	0.0000	0.0000
H	1.5246	0.9493	0.0000
O	0.9451	2.6455	-0.0296
H	0.3767	2.8323	0.7114
H	0.4584	2.8308	-0.8269

Table S24. Cartesian coordinates (in Å) of HOF(H₂O) at MP2/6-31+G* level

Atom	X	Y	Z
O	0.845726	0.756510	-0.000182
F	1.369289	-0.603678	0.000189
H	-0.116883	0.514916	0.000392
O	-1.841544	-0.010185	-0.000163
H	-2.118776	-0.527668	-0.775438
H	-2.121397	-0.524752	0.776107

Table S25. Cartesian coordinates (in Å) of HOF(H₂O) at MP2/ADZP level

Atom	X	Y	Z
O	0.851612	0.750716	-0.000534
F	1.362225	-0.603451	0.000559
H	-0.108005	0.520574	0.000548
O	-1.830417	-0.010055	-0.000478
H	-2.157686	-0.512129	-0.760482
H	-2.163890	-0.502681	0.762995

Table S26. Cartesian coordinates (in Å) of HOF(H₂O) at MP2/aug-cc-pVDZ level

Atom	X	Y	Z
O	0.828895	0.752017	-0.000267
F	1.368602	-0.594085	0.000301
H	-0.125083	0.499742	0.000338
O	-1.838579	-0.006844	-0.000362
H	-2.055382	-0.559883	-0.763290
H	-2.059480	-0.554474	0.765278

Table S27. Cartesian coordinates (in Å) of HOF(H₂O) at MP2/aug-cc-pVTZ level

Atom	X	Y	Z
O	0.842554	0.745727	-0.000029
F	1.331704	-0.600241	0.000033
H	-0.116456	0.532108	0.000016
O	-1.817292	-0.000486	-0.000043
H	-2.035301	-0.546254	-0.762452
H	-2.035678	-0.545610	0.762718

Table S28. Cartesian coordinates (in Å) of the E2 transition state (C₂H₅Cl + OF⁻) at PM3-SRP level

Atom	X	Y	Z
C	-0.5664	-0.2997	0.2007
C	0.8252	-0.2997	0.2007
H	-0.9924	0.9780	0.2007
Cl	1.5071	-2.1593	0.2116
O	-1.3548	2.2449	0.3178
F	-1.8076	2.5231	-0.9693
H	1.3286	0.0635	-0.6847
H	1.3291	0.0713	1.0829
H	-1.0912	-0.6096	1.0869
H	-1.0915	-0.6029	-0.6878

Table S29. Cartesian coordinates (in Å) of the E2 transition state ($C_2H_5Cl + OF^-$) at MP2/6-31+G* level

Atom	X	Y	Z
H	-1.506540	0.663213	-0.041227
C	-0.127562	0.978056	0.264810
O	-2.677615	0.504286	-0.297329
C	0.565703	-0.180452	-0.192721
H	0.081018	1.894244	-0.294709
H	-0.098888	1.142866	1.344682
F	-2.851869	-0.870290	0.196420
Cl	2.649878	-0.190959	0.003939
H	0.385977	-1.093172	0.369798
H	0.549414	-0.348155	-1.267189

Table S30. Cartesian coordinates (in Å) of the E2 transition state ($C_2H_5Cl + OF^-$) at MP2/ADZP level

Atom	X	Y	Z
H	-1.492842	0.653025	-0.045820
C	-0.130774	0.955163	0.285340
O	-2.656931	0.498212	-0.323419
C	0.586285	-0.185317	-0.215257
H	0.097336	1.900893	-0.233295
H	-0.097855	1.072827	1.380253
F	-2.876318	-0.845964	0.214044
Cl	2.642808	-0.186563	0.008208
H	0.397931	-1.133048	0.305597
H	0.576949	-0.313214	-1.305818

Table S31. Cartesian coordinates (in Å) of the E2 transition state ($C_2H_5Cl + OF^-$) at MP2/aug-cc-pVDZ level

Atom	X	Y	Z
H	-1.493472	0.752679	-0.015102
C	-0.135110	1.093677	0.117260
O	-2.700797	0.495802	-0.137511
C	0.503544	-0.185121	-0.066760
H	0.068257	1.824686	-0.680063
H	-0.007320	1.528107	1.120213
F	-2.634175	-0.950772	0.091248
Cl	2.575774	-0.200969	-0.006957
H	0.345599	-0.918249	0.731384
H	0.402125	-0.631545	-1.062315

Table S32. Cartesian coordinates (in Å) of E2 transition state [$C_2H_5Cl + OF^-(H_2O)$] at PM3-SRP level

Atom	X	Y	Z
C	-0.5816	-0.9295	0.1906
C	0.8141	-0.9295	0.1906
H	-1.0312	0.3519	0.1906
Cl	1.4897	-2.7695	0.1904
O	-1.4216	1.5512	0.2965
F	-1.8733	1.7912	-1.0005
H	-0.2419	2.8638	0.4766
O	0.2292	3.6400	0.1408
H	-0.0739	3.7713	-0.7508
H	1.3107	-0.5480	-0.6919
H	1.3110	-0.5494	1.0737
H	-1.1024	-1.2493	1.0755
H	-1.1026	-1.2392	-0.6980

Table S33. Cartesian coordinates (in Å) of E2 transition state [$\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$] at MP2/6-31+G* level.

