

SUPPORTING INFORMATION

Thermodynamics of the CMMS approach and carbon surface chemistry in SO₂ adsorption

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1. Fitting of the data by Toth adsorption isotherm equation:

$$a = a_m \frac{Kh}{\left(1 + (Kh)^t\right)^{\frac{1}{t}}}$$

Table 1S. The results of the fitting of SO₂ adsorption data by Toth equation.

Carbon	a_m [mmole g ⁻¹]	K	t	DC
DH11733	21.04	43.09	0.3909	0.9993
DHe11733	15.46	61.65	0.4485	0.9988
DHe10233	19.15	75.91	0.3808	0.9994
DHe5733	15.00	62.96	0.4570	0.9992
DN10233	26.06	51.57	0.3761	0.9992
DN10236	25.81	47.46	0.3629	0.9987
DN10239	18.35	62.45	0.4158	0.9982
DN11733	50.00 ^{*)}	19.69	0.3026	0.9984
DN11736	50.00 ^{*)}	6.787	0.3975	0.9985
DN14233	25.53	24.57	0.3674	0.9997

^{*)} the upper limit of the parameter assumed during the fitting, note that due to the shapes of the isotherms the algorithm behaves in such a way that a_m is increased for some cases up to the upper limit (sometimes unphysical) and K and t decrease at the same time.

