Supplementary Information for

Christoph Buttersack

Modeling of type IV and V sigmoidal adsorption isotherms

appeared in PCCP 2019

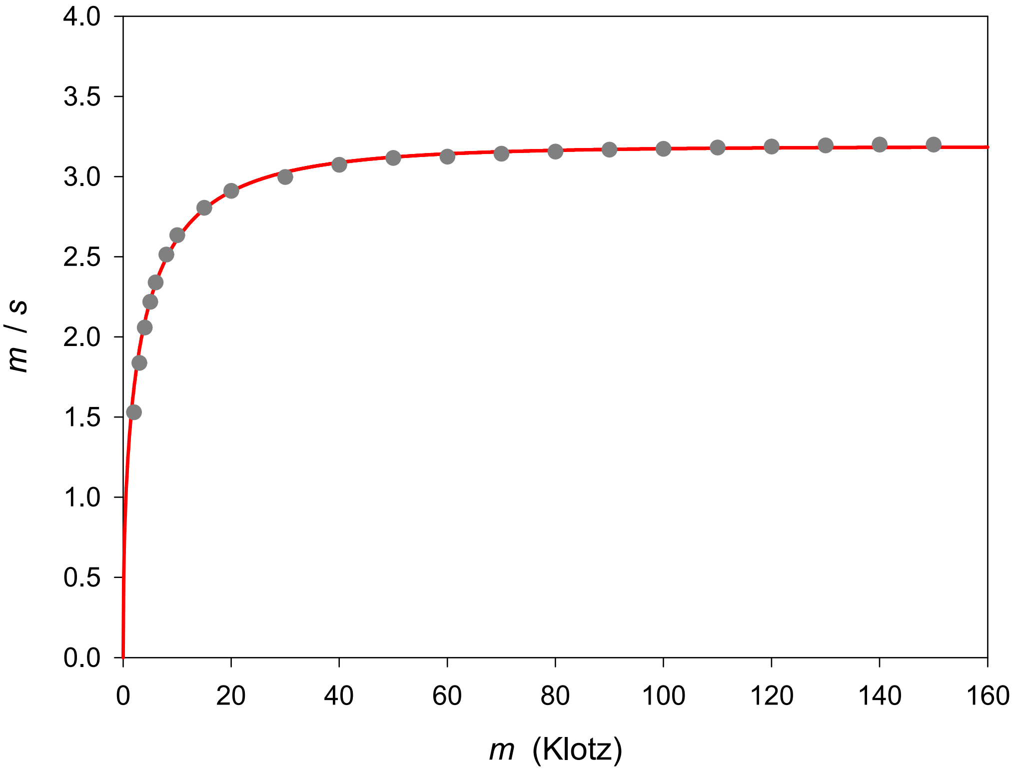

Figure A1: Conversion of the exponent m of the Klotz equation (20) to the exponent s of the Sips isotherm (eqn. 12) from non-linear regression in the range of θ = 0.2.... 0.8.

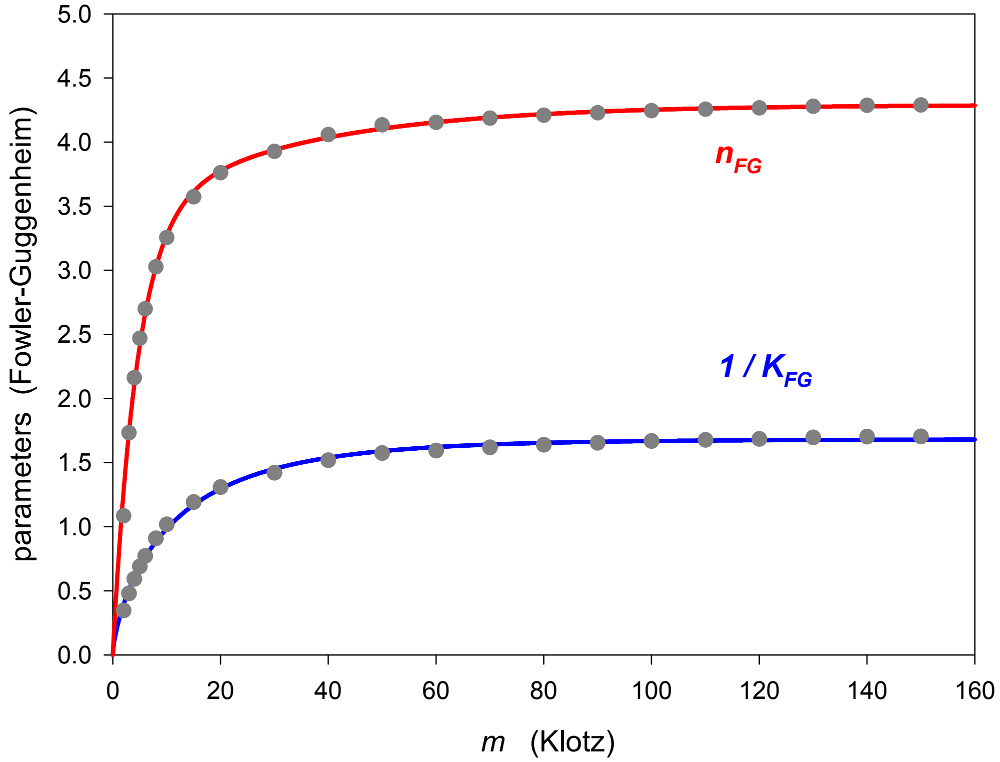

Figure A2: Conversion of the parameter *m* of the Klotz equation (20) to the adsorption constant K_{FG} and the exponent *n* of the Fowler-Guggenheim equation (4) from non-linear regression in the range of θ = 0.2.... 0.8..

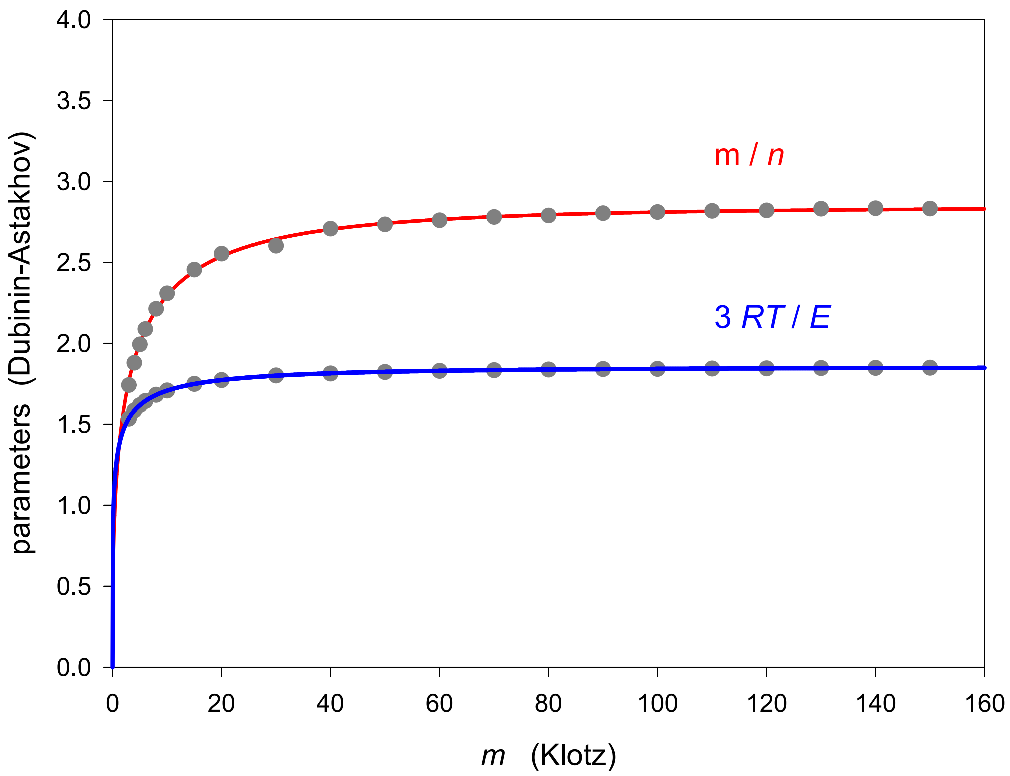

Figure A3: Conversion of the parameters *m* of the Klotz equation (20) **with *K* = 5** to the energy term *E* / RT and the exponent *n* of the Dubinin-Asthakov equation (13) from non-linear regression in the range *of* θ = 0.2.... 0.8.