Atom	X	Y	Z
C	0.610085	-0.813056	0.893719
C	1.088165	0.042997	-0.117441
H	-0.846260	-0.814629	0.583466
Cl	3.248524	0.420479	-0.161843
O	-2.011815	-0.877905	0.433881
F	-2.061057	-0.943299	-1.030602
H	-2.969330	0.744266	0.453863
O	-3.407264	1.603804	0.247422
H	-3.151102	1.756966	-0.676153
H	1.064756	-0.331165	-1.136158
H	0.837499	1.096436	-0.034208
H	0.663105	-0.432261	1.915478
H	0.889069	-1.864907	0.812372

Table S34. Cartesian coordinates (in Å) of E2 transition state [C₂H₅Cl + OF⁻(H₂O)] at MP2/ADZP level

Atom	X	Y	Z
C	-0.539160	-0.890219	0.309831
C	-1.343499	0.258581	0.111903
H	0.777773	-0.248152	0.526705
Cl	-3.472792	-0.064218	-0.231444
O	1.855499	0.154640	0.737724
F	1.870697	1.321020	-0.136504
H	3.438536	-0.551187	0.061676
O	4.258887	-0.756412	-0.439956
H	4.182085	-0.128804	-1.170142
H	-1.511575	0.908037	0.978639
H	-1.204851	0.813479	-0.822644
H	-0.389350	-1.538300	-0.565696
H	-0.710559	-1.448543	1.241994

Table S35. Cartesian coordinates (in Å) of E2 transition state [C₂H₅Cl + OF⁻(H₂O)] at MP2/aug-cc-pVDZ level

Atom	X	Y	Z
C	0.340549	0.049761	1.084523
C	1.017394	-0.274427	-0.125945
H	-1.002216	-0.428971	0.769661
Cl	3.107135	0.237782	-0.222249
O	-2.133850	-0.757568	0.576992
F	-1.948867	-1.436273	-0.700084
H	-2.721301	0.851161	-0.020734
O	-2.922123	1.771382	-0.311926
H	-2.040303	2.139020	-0.450819
H	1.182027	-1.335521	-0.335513
H	0.752269	0.303057	-1.017097
H	0.211154	1.121392	1.291474
H	0.636997	-0.528500	1.970018

Table S36. Cartesian coordinates (in Å) of the reactant-side complex [C₂H₅Cl + OF⁻(H₂O)] at PM3-SRP level

Atom	X	Y	Z
Cl	-2.9287	-0.2735	-0.1192
C	-1.1031	-0.2735	-0.1192
C	-0.6122	1.0921	-0.1192
H	-0.8120	-0.8494	0.7551
H	-0.8109	-0.8493	-0.9934
H	-0.9060	1.6664	-0.9896
H	-0.8897	1.6612	0.7599
H	0.5159	1.0988	-0.1298
O	2.2517	0.8374	-0.3060
F	2.8015	0.8054	0.9797
H	2.0511	-0.8517	-0.5892
O	2.0930	-1.8034	-0.3693
H	2.5365	-1.8570	0.4697

Table S37. Cartesian coordinates (in Å) of the reactant-side complex [C₂H₅Cl + OF⁻(H₂O)] at MP2/6-31+G* level

Atom	X	Y	Z
Cl	2.772524	0.222981	-0.159133
C	0.970274	-0.042634	-0.178485
C	0.578400	-1.172706	0.743820
H	0.509881	0.897999	0.118140
H	0.699380	-0.262428	-1.209013
H	1.071349	-2.106648	0.454651
H	0.847449	-0.943403	1.780100
H	-0.505172	-1.297111	0.661242
O	-2.082228	-0.309119	-1.021467
F	-2.724405	-0.939435	0.173186
H	-1.855616	1.117385	-0.220075
O	-1.719089	1.918291	0.397058
H	-2.262048	1.677102	1.164809

Table S38. Cartesian coordinates (in Å) of the reactant-side complex [C₂H₅Cl + OF⁻(H₂O)] at MP2/ADZP level

Atom	X	Y	Z
Cl	2.790548	0.190500	-0.188745
C	0.973447	-0.026397	-0.160762
C	0.571746	-1.128984	0.796184
H	0.547630	0.942112	0.131484
H	0.674613	-0.256069	-1.191149
H	1.031045	-2.089859	0.509525
H	0.876304	-0.885356	1.827525
H	-0.525214	-1.220206	0.743112
O	-2.110450	-0.208941	-0.976210
F	-2.749488	-1.020363	0.091381
H	-1.852048	1.060643	-0.156002
O	-1.675169	1.893124	0.435613
H	-2.432456	1.852321	1.033996

