

Measurement of surface area of molecular sieves using BET theory

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Starting from

$$E_t = \frac{1}{ak} \frac{E_0 - E_t}{t} + E_\infty \quad (1)$$

It is deduced that

$$E_t = \frac{E_0 + akE_\infty t}{1 + akt} \quad (2)$$

Thanks to machine learning integrated in *Mathematica*, the coefficients can be derived out immediately:

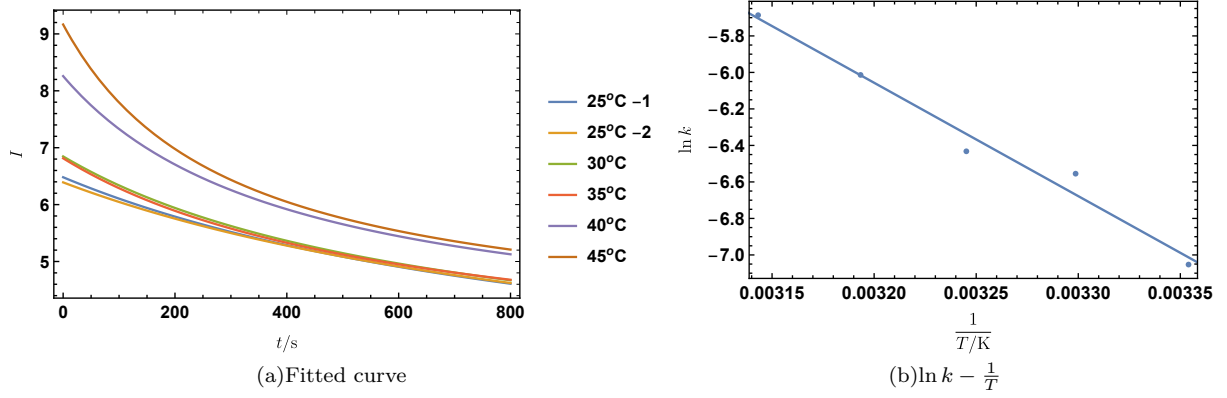
```
In[377]:= c1 /. (NonlinearModelFit[#, (-c2 + c1 c3 t)/(
  1 + c1 t), {c1, c2, c3}, t][
  "BestFitParameters"] & /@ (Transpose[{Range[Length
    [#]] +
    1, #}] & /@ react))

Out[377]= {0.000951675, 0.000865023, 0.00142327,
  0.0016089, \
  0.0024449, 0.00339182}
```

which is equivalent to the result shown in Table.I.

TABLE I. The fitting result of the reaction rate constant

$T/^{\circ}\text{C}$	25	30	35	40	45	
k	0.09517	0.08650	0.1423	0.1609	0.2445	0.3392

FIG. 1. The fitted curve of the reaction process with a fit of k according to Arrhenius equation