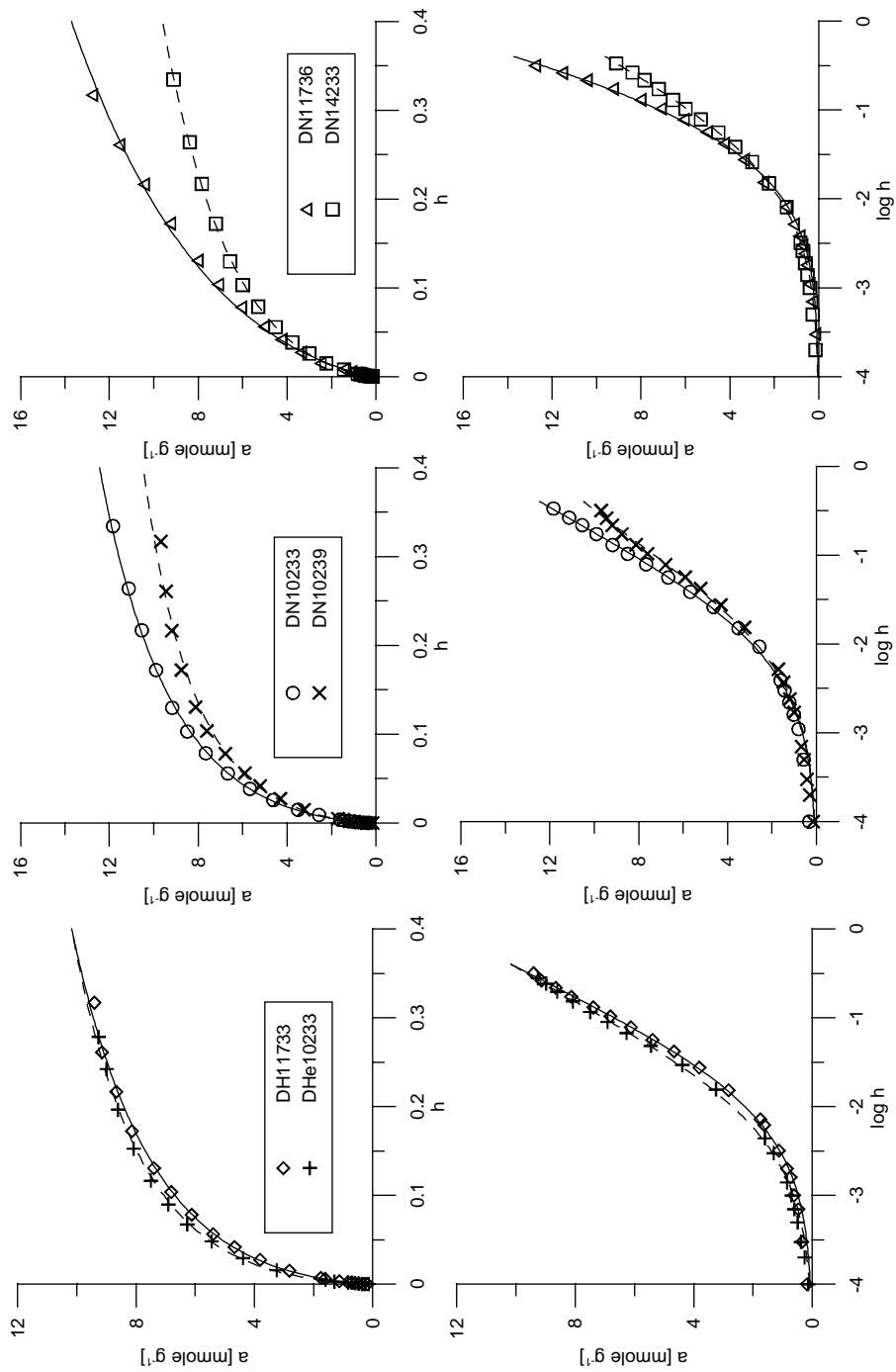


Figure 1S. The results of the fitting of adsorption isotherm applying the Toth model.

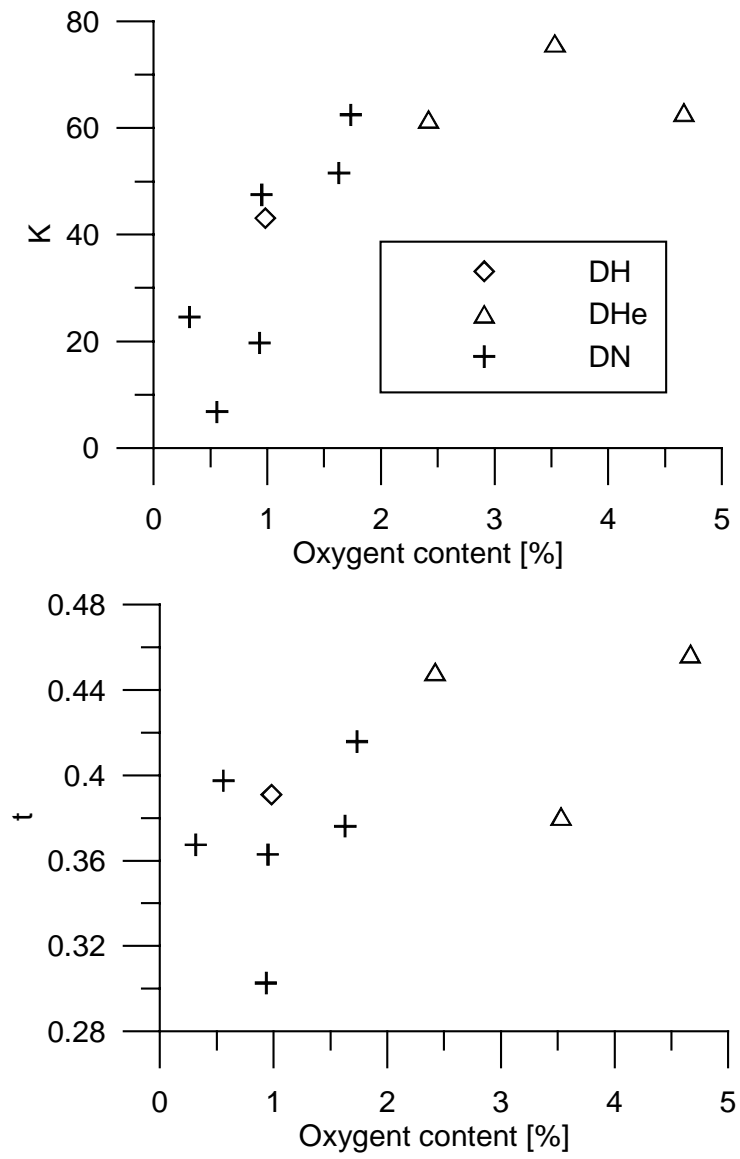


Figure 2S. The correlations as shown in the paper but for the parameters obtained from Toth adsorption isotherm equation.

2. Fitting of the data by BET adsorption isotherm equation:

$$a = \frac{a_m Ch}{(1-h)[1+(C-1)h]}$$

Table 2S. The results of the fitting of SO₂ adsorption data by BET equation.

