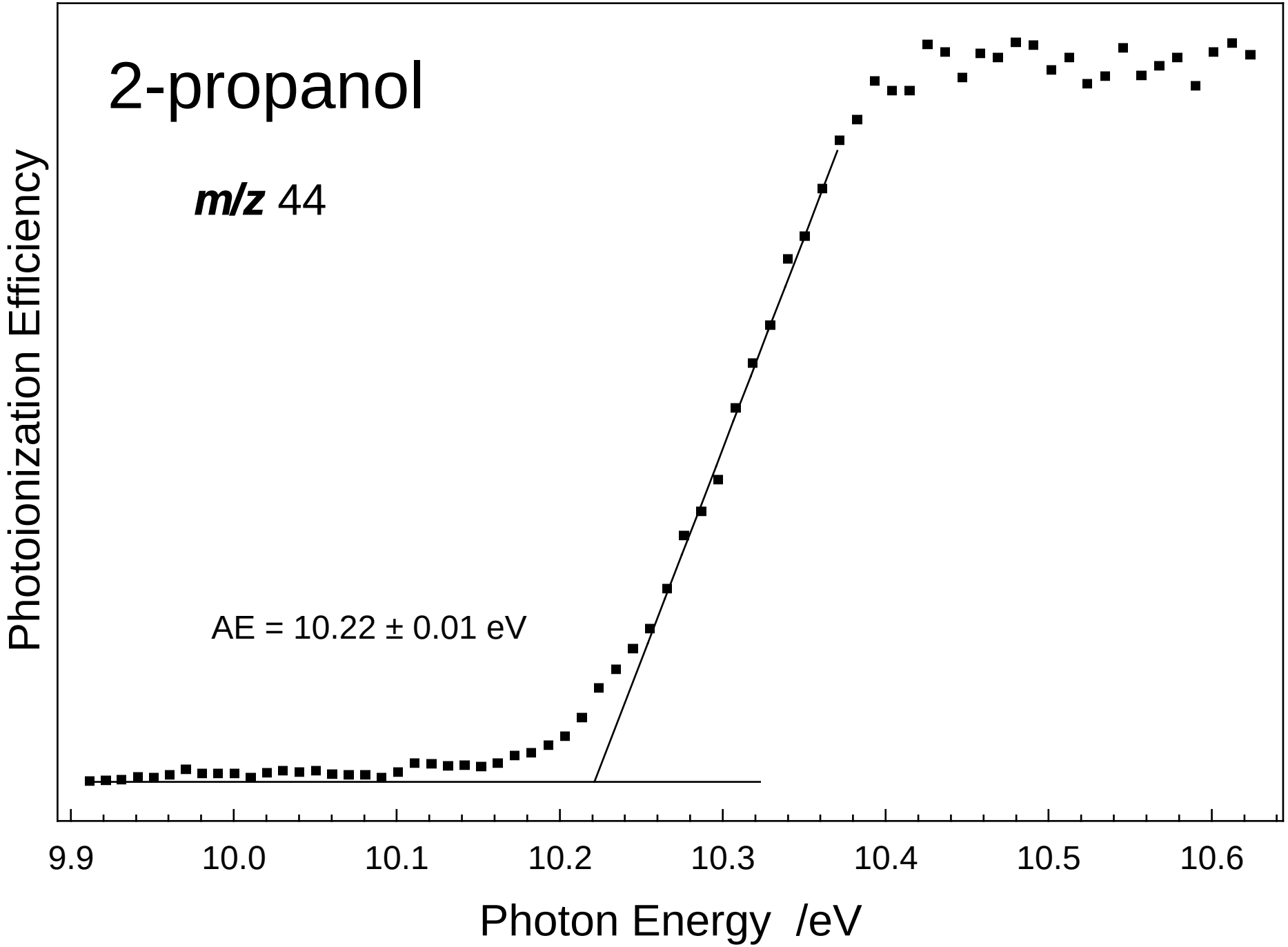
2-propanol
m/z 44
AE = 10.22 ± 0.01 eV
Photoionization Efficiency
9.9
10.0
10.1
10.2
10.3
10.4
10.5
10.6
Photon Energy /eV

Figure S1.