Table S39. Calculated vibrational frequencies (in cm^{-1}) of the reactants and products at MP2/ADZP level

	$\text{C}_2\text{D}_5\text{Cl}$	$\text{OF}^-(\text{D}_2\text{O})$	C_2D_4	$\text{DOF}(\text{H}_2\text{O})$	$\text{HOF}(\text{D}_2\text{O})$
ν_1	2384.9	2835.8	2466.0	3948.7	3567.6
ν_2	2372.2	1946.1	2449.0	3831.4	2892.2
ν_3	2362.3	1300.0	2373.8	2600.6	2763.3
ν_4	2278.9	893.0	2301.1	1647.4	1488.2
ν_5	2221.5	755.6	1568.2	1087.3	1205.3
ν_6	1207.5	446.2	1087.3	923.1	924.3
ν_7	1095.2	307.3	1006.8	571.6	715.0
ν_8	1072.3	107.8	1000.4	298.4	237.7
ν_9	1066.9	75.9	773.0	222.8	223.2
ν_{10}	1047.2		753.7	221.3	181.4
ν_{11}	992.2		735.9	89.7	84.3
ν_{12}	919.2		593.3	54.6	39.7
ν_{13}	820.6				
ν_{14}	800.5				
ν_{15}	647.5				
ν_{16}	580.8				
ν_{17}	300.0				
ν_{18}	203.7				

Table S40. Calculated vibrational frequencies (in cm^{-1}) of the E2 transition states at MP2/ADZP level

	$\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$	$\text{C}_2\text{D}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$	$\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{D}_2\text{O})$
ν_1	3914.5	3914.4	3276.4
ν_2	3584.7	3583.7	3217.9
ν_3	3276.4	2439.7	3180.3
ν_4	3217.9	2392.6	3133.9
ν_5	3180.3	2321.4	2851.3
ν_6	3133.9	2274.3	2602.5
ν_7	1719.0	1718.1	1617.4
ν_8	1617.3	1371.9	1548.0
ν_9	1548.0	1170.4	1459.1
ν_{10}	1459.1	1080.2	1311.5
ν_{11}	1312.0	1008.1	1565.0
ν_{12}	1263.1	980.4	1259.4
ν_{13}	1259.0	957.8	1252.8
ν_{14}	1176.5	920.0	1175.3
ν_{15}	1048.9	885.7	1048.8
ν_{16}	998.4	782.1	997.7
ν_{17}	923.7	747.8	923.7
ν_{18}	769.7	709.7	769.6
ν_{19}	719.1	559.4	621.8
ν_{20}	604.8	514.6	588.7
ν_{21}	586.3	434.1	504.6
ν_{22}	454.8	409.9	454.5
ν_{23}	402.0	398.3	307.3
ν_{24}	299.7	285.0	284.5
ν_{25}	204.7	202.2	201.1
ν_{26}	163.9	159.4	162.0
ν_{27}	111.8	111.2	92.9
ν_{28}	92.4	88.6	87.1
ν_{29}	66.1	64.7	62.2
ν_{30}	60.1	56.7	59.1
ν_{31}	22.0	21.4	21.0
ν_{32}	5.4	4.9	5.4
ν_{33}	696.3 <i>i</i>	585.9 <i>i</i>	694.9 <i>i</i>

Table S41. Calculated vibrational frequencies (in cm^{-1}) of the reactant-side complex at MP2/ADZP level

	$\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$	$\text{C}_2\text{D}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$	$\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{D}_2\text{O})$
ν_1	3899.3	3899.3	3252.2
ν_2	3252.2	2581.8	3204.5
ν_3	3204.5	2418.2	3176.4
ν_4	3176.4	2374.9	3170.0
ν_5	3170.1	2354.8	3080.1
ν_6	3080.1	2305.6	2836.2
ν_7	2581.4	2213.1	1890.5
ν_8	1773.8	1773.6	1499.7
ν_9	1499.4	1210.9	1497.6
ν_{10}	1497.7	1104.0	1488.9
ν_{11}	1489.0	1093.8	1397.7
ν_{12}	1397.8	1079.0	1310.5
ν_{13}	1310.0	1059.2	1285.8
ν_{14}	1279.5	1021.7	1279.4
ν_{15}	1113.8	995.5	1113.7
ν_{16}	1105.2	917.7	1070.9
ν_{17}	1068.3	900.3	1001.9
ν_{18}	1000.5	801.5	901.1
ν_{19}	900.3	787.5	804.6
ν_{20}	804.7	613.9	791.2
ν_{21}	654.0	603.7	653.2
ν_{22}	607.9	588.6	444.3
ν_{23}	341.2	335.3	338.9
ν_{24}	330.7	298.3	323.3
ν_{25}	297.4	216.6	297.3
ν_{26}	186.0	185.1	150.4
ν_{27}	122.1	116.1	121.7
ν_{28}	107.0	105.3	100.7
ν_{29}	79.5	77.0	78.8
ν_{30}	76.0	73.8	74.7
ν_{31}	68.7	60.9	64.1
ν_{32}	50.3	48.4	50.0
ν_{33}	28.7	26.8	28.5

Figure Captions.