Carbon	a_m [mmole g ⁻¹]	C	DC
DH11733	7.142	44.26	0.9949
DHe11733	6.866	59.45	0.9920
DHe10233	7.253	56.84	0.9953
DHe5733	6.932	59.33	0.9950
DN10233	8.672	48.27	0.9937
DN10236	7.958	44.28	0.9919
DN10239	7.432	56.20	0.9910
DN11733	8.569	25.20	0.9944
DN11736	9.795	17.38	0.9973
DN14233	6.672	32.65	0.9970

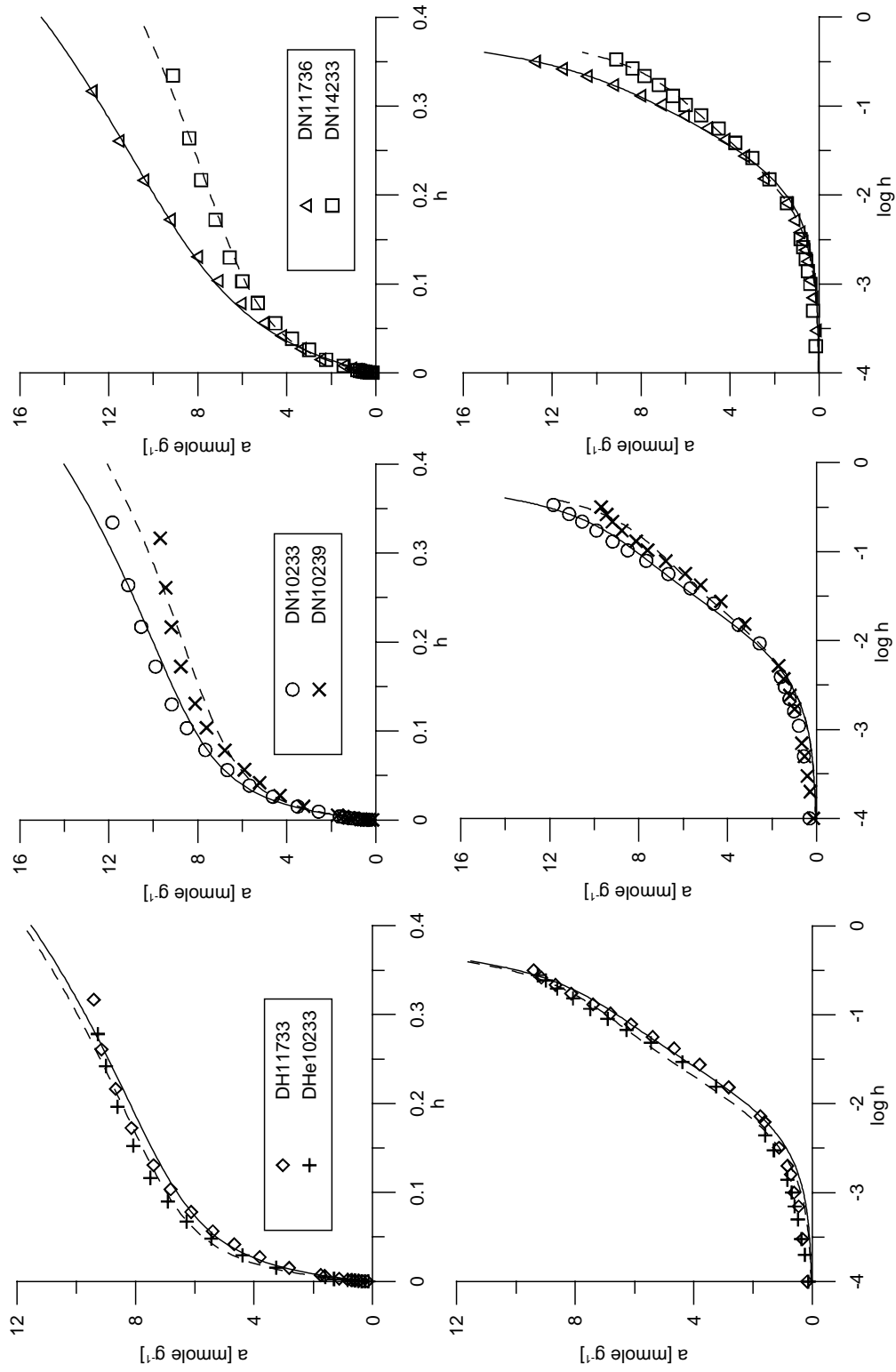


Figure 3S. The results of the fitting of adsorption isotherm applying the BET model.