$m / n = 2.84\ (1\text{-}\exp(-0.60\ m^{0.44}))$; $RT / E = 0.618\ (1\text{-}\exp(-1.27\ m^{0.30}))$

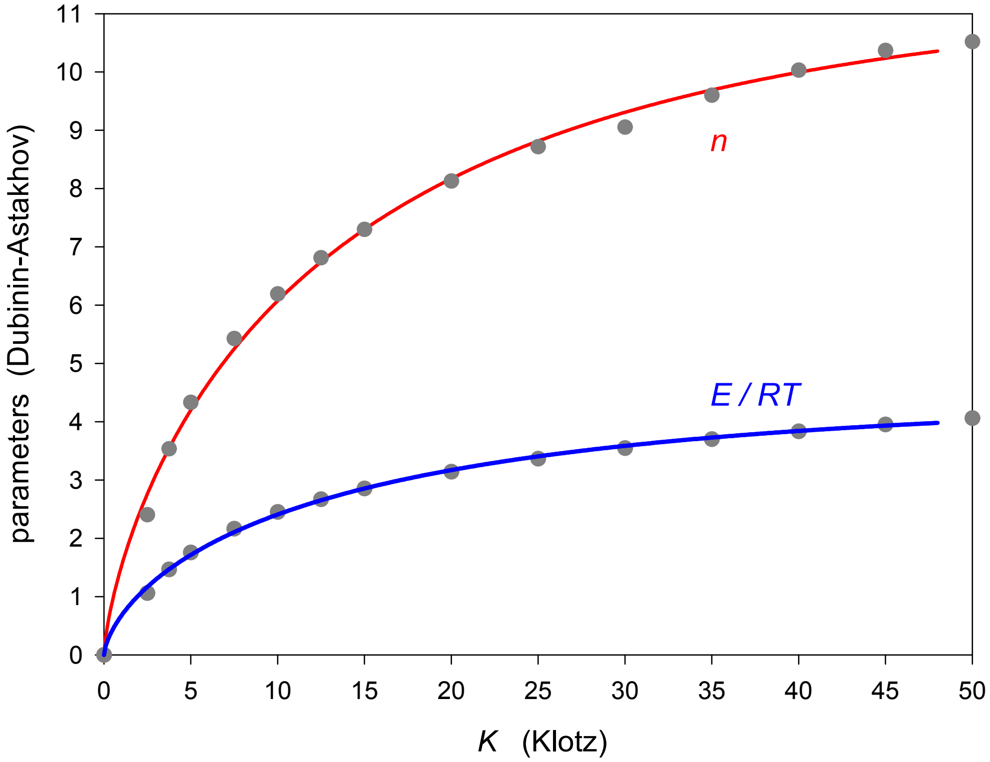

Figure A4: Conversion of the parameters K of the Klotz equation (20) **with m = 10** to the energy term E / RT and the exponent n of the Dubinin-Asthakov equation (13) from non-linear regression in the range of θ = 0.2.... 0.8.

$n = 11.4\ (1\text{-}\exp(-0.14\ K^{0.73}))$; $E / RT = 4.4\ (1\text{-}\exp(-0.16\ K^{0.68}))$

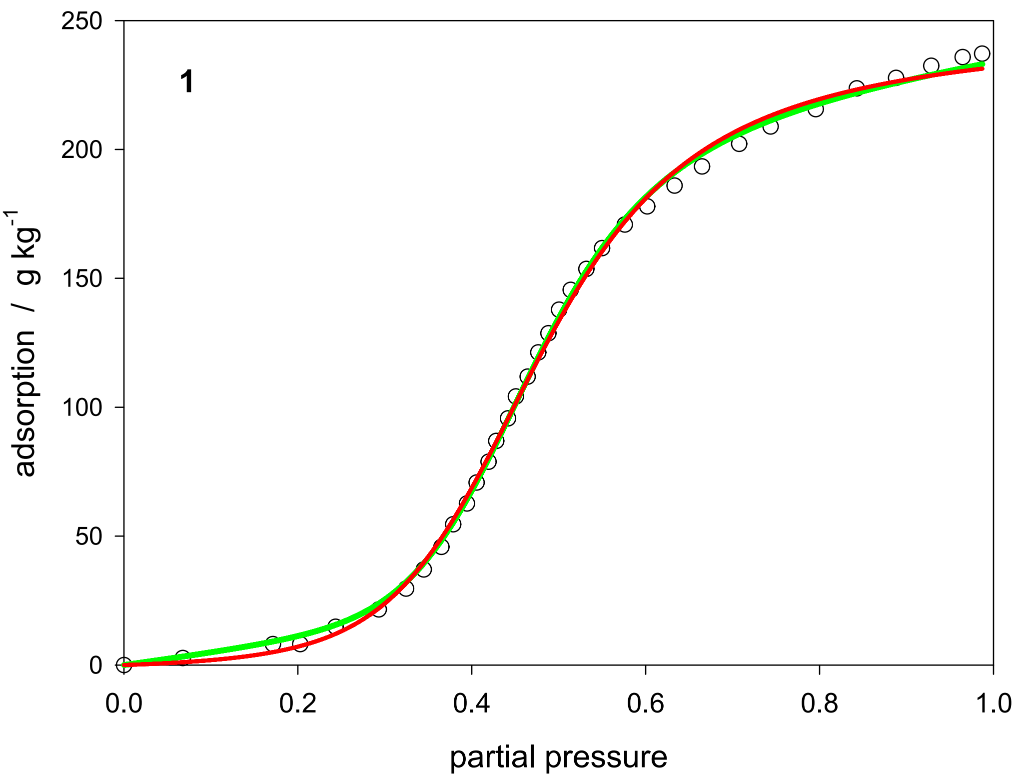

Figure A5: Modeling of the adsorption of water on carbon no. 1 with the Klotz isotherm (eqn. (24)), green line: modeled with eqn. (31)

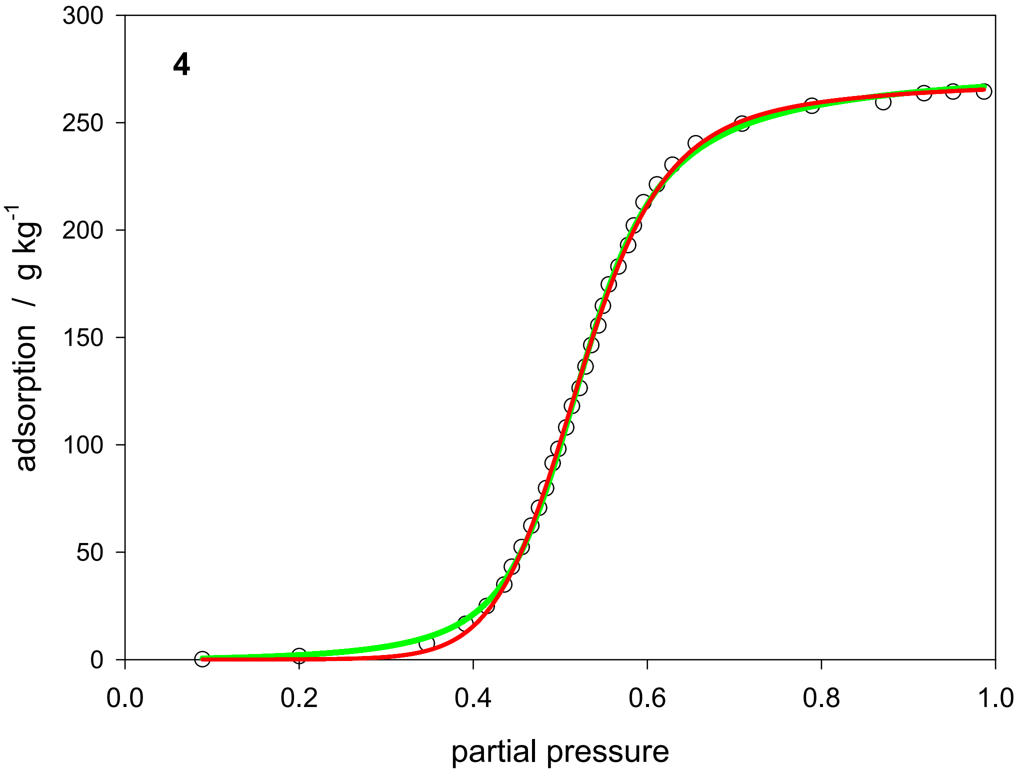

Figure A6: Modeling of the adsorption of water on carbon no. 4 with the Klotz isotherm (eqn. (24)), green line: modeled with eqn. (31).