Figure S1. Arrhenius plot of the calculated rate constants of $\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$ reaction with a classical barrier height of 3 kcal/mol.

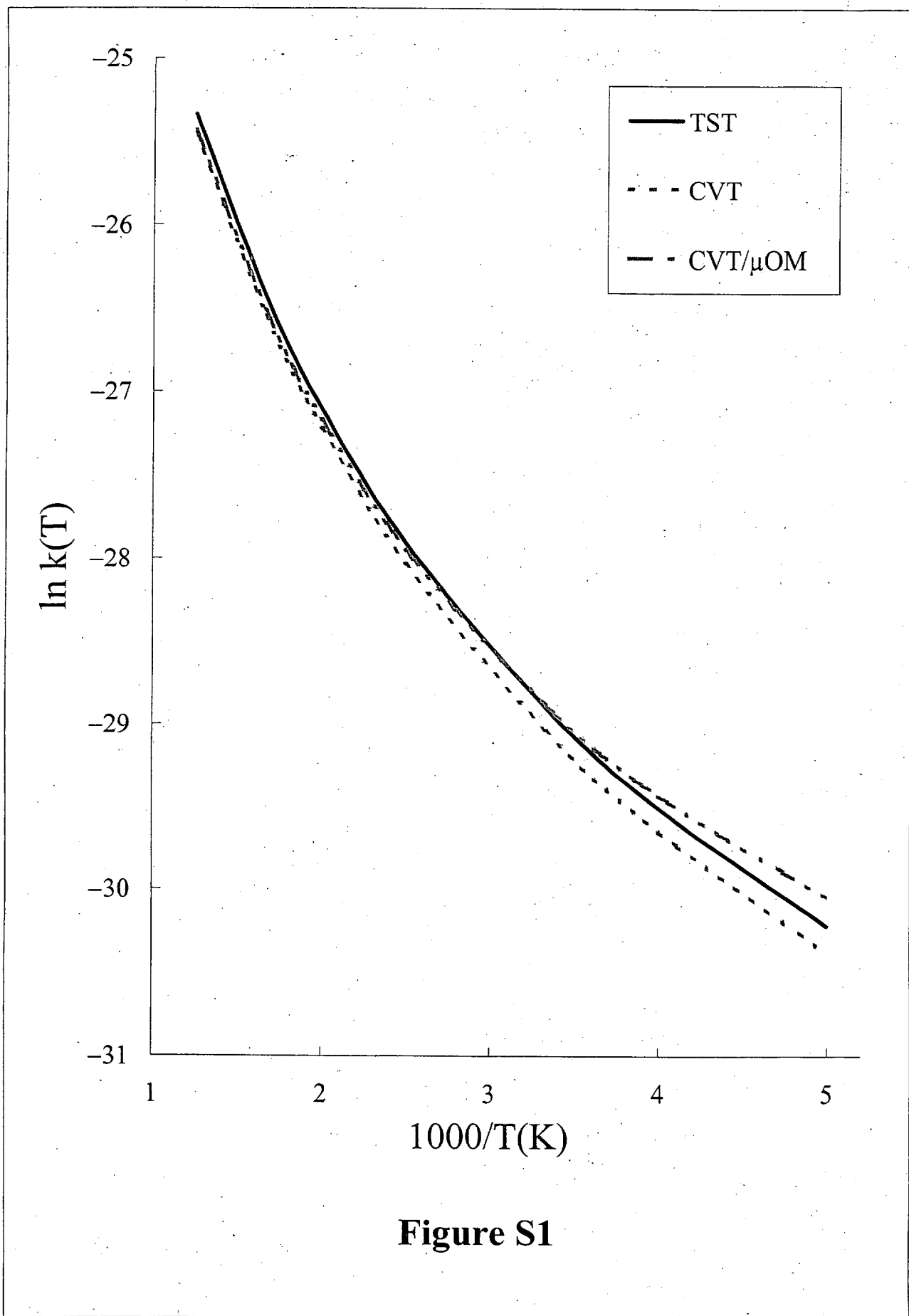
Figure S2. Arrhenius plot of the calculated rate constants of $\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$ reaction with a classical barrier height of 5 kcal/mol.

Figure S3. Arrhenius plot of the calculated rate constants of $\text{C}_2\text{D}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$ reaction with a classical barrier height of 3 kcal/mol.

Figure S4. Arrhenius plot of the calculated rate constants of $\text{C}_2\text{D}_5\text{Cl} + \text{OF}^-(\text{H}_2\text{O})$ reaction with a classical barrier height of 5 kcal/mol.

Figure S5. Arrhenius plot of the calculated rate constants of $\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{D}_2\text{O})$ reaction with a classical barrier height of 3 kcal/mol.