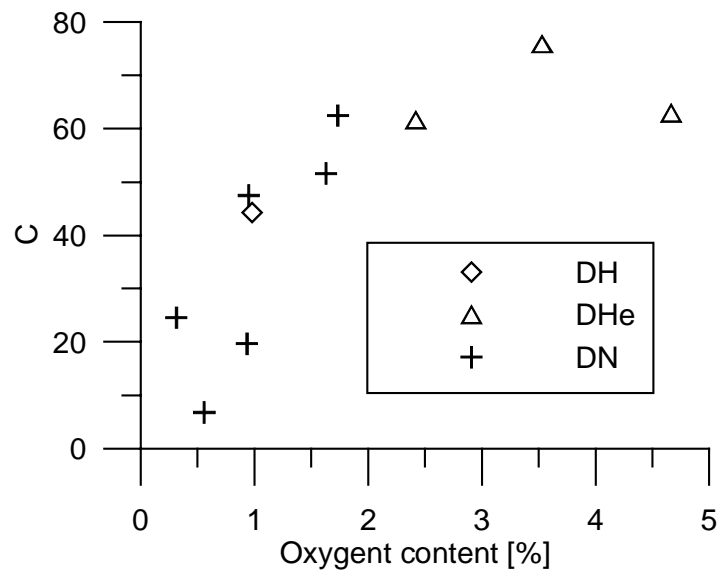


Figure 4S. The correlations as shown in the paper but for the C parameter of the BET adsorption isotherm equation.

3. Fitting the data of Beebe and Dell:

[Beebe, R.A.; Dell, R.M. *J. Phys. Chem.* **1955**, *59*, 746.]

Table 3S. The results of the fitting of SO₂ adsorption data on carbon blacks by CMMS equation.

Spheron	a_m [cm ³ (STP) g ⁻¹]	K_0	K_1	K_{as}	DC
(1000 °)	21.25	3.816	4.501	0.4661	0.9993
(1500 °)	14.87	2.469	6.536	0.6213	0.9997
(2700 °)	13.06	1.341	6.968	0.6872	0.9997