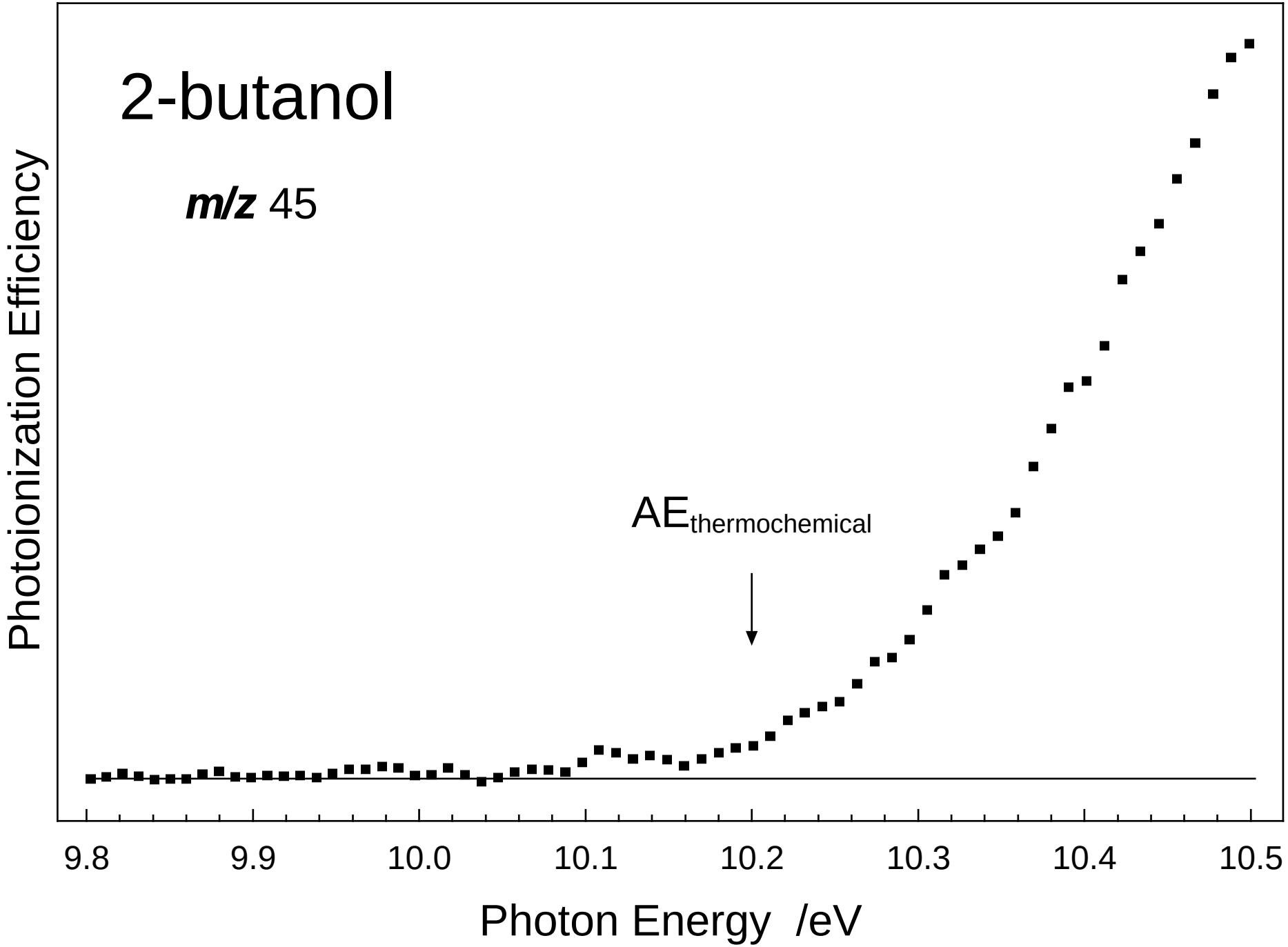
2-butanol
m/z 45
AEthermochemical
Photoionization Efficiency
9.8
9.9
10.0
10.1
10.2
10.3
10.4
10.5
Photon Energy /eV

Figure S2.