Figure S6. Arrhenius plot of the calculated rate constants of $\text{C}_2\text{H}_5\text{Cl} + \text{OF}^-(\text{D}_2\text{O})$ reaction with a classical barrier height of 5 kcal/mol.



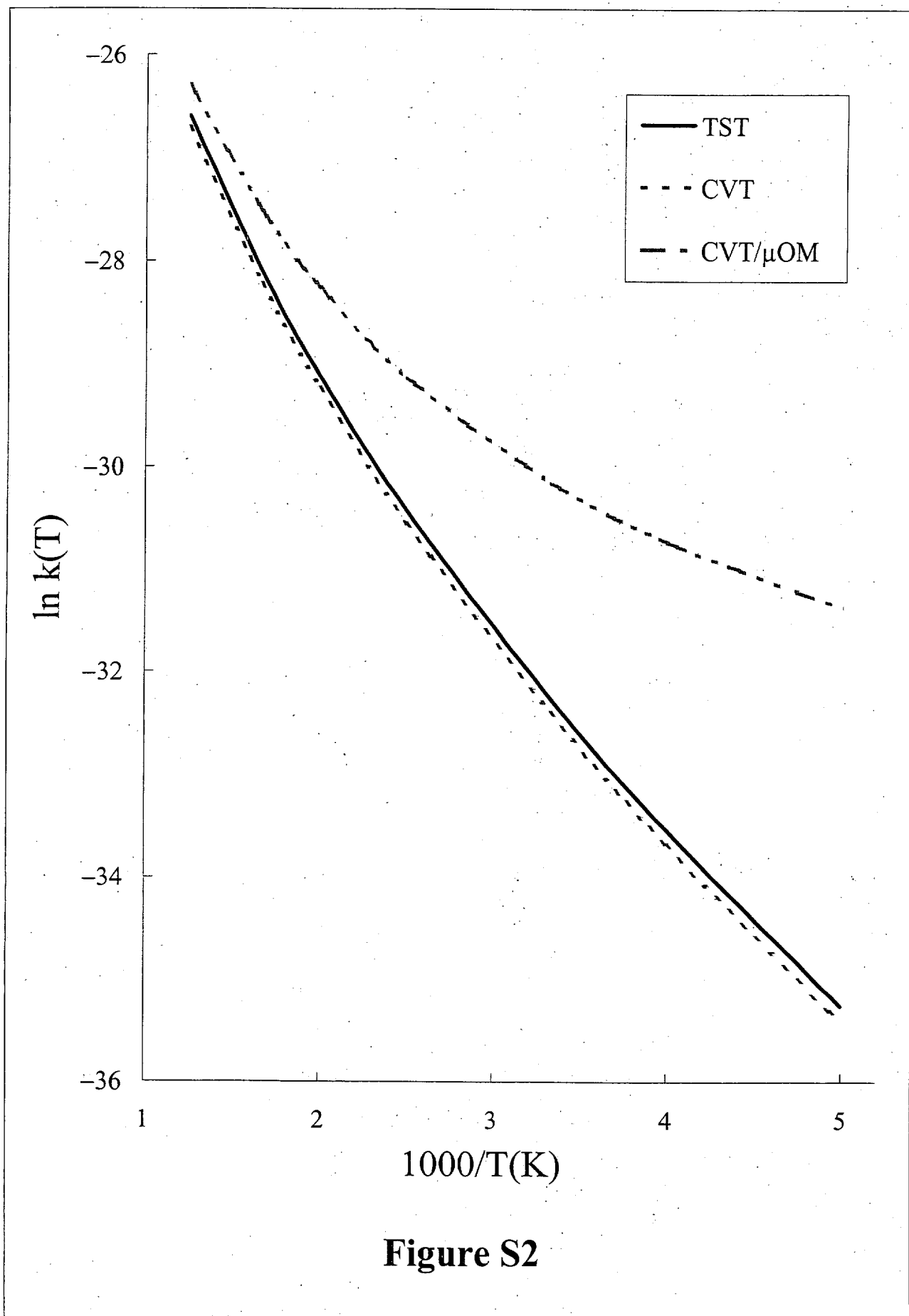