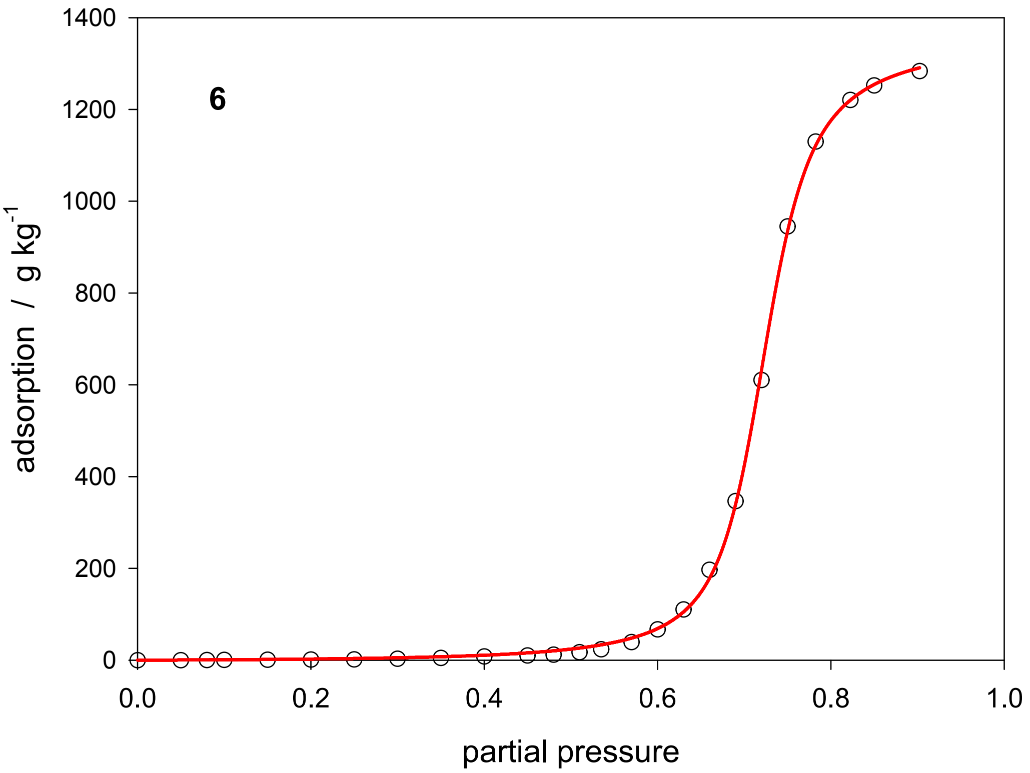

Figure A7: Modeling of the adsorption of water on carbon no. 6 with the Klotz isotherm (eqn. (24)).

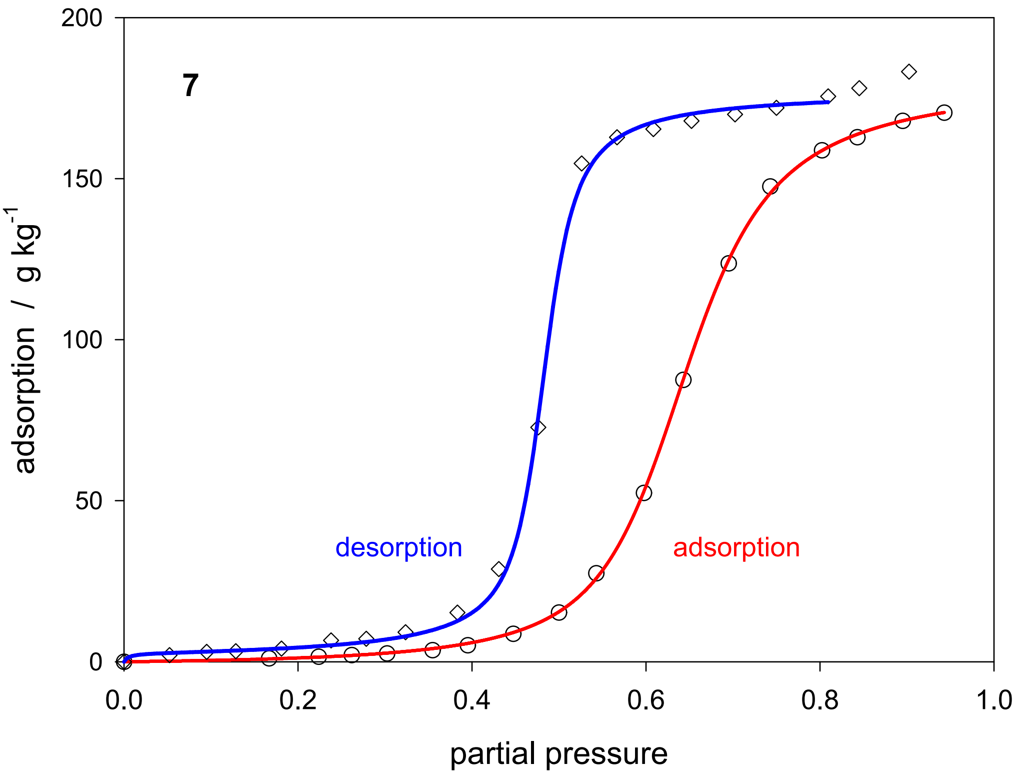

Figure A8: Modeling of the adsorption desorption hysteresis of water on carbon no. 7 with the Klotz isotherm (eqn. (24))

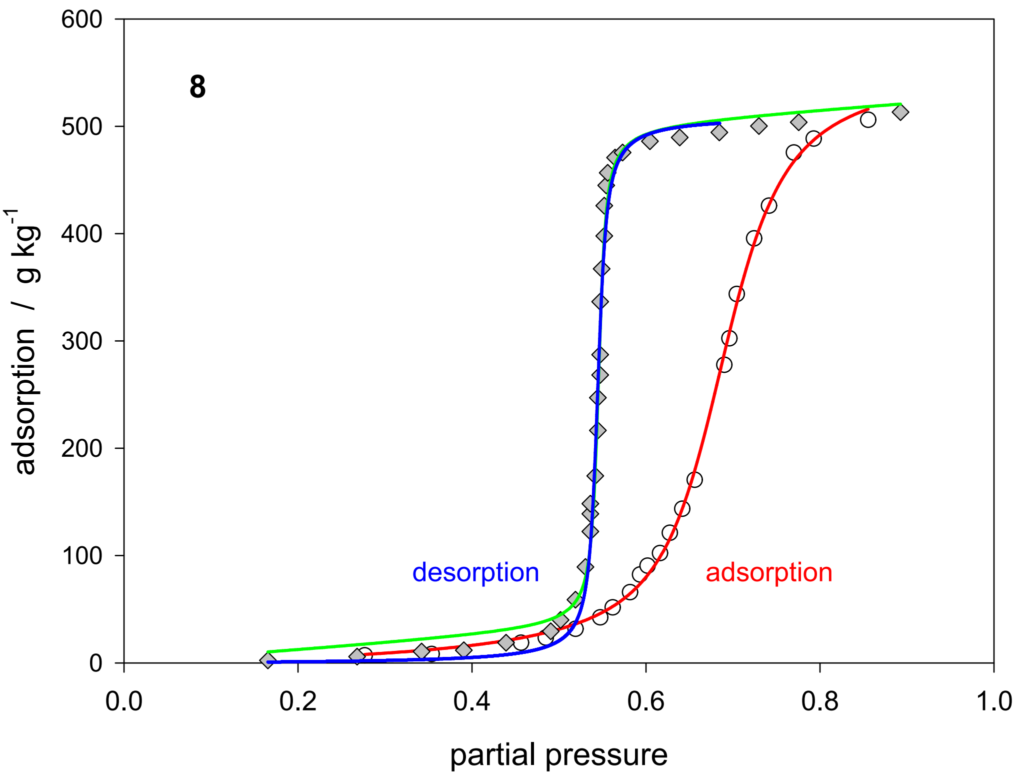

Figure A9: Modeling of the adsorption desorption hysteresis of water on carbon no. 8 with the Klotz isotherm (eqn. (24)), green line: desorption modeled with eqn. (29)