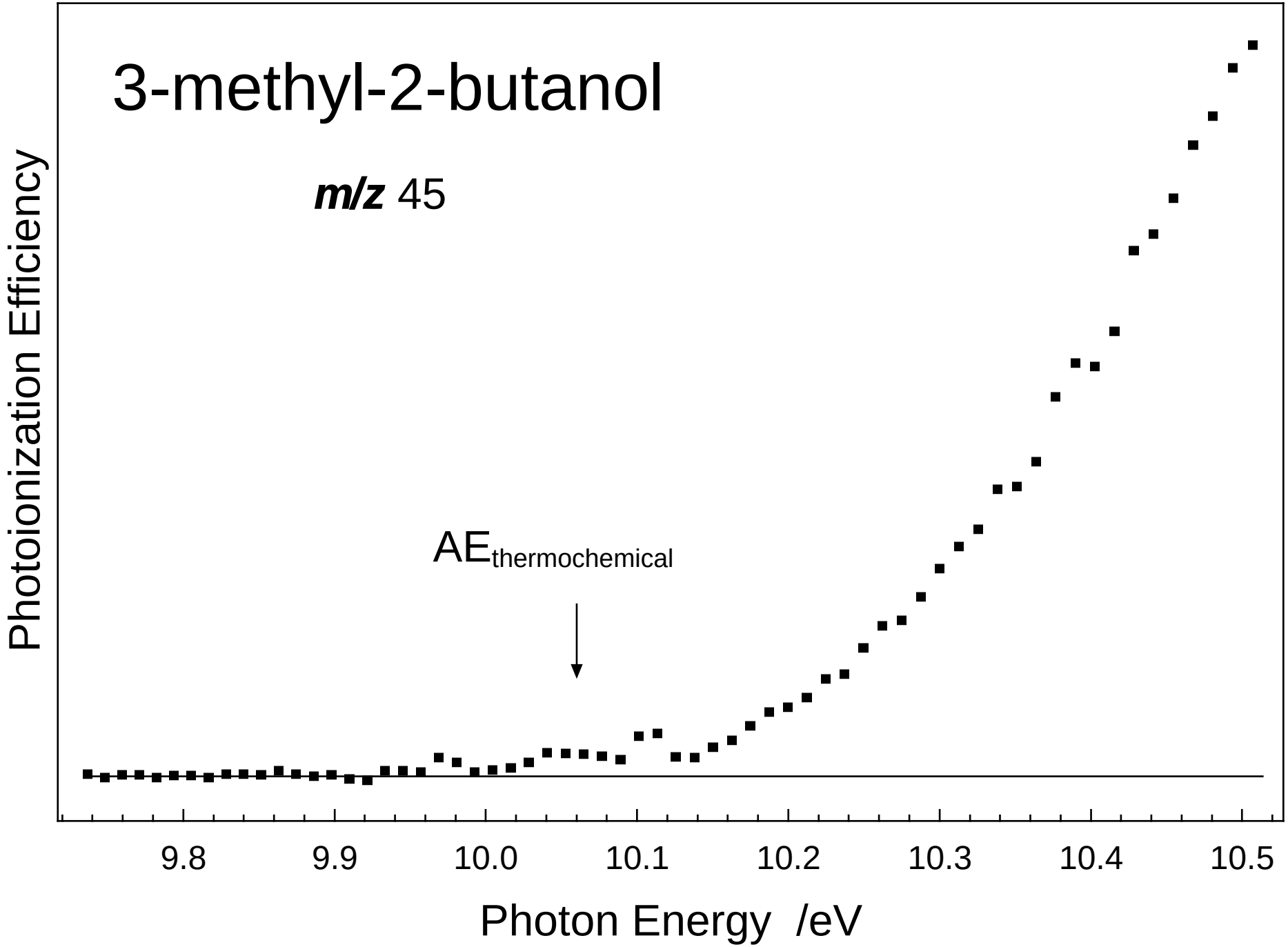
3-methyl-2-butanol
m/z 45
AEthermochemical
Photoionization Efficiency
9.8
9.9
10.0
10.1
10.2
10.3
10.4
10.5
Photon Energy /eV

Figure S3.

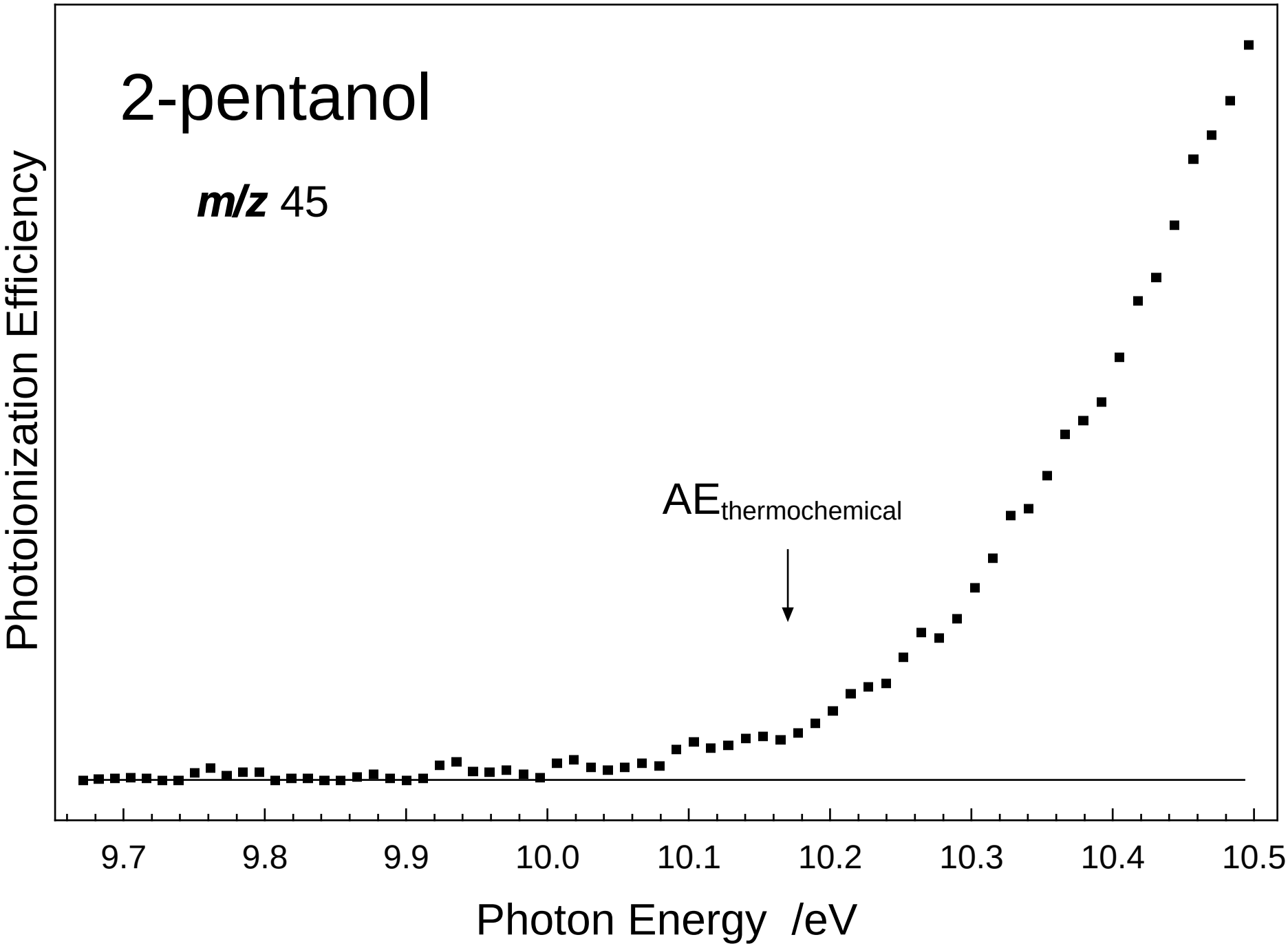
2-pentanol
m/z 45
AEthermochemical
Photoionization Efficiency
9.7
9.8
9.9
10.0
10.1
10.2
10.3
10.4
10.5
Photon Energy /eV