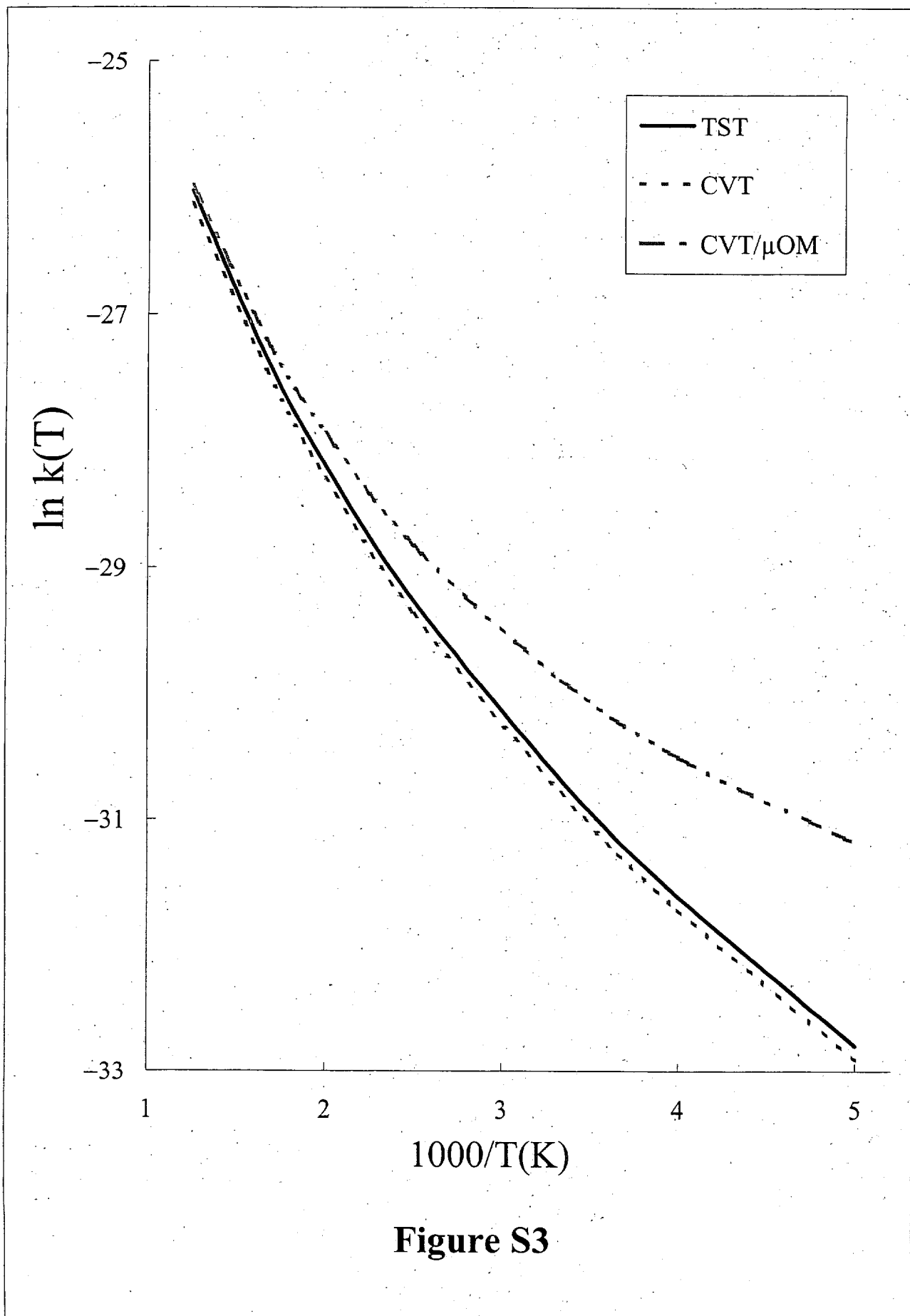
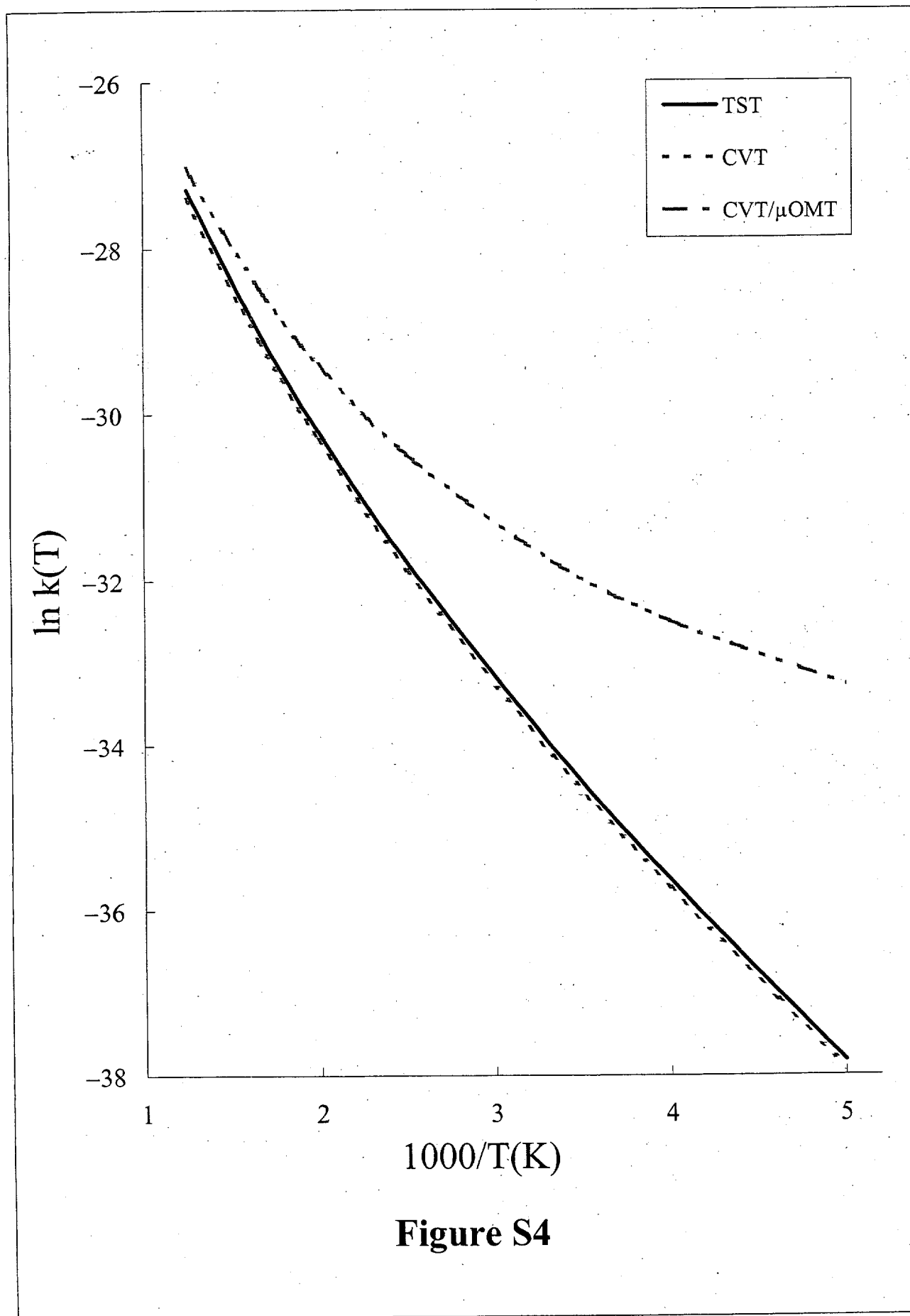
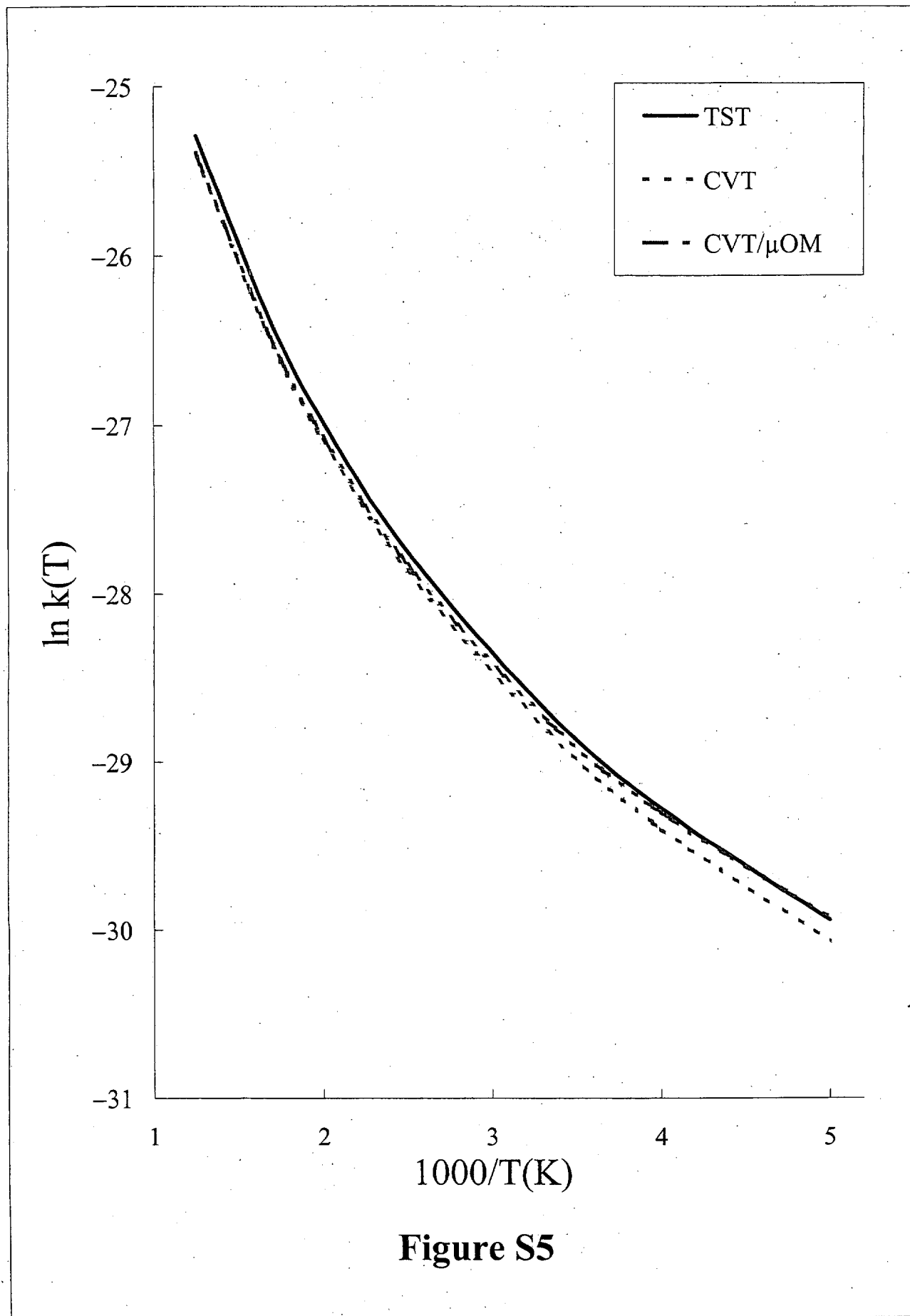