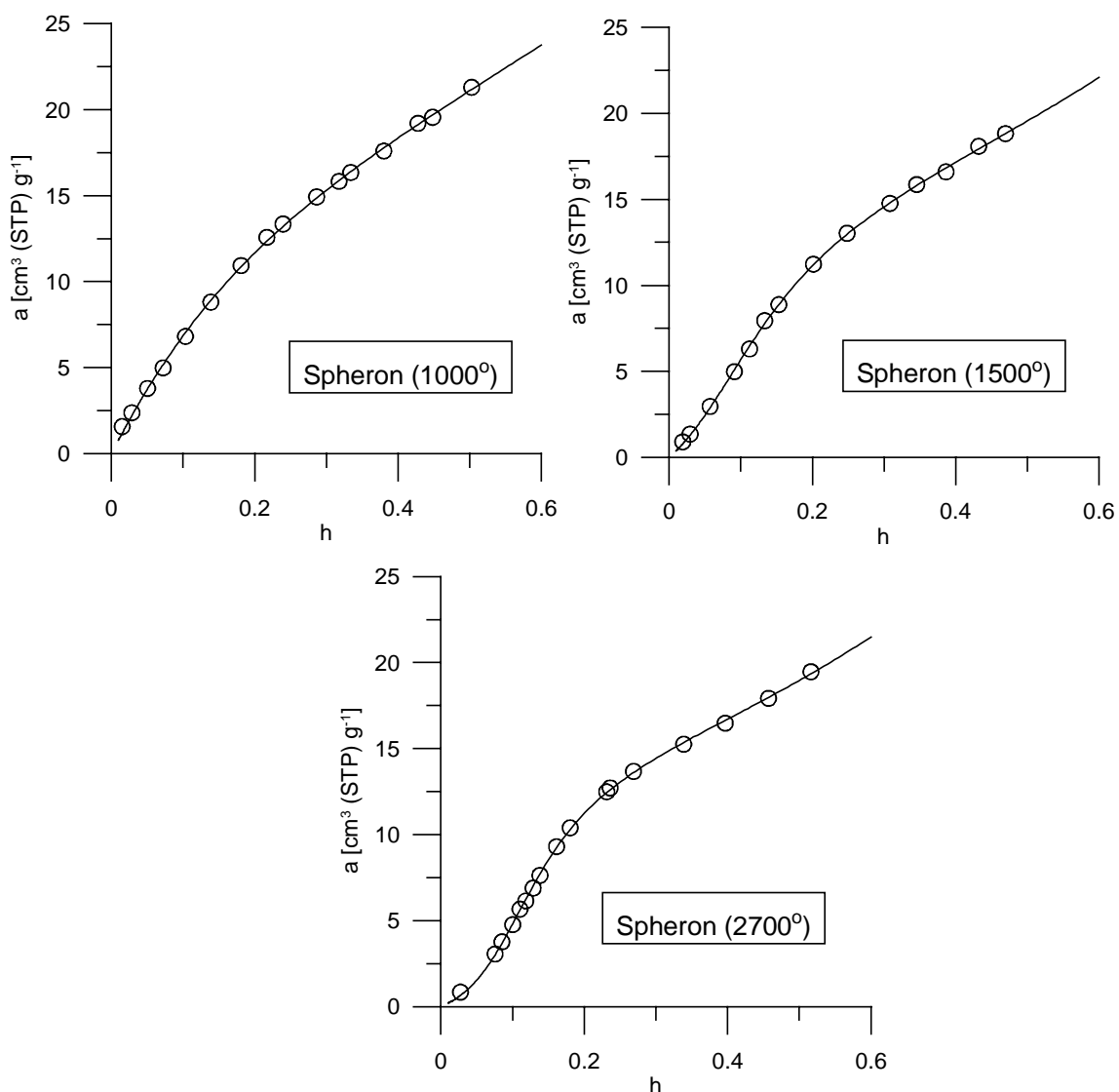


Figure 5S. The results of the fitting of adsorption isotherms on carbon black reported by Beebe and Dell applying the CMMS model.

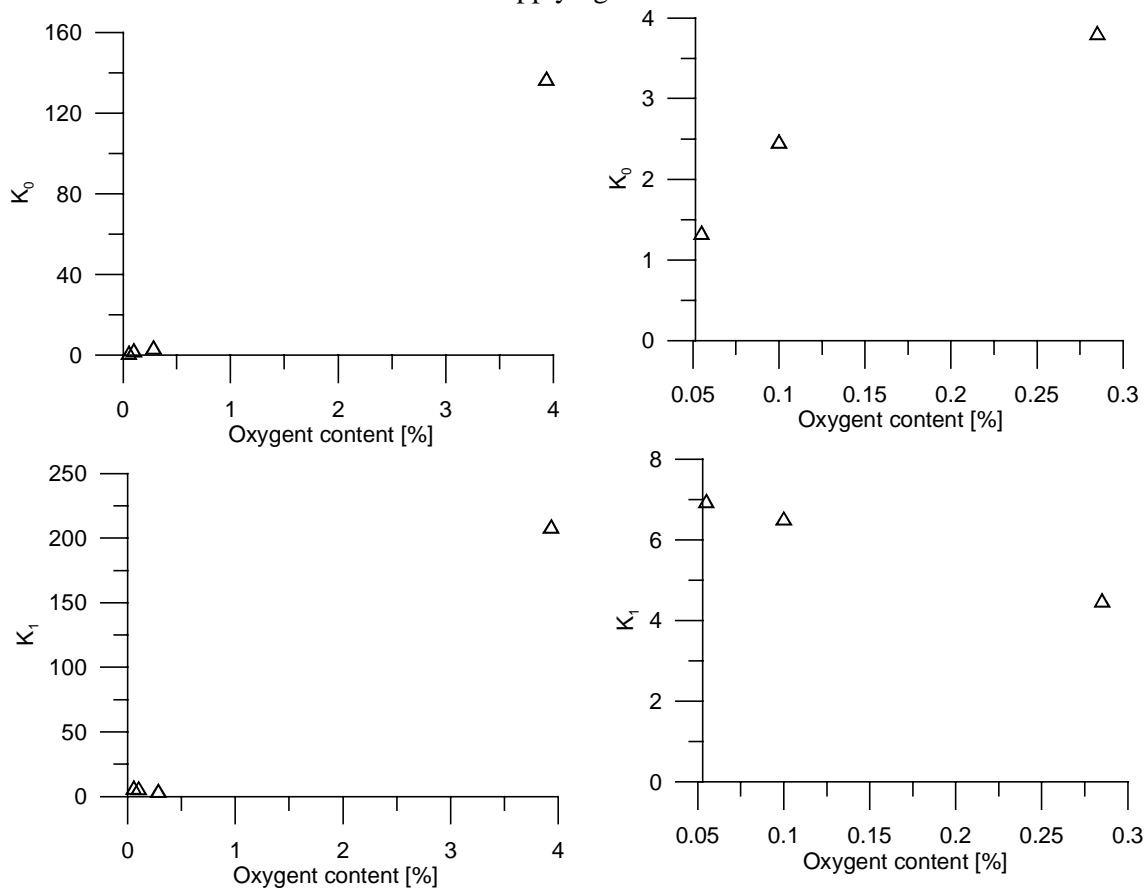


Figure 6S. The correlations as shown in the paper but for the data reported by Beebe and Dell.