Figure S4.

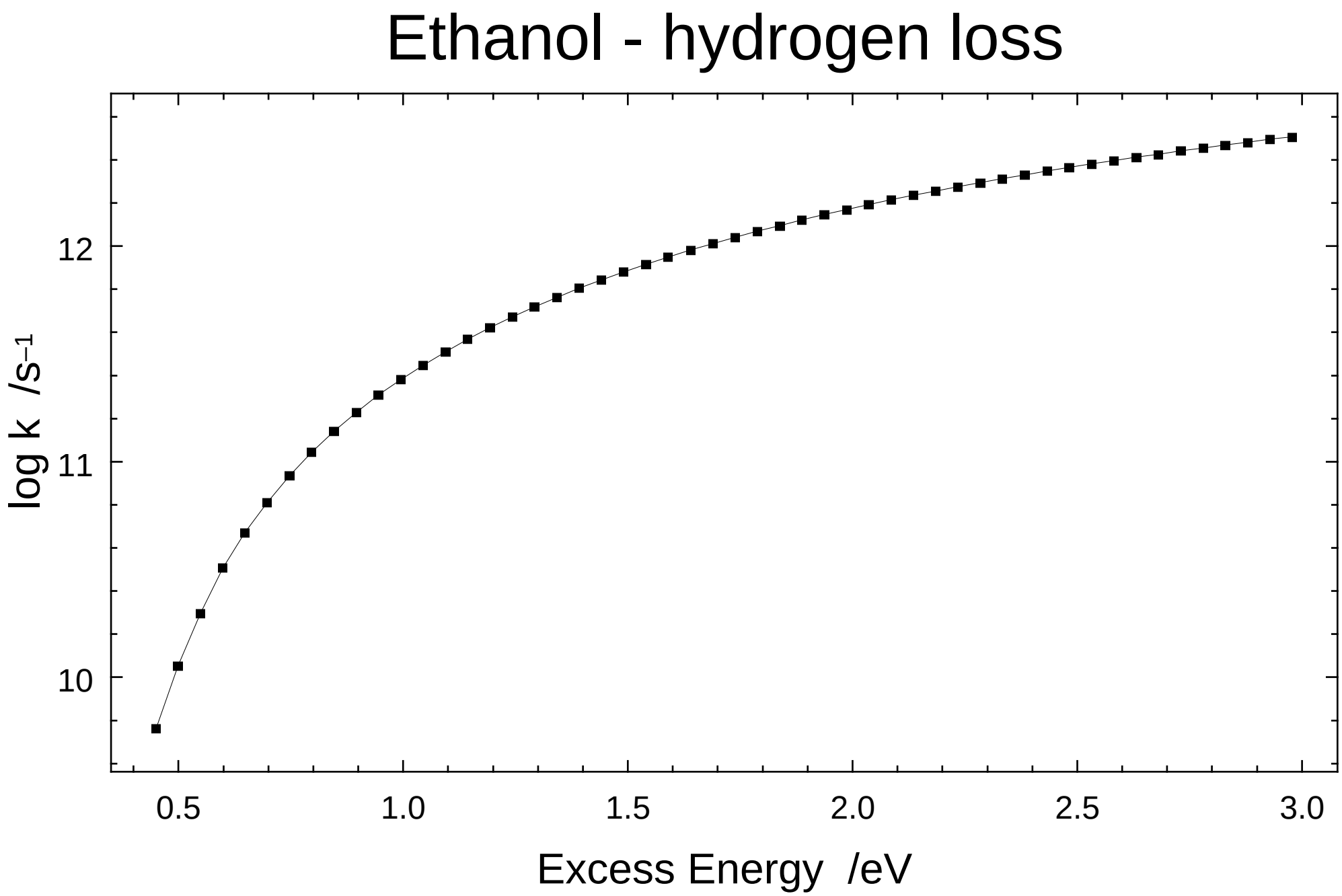
Ethanol - hydrogen loss
log k /s−1
12
11
10
0.5
1.0
1.5
2.0
2.5
3.0
Excess Energy /eV