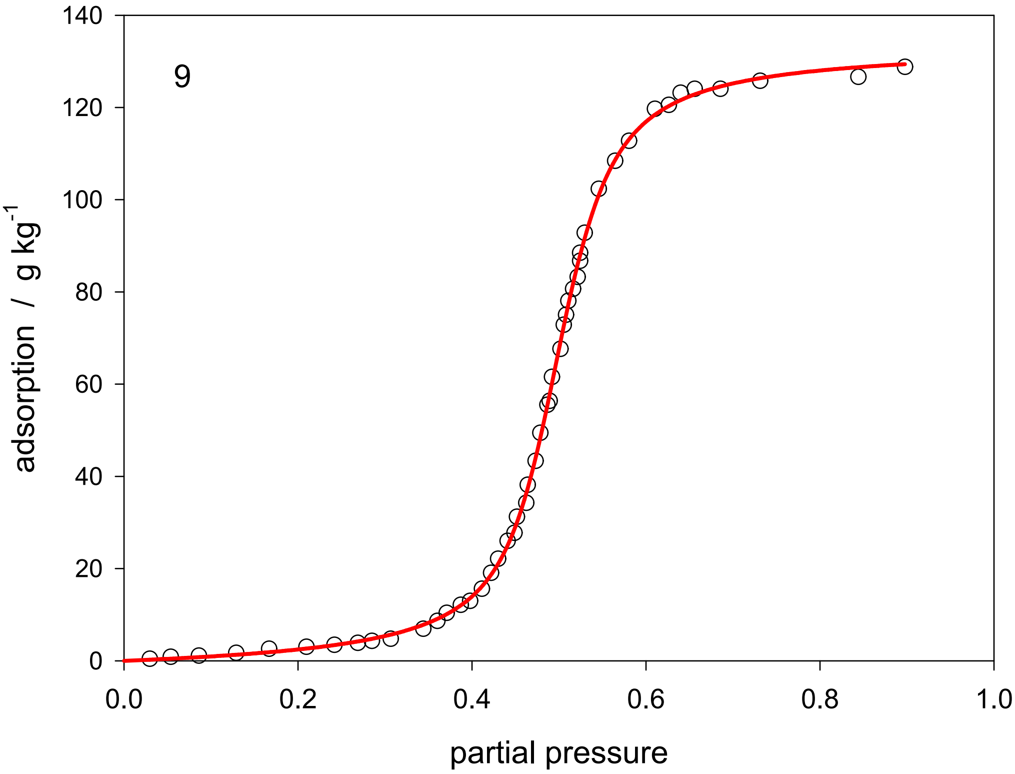

Figure A10: Modeling of the adsorption of water on carbon no. 9 with the Klotz isotherm (eqn. (24)).

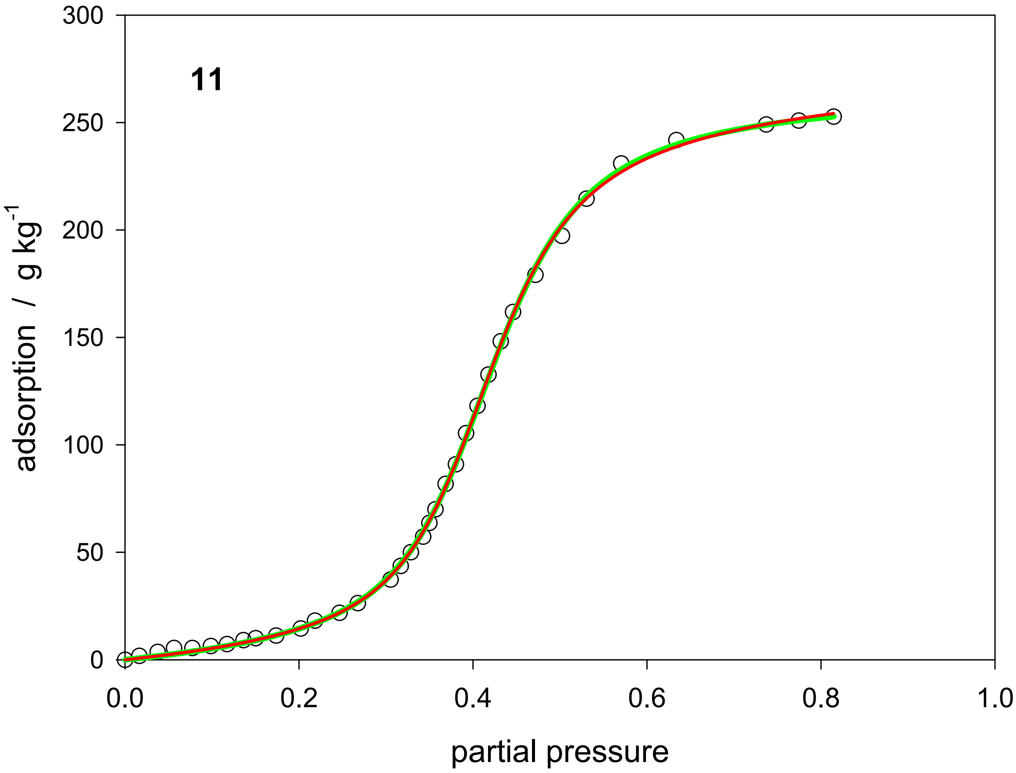

Figure A11: Modeling of the adsorption of water on carbon no. 11 with the Klotz isotherm (eqn. (24)), green line: modeled with eqn. (31).

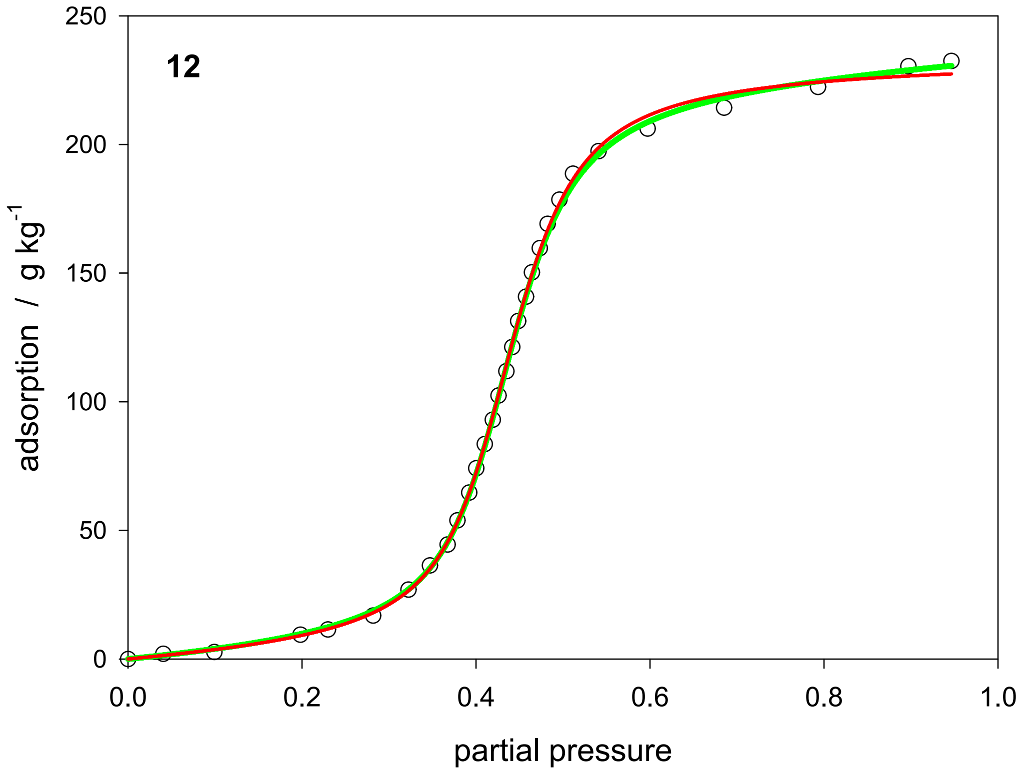

Figure A12: Modeling of the adsorption of water on carbon no. 12 with the Klotz isotherm (eqn. (24)), green line: modeled with eqn. (31).