Figure S2







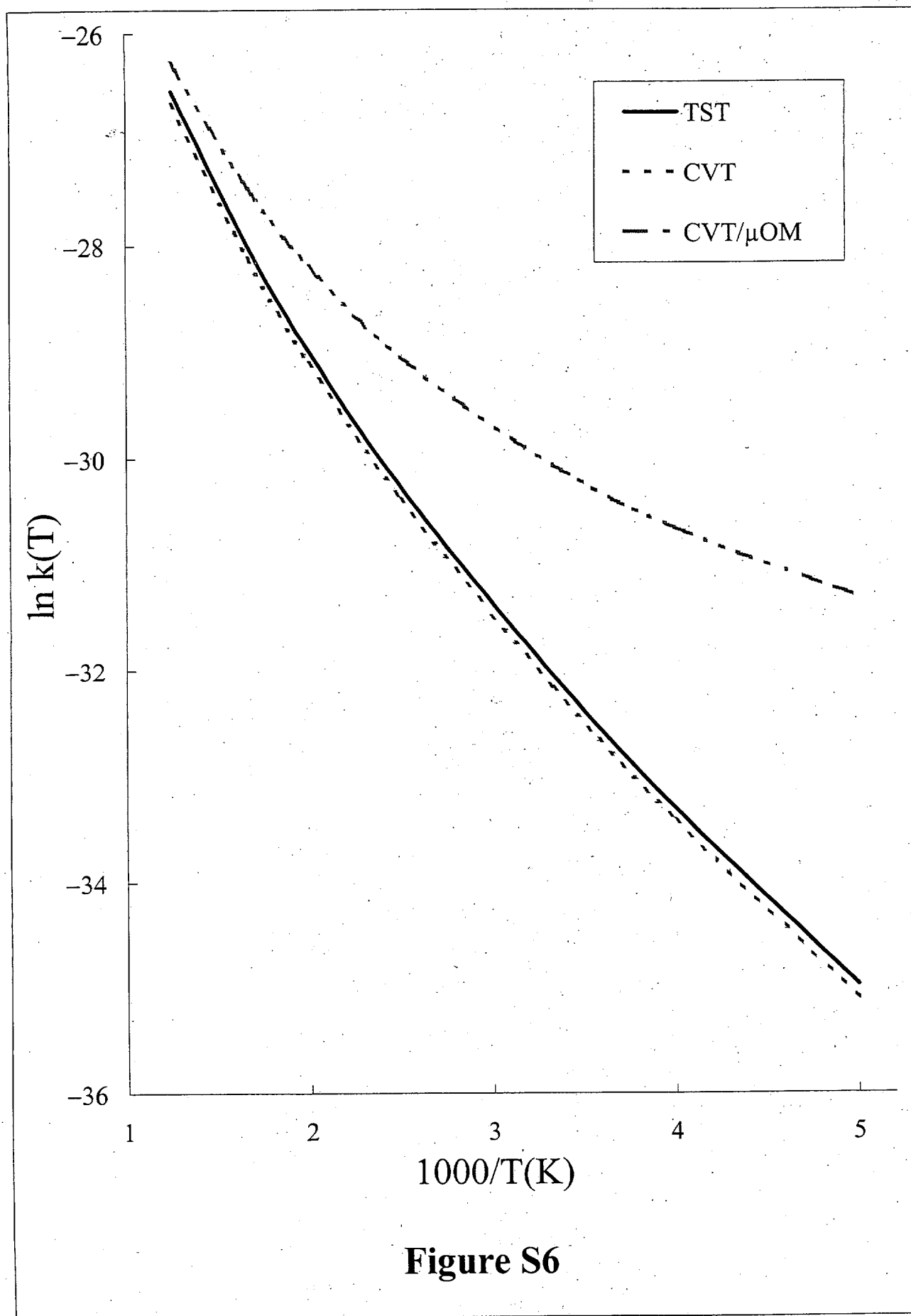


Figure S6