Figure S5.

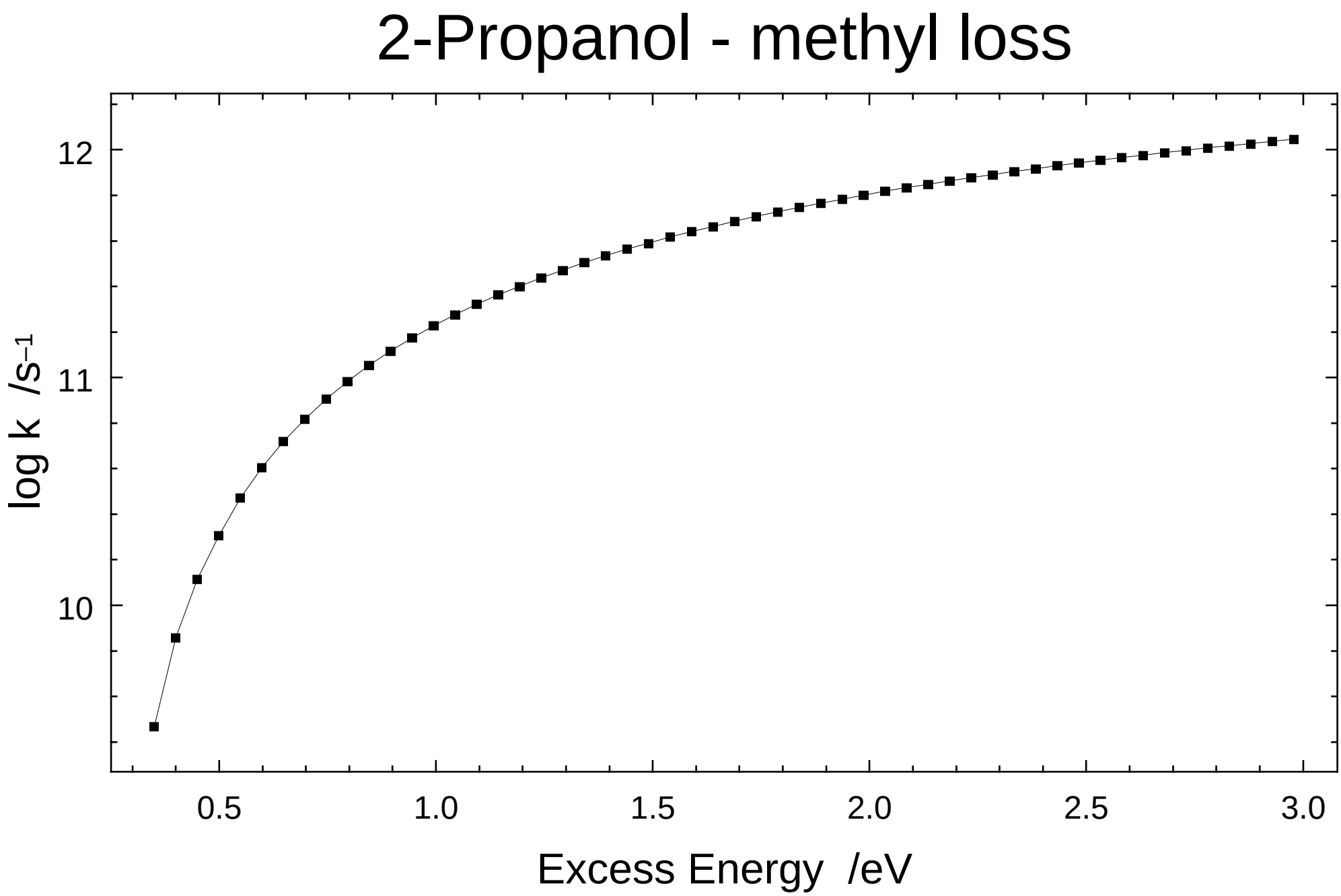
2-Propanol - methyl loss
log k /s–1
12
11
10
0.5
1.0
1.5
2.0
2.5
3.0
Excess Energy /eV

Figure S6.