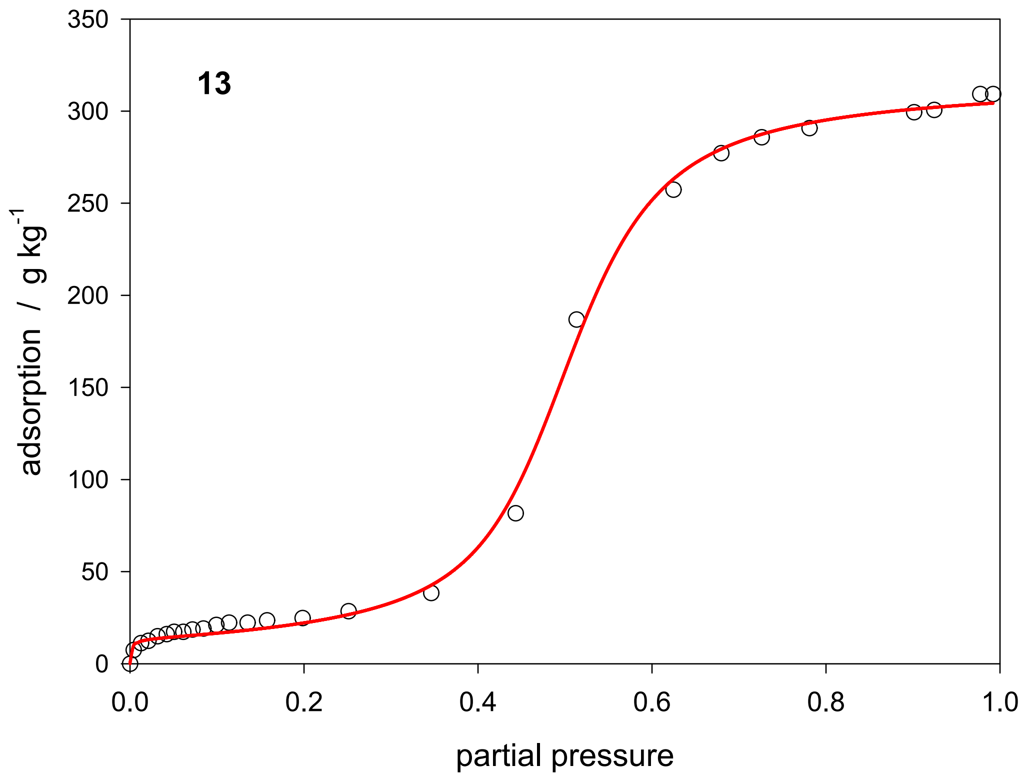

Figure A13: Modeling of the adsorption of water on carbon no. 13 with the Klotz isotherm (eqn. (24)).

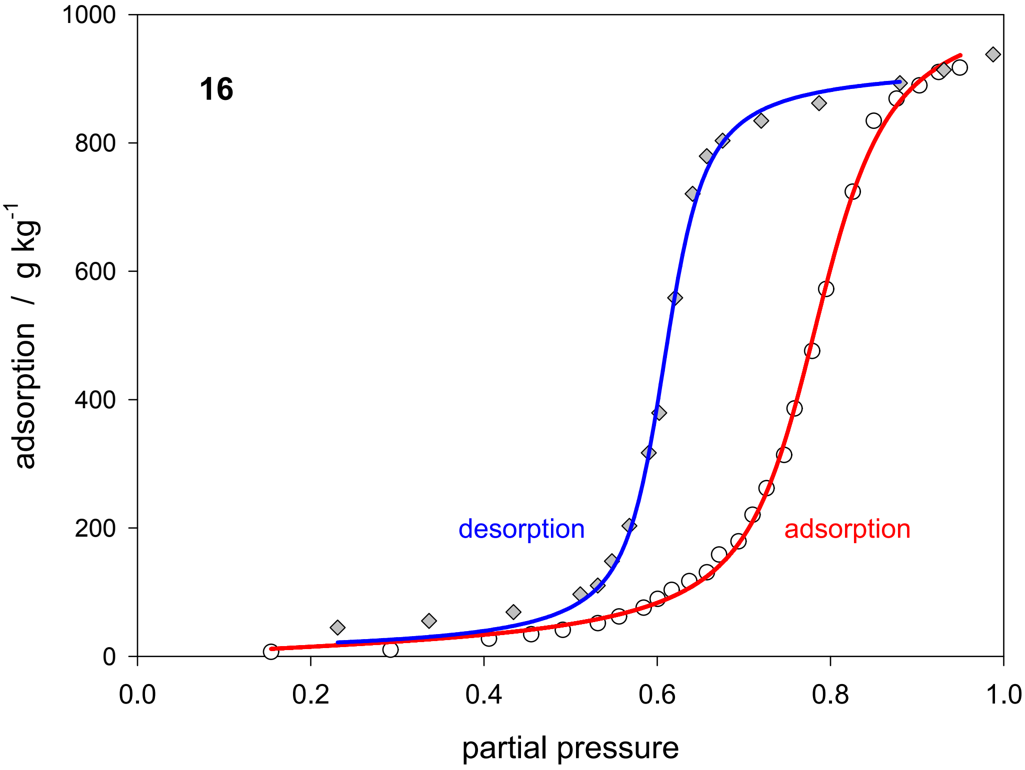

Figure A14: Modeling of the adsorption desorption hysteresis of water on carbon no. 16 with the Klotz isotherm (eqn. (24))

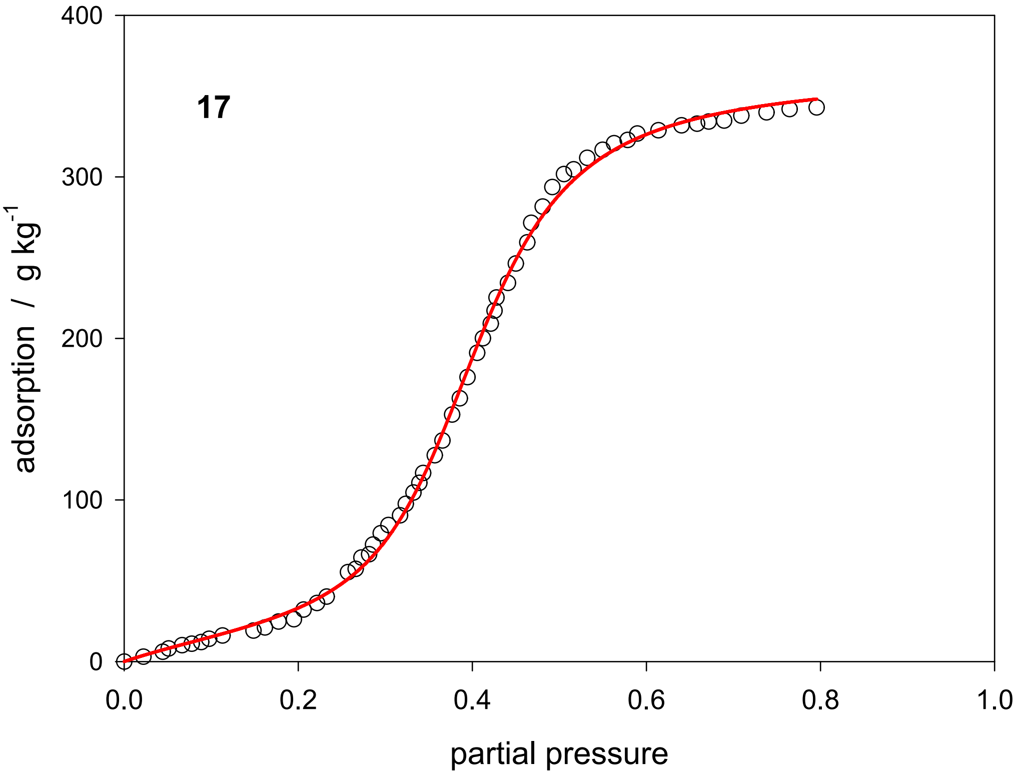

Figure A15: Modeling of the adsorption of water on carbon no. 17 with the Klotz isotherm (eqn. (24)).

