Electronic Supplementary Material (ESI) for CrystEngComm.

Drastic and Subtle Thermally and Gas-Induced Transformations of Pure 4-*tert*-Butylcalix[4]arene

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Supporting Information

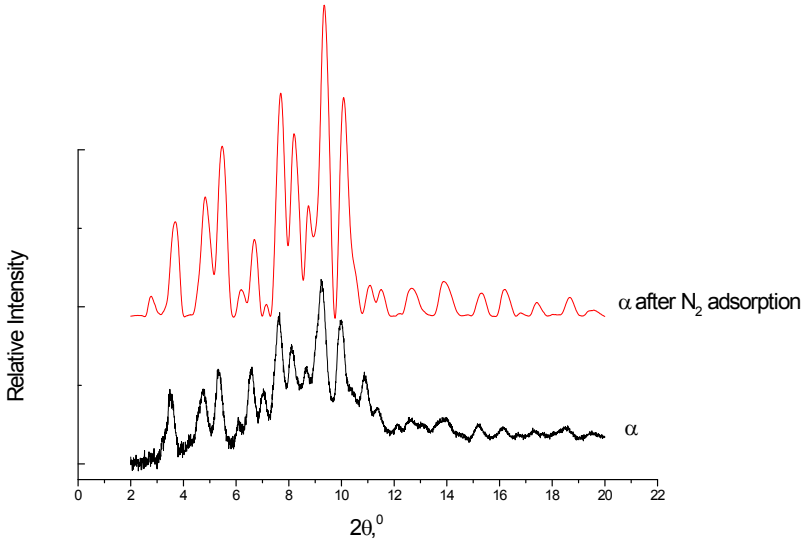

Fig. S1. X-Ray powder diffraction patterns for *t*BC α-form.

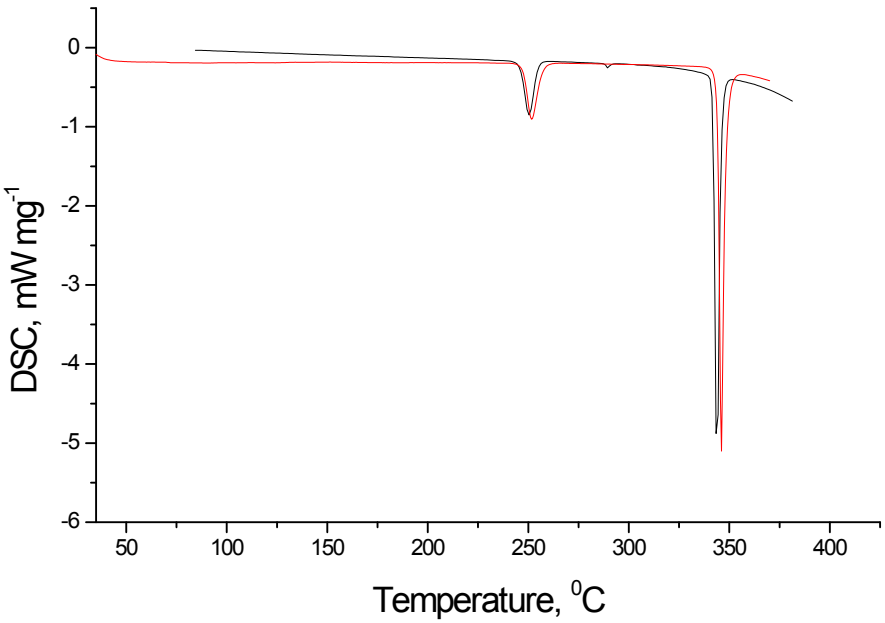

Fig. S2. DSC traces for *t*BC samples: α-form (black) and α-form after low-temperature N_2 adsorption (red).

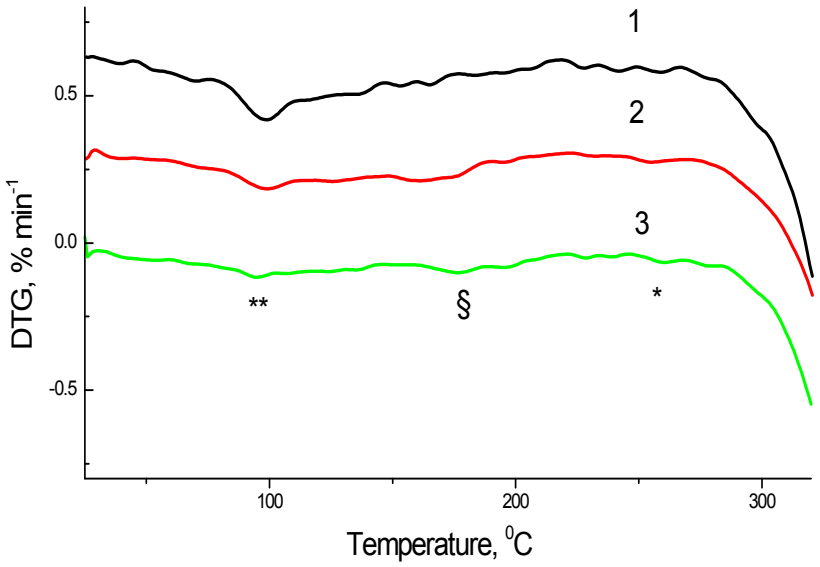

Fig. S3. DTG traces for *t*BC samples after air storage: *(1)* β_0 form; *(2)* α form treated by vacuum heating at 260^{0}C for 30 minutes; *(3)* β_0 form after the low-temperature N_2 adsorption. Signs *, ** and § correspond to marks for phase transitions in Fig.3.