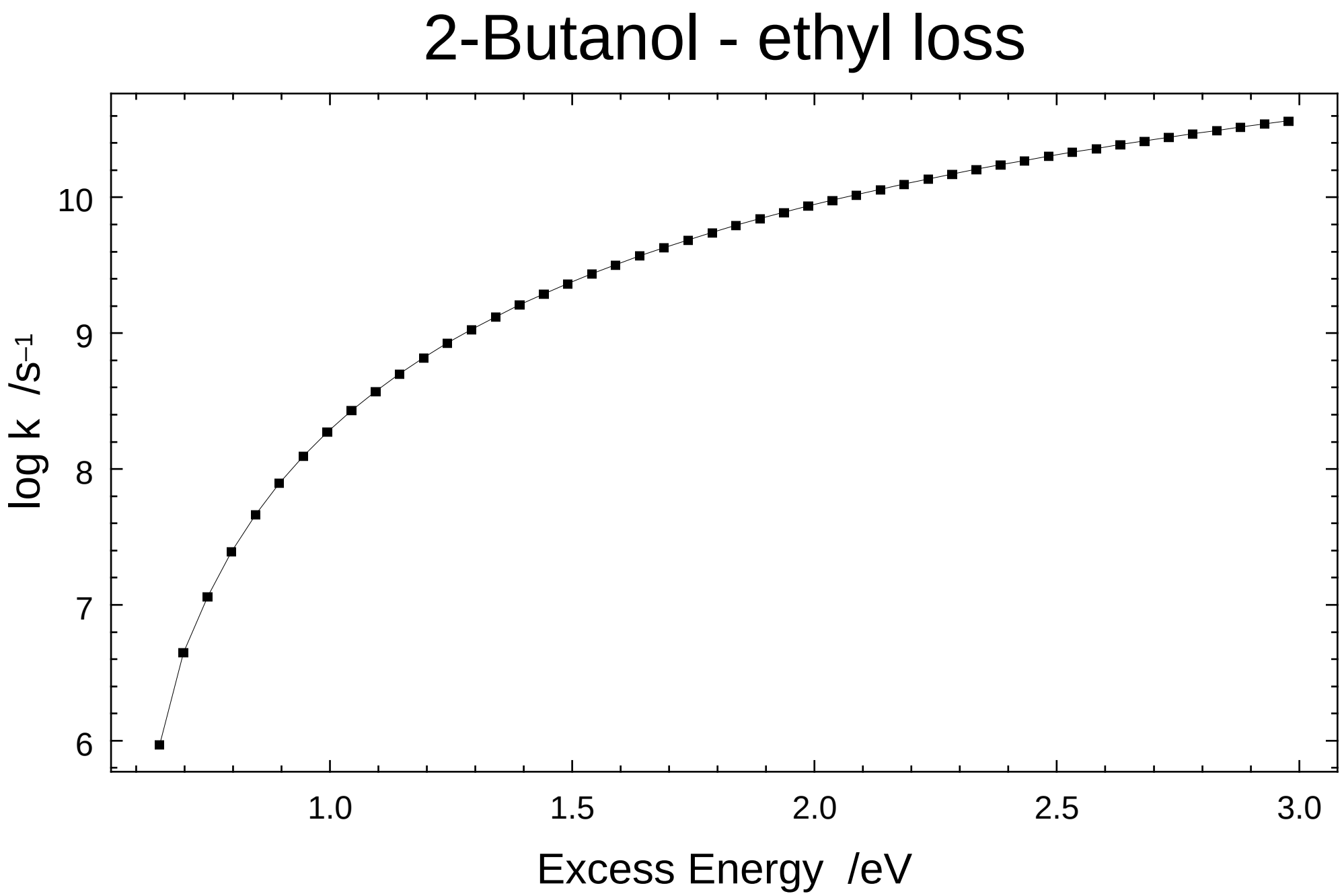
2-Butanol - ethyl loss
log k /s–1
10
9
8
7
6
1.0
1.5
2.0
2.5
3.0
Excess Energy /eV

Figure S7.