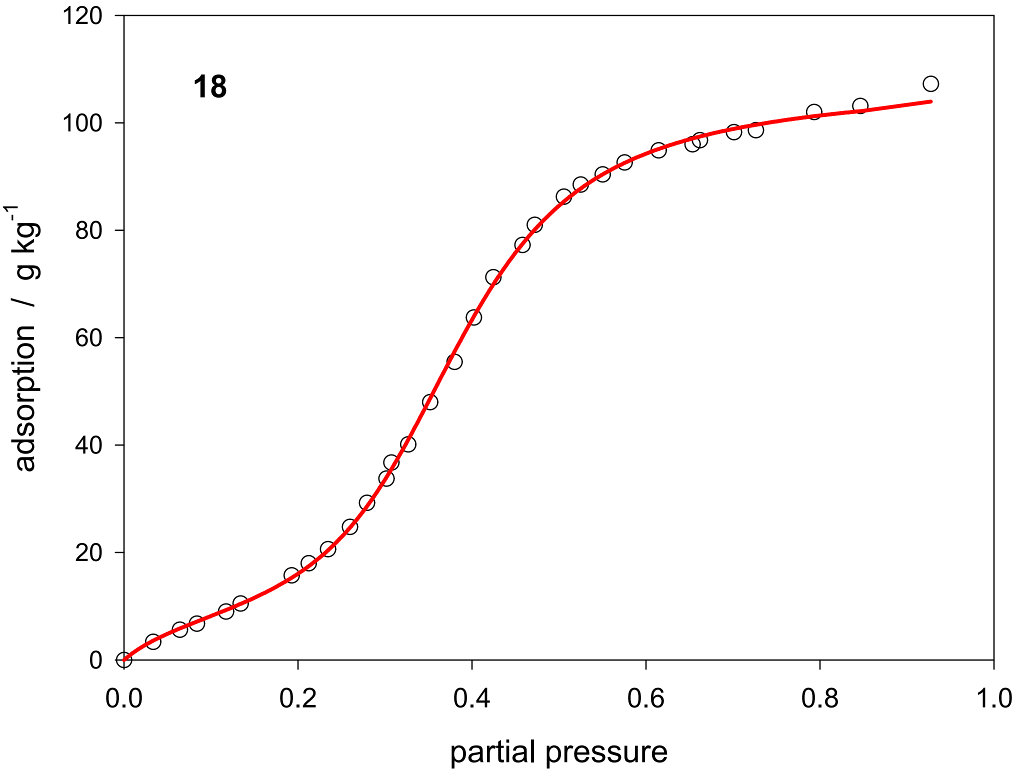

Figure A16: Modeling of the adsorption of water on carbon no. 18 with the Klotz isotherm (eqn. (24)).

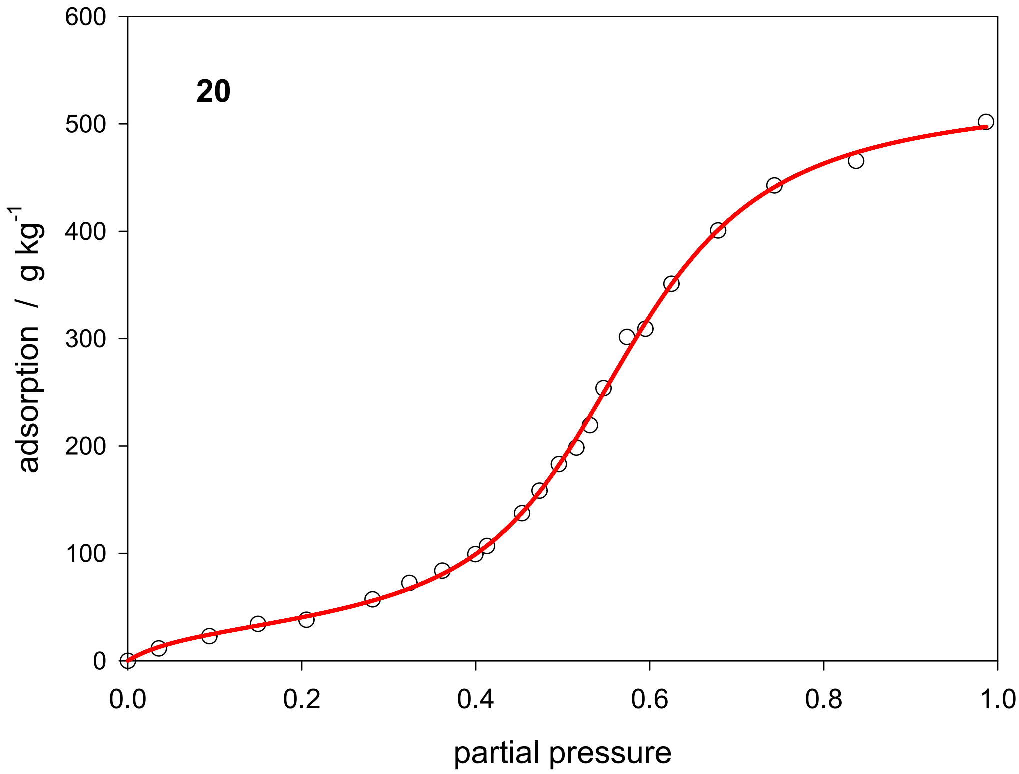

Figure A17: Modeling of the adsorption of water on carbon no. 20 with the Klotz isotherm (eqn. (24)).

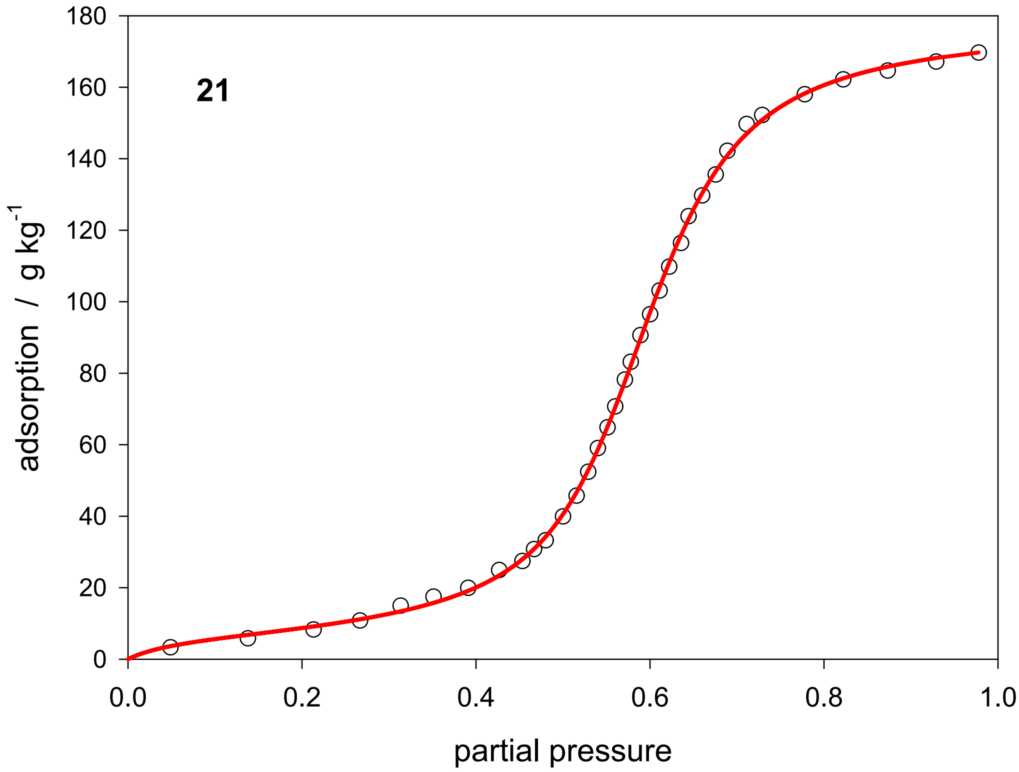

Figure A18: Modeling of the adsorption of water on carbon no. 21 with the Klotz isotherm (eqn. (24)).

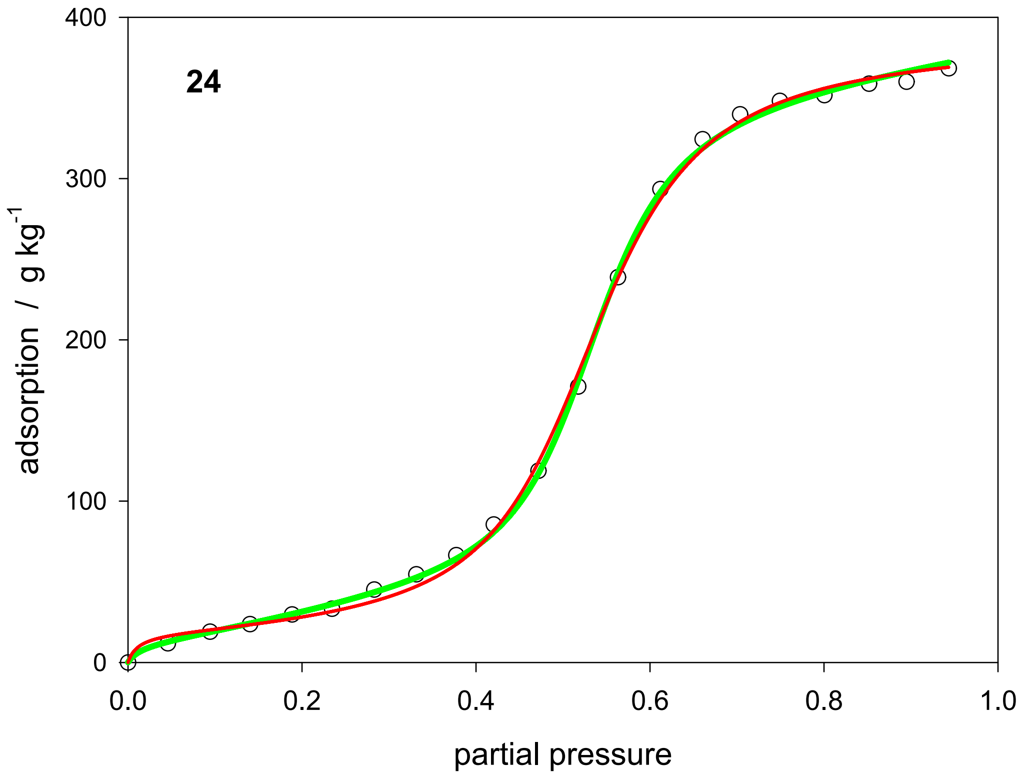

Figure A19: Modeling of the adsorption of water on carbon no. 24 with the Klotz isotherm (eqn. (24)), green line: modeled with eqn. (31)