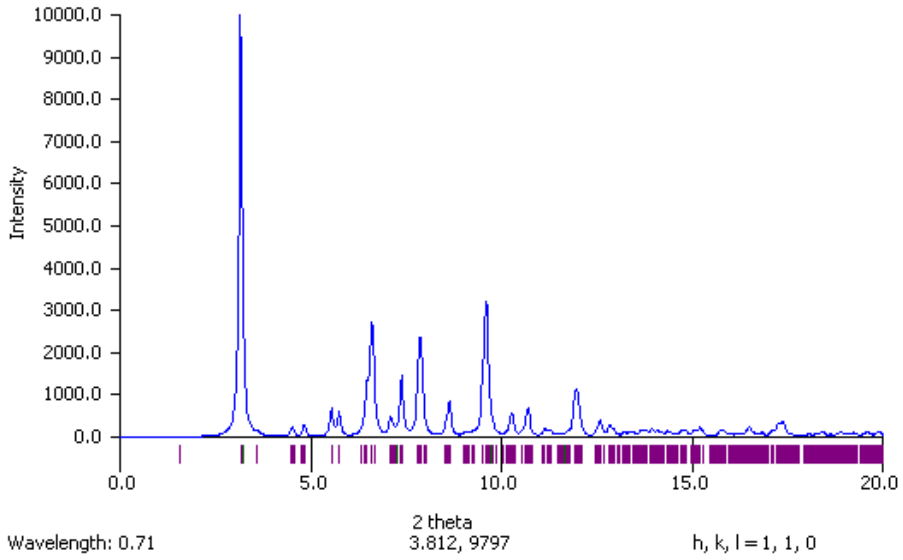

Fig. S4. Simulated diffraction pattern of single crystals of β_0 form of *t*BC partially loaded by xenon (Xe/tBC ratio up to 0.25).[34]

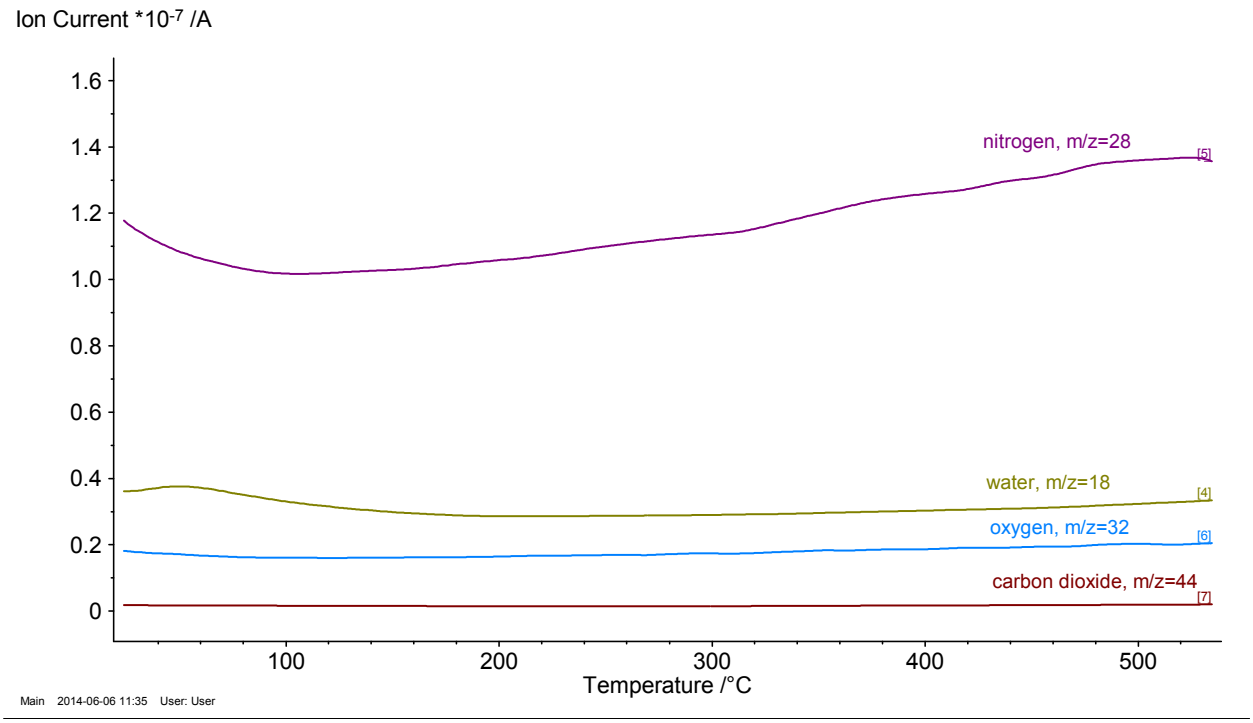

Fig. S5. Background ion currents for N_2, O_2, H_2O and CO_2.