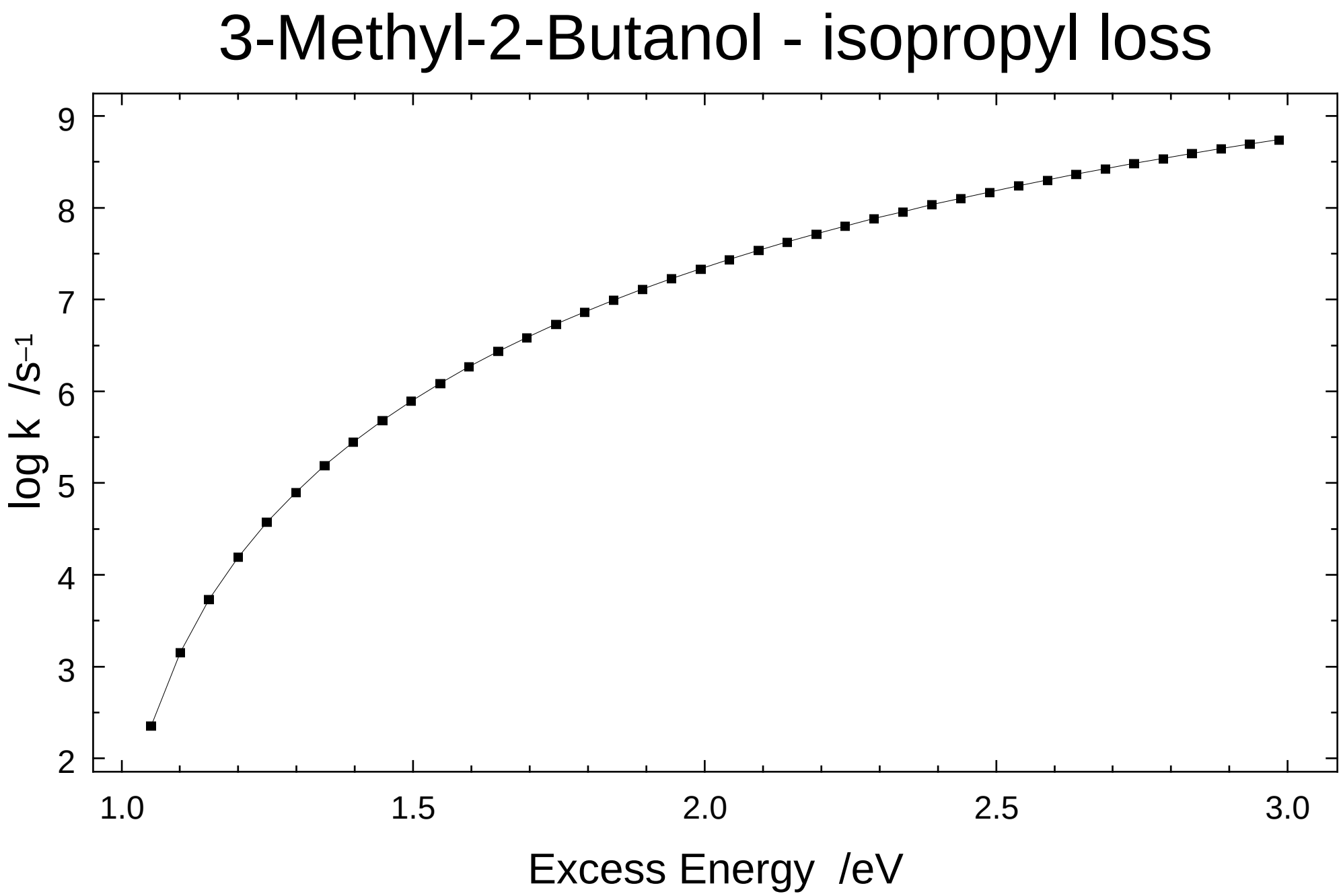
3-Methyl-2-Butanol - isopropyl loss
log k /s–1
9
8
7
6
5
4
3
2
1.0
1.5
2.0
2.5
3.0
Excess Energy /eV

Figure S8.