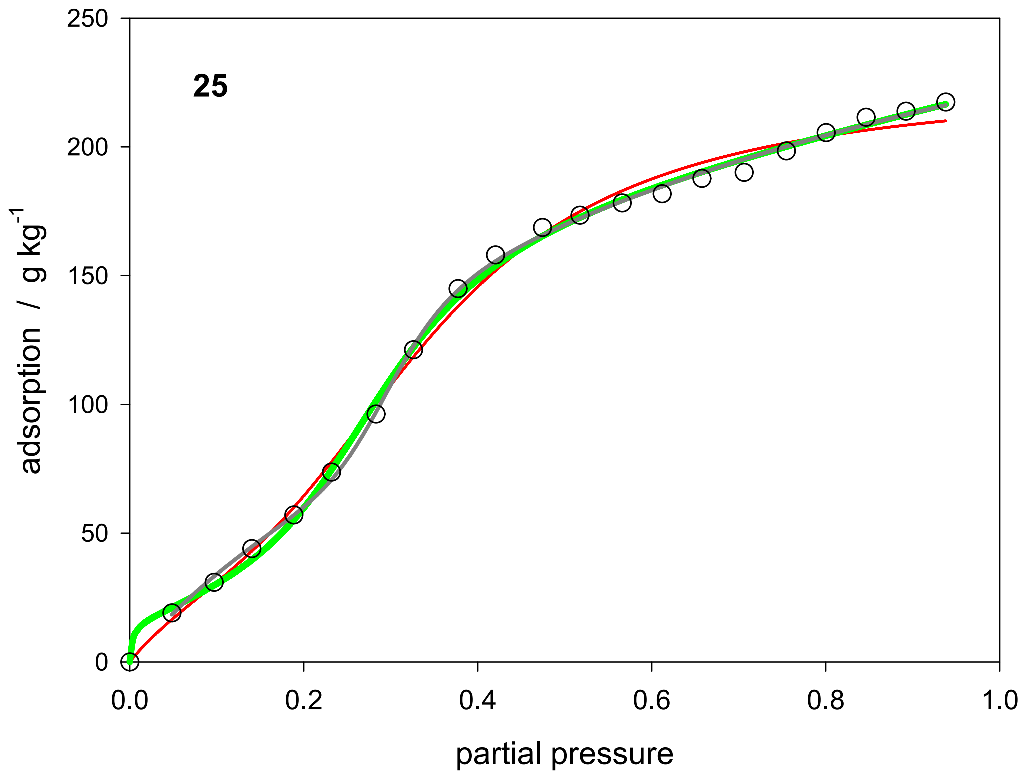

Figure A20: Modeling of the adsorption of water on carbon no. 25 with the Klotz isotherm (eqn. (24)), green line: modeled with eqn. (31).; gray line modeling with DD (eqn. (30)).

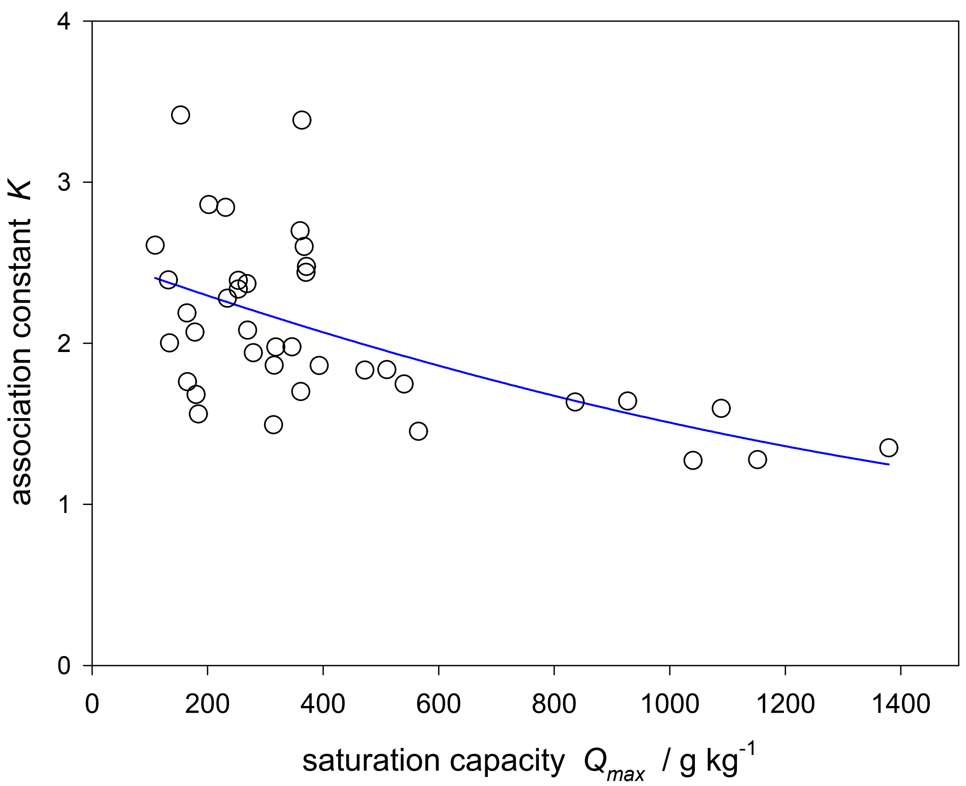

Figure A21: Correlation between K and Q_{max} (all values of Table 1).

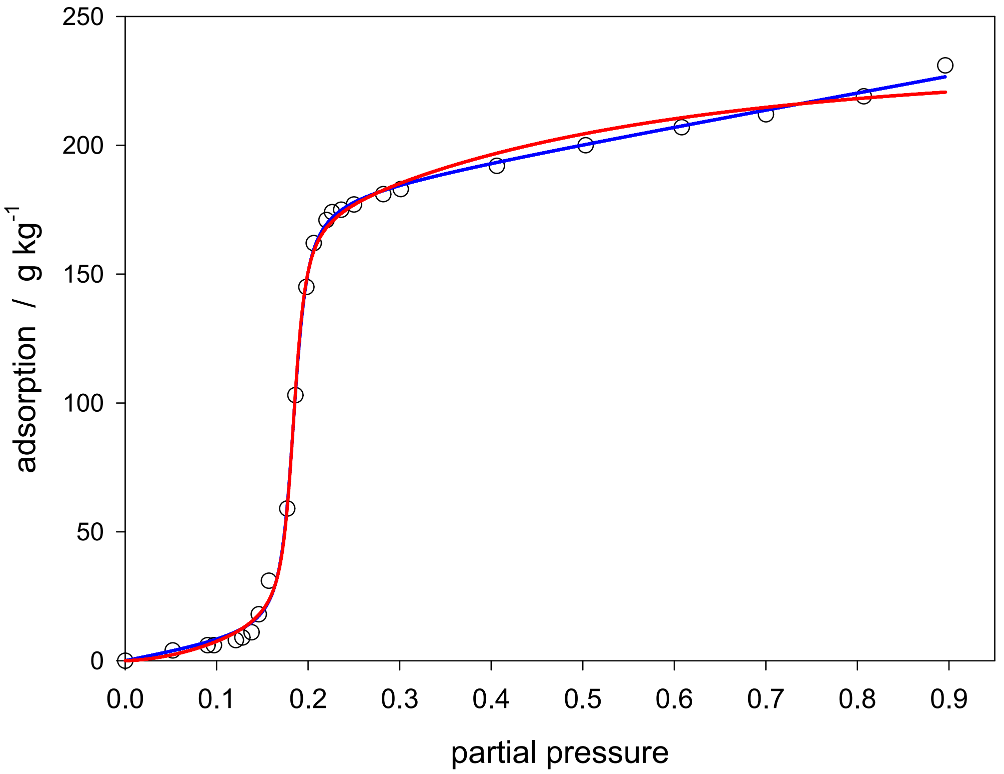

Figure A22: Modeling of the adsorption of water on an ferro aluminophosphate molecular sieve (No. 28 in Table 1) at 25°C. Blue: extended Klotz isotherm (eqn. (31)). Red: additive superposition of the original Klotz isotherm (eqn. (24)) with the part of the Sips-isotherm used in the fitting of the same underlying data by the "universal isotherm" [50].

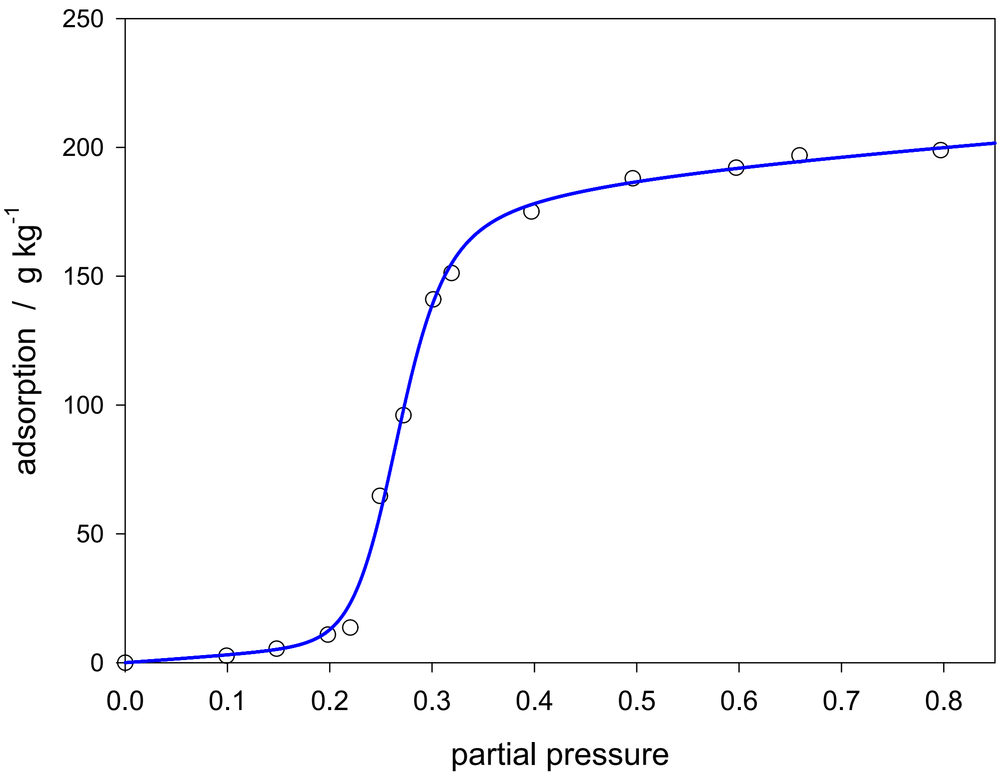

Figure A23: Modeling of the adsorption of water on ferro aluminophosphate molecular sieve (No. 29 in Table 1) at 60°C by the extended Klotz isotherm (eqn. (31))

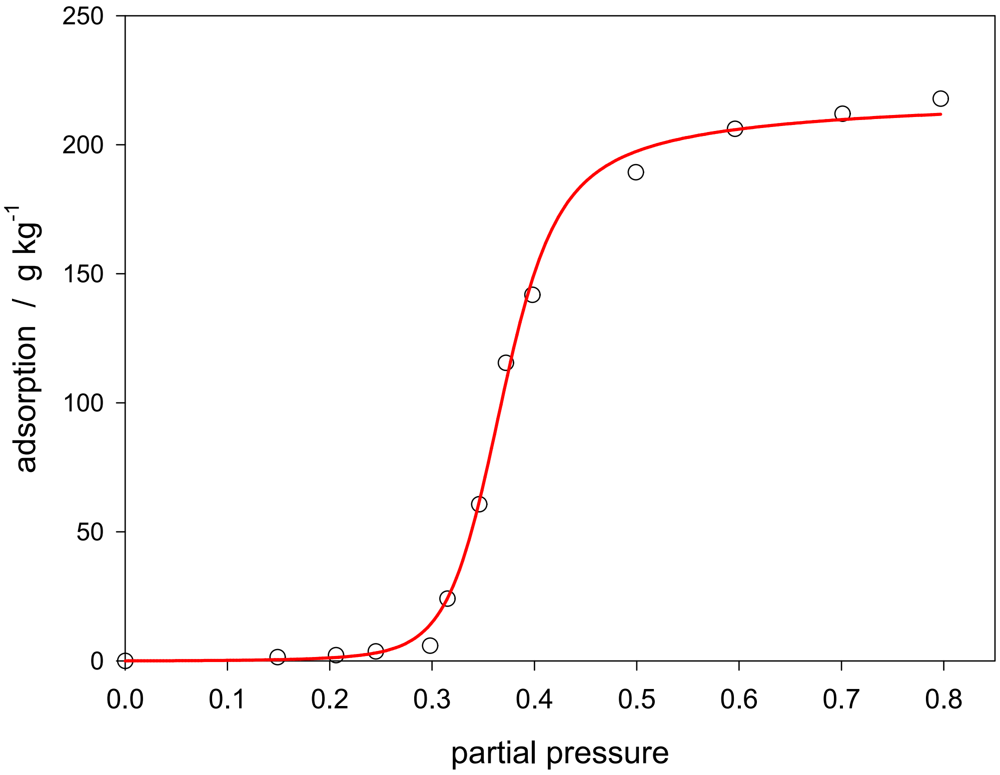

Figure A24: Modeling of the adsorption of water on aluminophosphate molecular sieve (No. 30 in Table 1) at 45°C by the Klotz isotherm (eqn. (24)).

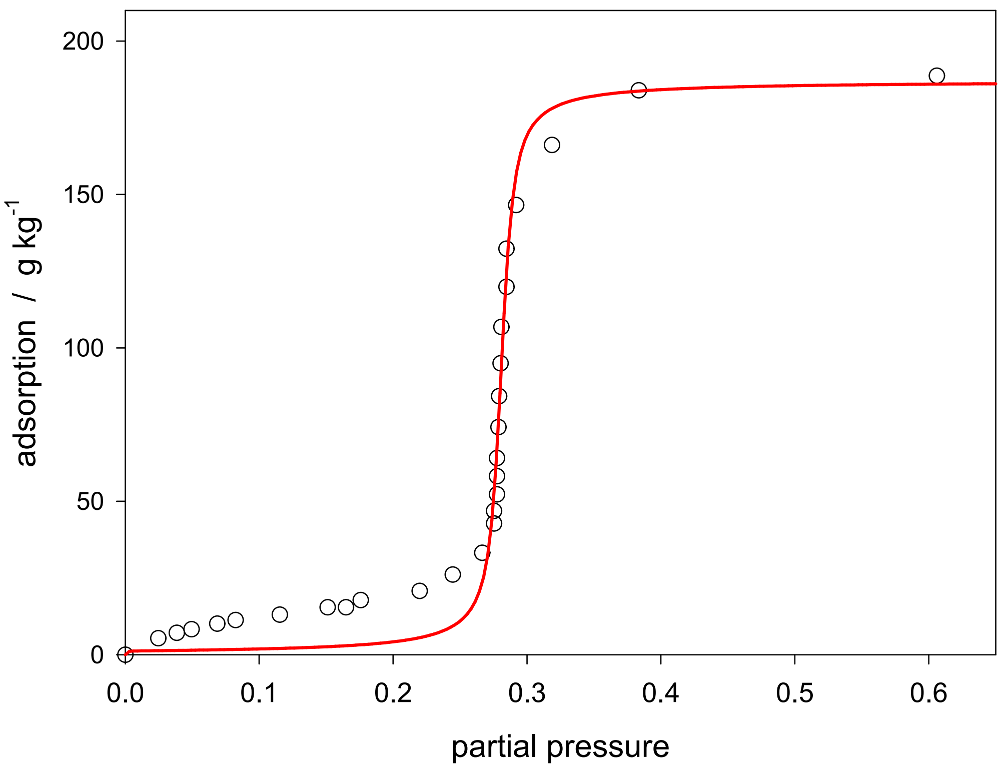

Figure A25: Unsuccessful fitting of the adsorption of water on aluminophosphate molecular sieve $AlPO_4$-5 (AFI-structure) [6] by the Klotz isotherm (eqn.(24)).