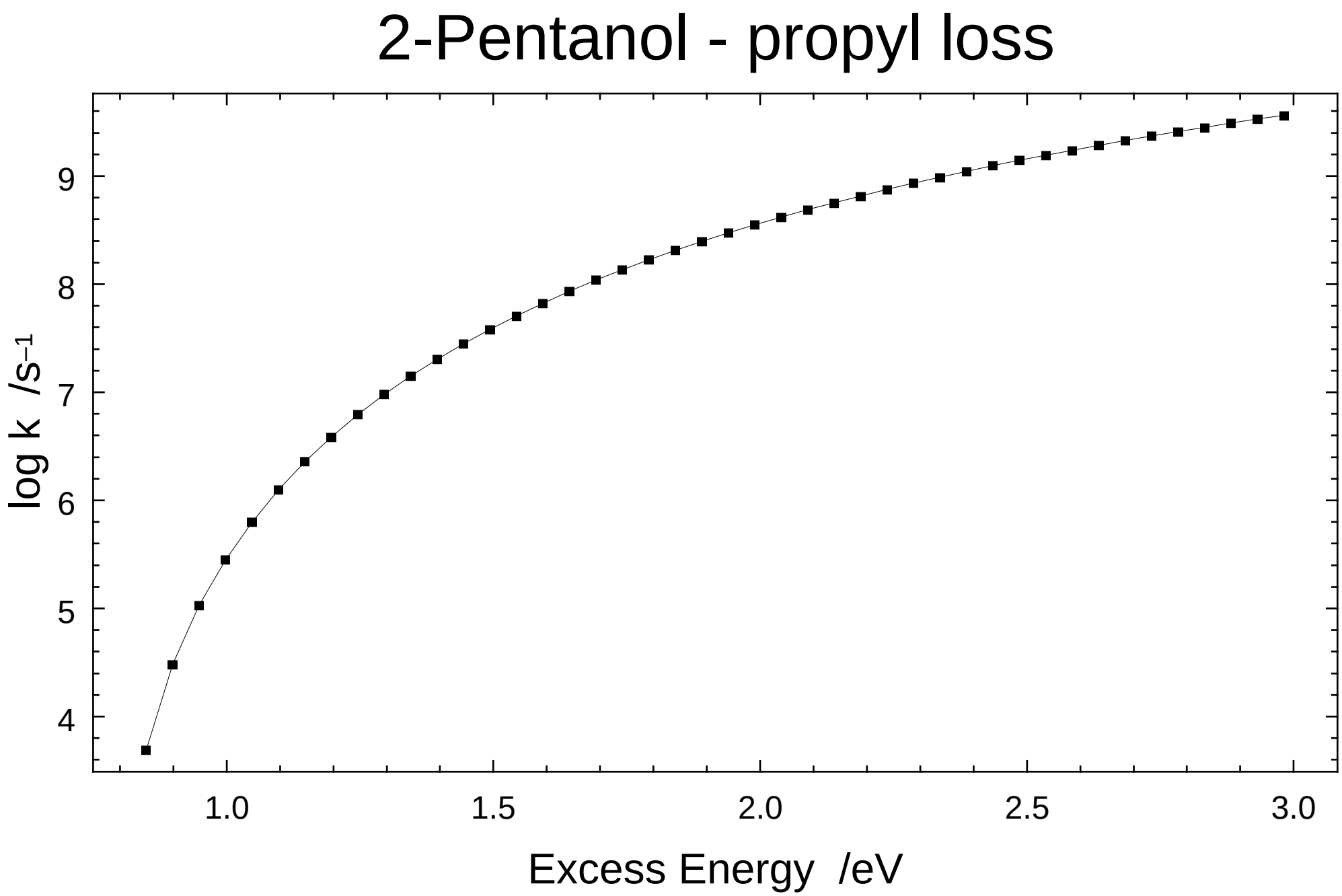
2-Pentanol - propyl loss
log k /s−1
9
8
7
6
5
4
1.0
1.5
2.0
2.5
3.0
Excess Energy /eV

Figure S9.

TABLE S1: Gaussian 0 K Energies

Molecule	H298-H0 (kJ/mol)	G3 0K energy (au)	G3B3 0K energy (au)	G2 0K energy (au)	G2(MP2) 0K energy (au)	CBS-APNO 0K energy (au)	W1U 0K energy (au)
CH_3CHOH^+ (anti)	13.4	-154.006556	-154.009734	-153.867951	-153.864336	-154.061967	-154.134813
CH_3CHO	12.9	-153.714796	-153.718193	-153.576848	-153.572975	-153.770771	-153.842898
t-$C_4H_9^+$	17.6	-157.362907	-157.366125	-157.180569	-157.176801	-157.414712	-157.458768
i-C_4H_8	16.8	-157.058913	-157.062303	-156.876343	-156.873030	-157.110608	-157.154314
ethanol	13.9	-154.904746	-154.908093	-154.764463	-154.760512		
$C_2H_5OH^{+\bullet}$	15.4	-154.523164	-154.525481	-154.382319	-154.378407		
H	6.2	-0.501003	-0.501087	-0.500000	-0.500000		
H-loss Transition State	13.8	-154.502554	-154.507762	-154.361590	-154.357681		
2-propanol	16.0	-194.183072	-194.186524	-193.996458	-193.991653		
$CH_3CH(CH_3)OH^{+\bullet}$	19.1	-193.811594	-193.815014	-193.625046	-193.620210		
CH_3	11.1	-39.793293	-39.793620	-39.745085	-39.743906		
CH_3-loss Transition State	17.1	-193.807773		-193.621408	-193.616553		
2-butanol	20.7	-233.453556	-233.458478	-233.221945	-233.216316		
$C_2H_5CH(CH_3)OH^{+\bullet}$	23.2	-233.096395	-233.101430	-232.864624	-232.858891		
C_2H_5	13.0	-79.063991	-79.065686	-78.970170	-78.968123		
C_2H_5-loss Transition State	20.7	-233.092507		-232.860753	-232.855033		
2-pentanol	24.3	-272.724539	-272.730172	-272.447408	-272.440957		
n-$C_3H_7CH(CH_3)OH^{+\bullet}$	26.3	-272.370465	-272.375655	-272.092399	-272.085877		
n-C_3H_7	15.6	-118.333913	-118.336443	-118.194457	-118.191643		
n-C_3H_7-loss Transition State	24.4	-272.351375		-272.073079	-272.066665		
3-methyl-2-butanol	24.1	-272.726306	-272.731883	-272.449311	-272.442877		
i-$C_3H_7CH(CH_3)OH^{+\bullet}$	26.5	-272.380206	-272.385529	-272.102879	-272.096248		
i-C_3H_7	16.0	-118.338136	-118.340882	-118.198873	-118.195958		