Table S1. BET specific surface area of *t*BC α form.

Quantachrome NovaWin - Data Acquisition and Reduction
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Analysis Report
Operator:MISI Date:2013/06/26 Operator:111 Date:4/23/2014
Sample ID: 1 Filename: D:\Мои документы\2013\Quantachrome\адсобция\Kalixaren_4tert_Butyl.qps
Sample Desc: Comment:
Sample weight: 0.1083 g Sample Volume: 0.1092 cc
Outgas Time: 14.0 hrs OutgasTemp: 120.0 C
Analysis gas: Nitrogen Bath Temp: 77.3 K
Press. Tolerance:0.100/0.100 (ads/des)Equil time: 60/60 sec (ads/des) Equil timeout: 240/240 sec (ads/des)
Analysis Time: 85.1 min End of run: 2013/06/26 10:34:49 Instrument: Nova Station A
Cell ID: 1 F/W version: 0.00
Adsorbate Nitrogen Temperature 77.350K
Molec. Wt.: 28.013 g Cross Section: 16.200 El Liquid Density: 0.808 g/cc

Relative Pressure P/Po	Volume @ STP cc/g	1 / [W((Po/P) - 1)]
7.32790e-02	0.7409	8.5390e+01
1.45115e-01	1.2417	1.0938e+02
2.16148e-01	1.7854	1.2357e+02
2.87962e-01	2.3995	1.3485e+02
3.58916e-01	3.1035	1.4434e+02
4.28030e-01	3.8566	1.5525e+02
4.16593e-01	6.4722	8.8275e+01
3.45624e-01	5.4887	7.6994e+01
2.71846e-01	4.4235	6.7528e+01
2.03701e-01	3.4323	5.9633e+01
1.34493e-01	2.3921	5.1976e+01
6.20370e-02	1.1891	4.4505e+01

BET summary
Slope = 167.327
Intercept = 5.409e+01
Correlation coefficient, r = 0.563521
C constant= 4.093

Surface Area = 15.728 ml/g

Table S2. BET specific surface area of *t*BC β_0 form (1).

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Analysis Report
Operator:MISI Date:2013/06/22 Operator:111 Date:4/23/2014
Sample ID: 1 Filename: D:\Мои документы\2013\Quantachrome\адсобция\Kalixaren_tBcb0.qps
Sample Desc: Comment:
Sample weight: 0.1081 g Sample Volume: 0.10326 cc
Outgas Time: 14.0 hrs OutgasTemp: 120.0 C
Analysis gas: Nitrogen Bath Temp: 77.3 K
Press. Tolerance:0.100/0.100 (ads/des)Equil time: 60/60 sec (ads/des) Equil timeout: 240/240 sec (ads/des)
Analysis Time: 32.9 min End of run: 2013/06/22 10:54:10 Instrument: Nova Station A
Cell ID: 1 F/W version: 0.00
Adsorbate Nitrogen Temperature 77.350K
Molec. Wt.: 28.013 g Cross Section: 16.200 El Liquid Density: 0.808 g/cc

Relative Pressure P/Po	Volume @ STP cc/g	1 / [W((Po/P) - 1)]
1.12613e-01	0.6860	1.4801e+02
2.23228e-01	1.2287	1.8713e+02
3.34947e-01	1.9601	2.0559e+02
4.43202e-01	2.8235	2.2556e+02

BET summary
Slope = 227.651
Intercept = 1.282e+02
Correlation coefficient, r = 0.982471
C constant= 2.776

Surface Area = 9.787 ml/g

Table S3. BET specific surface area of *t*BC β_0 form (2).

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Analysis Report
Operator:MISI Date:2013/06/25 Operator:111 Date:4/23/2014
Sample ID: 1 Filename: D:\Мои документы\2013\Quantachrome\адсобция\Kalixaren_tBcb02.qps
Sample Desc: Comment:
Sample weight: 0.1095 g Sample Volume: 0.10086 cc
Outgas Time: 14.0 hrs OutgasTemp: 120.0 C
Analysis gas: Nitrogen Bath Temp: 77.3 K
Press. Tolerance:0.100/0.100 (ads/des)Equil time: 60/60 sec (ads/des) Equil timeout: 240/240 sec (ads/des)
Analysis Time: 79.7 min End of run: 2013/06/25 10:51:05 Instrument: Nova Station A
Cell ID: 1 F/W version: 0.00
Adsorbate Nitrogen Temperature 77.350K
Molec. Wt.: 28.013 g Cross Section: 16.200 El Liquid Density: 0.808 g/cc

Relative Pressure P/Po	Volume @ STP cc/g	1 / [W((Po/P) - 1)]
7.42340e-02	0.3783	1.6960e+02
1.46246e-01	0.5824	2.3532e+02
2.17571e-01	0.8306	2.6785e+02
2.88433e-01	1.1677	2.7776e+02
3.59121e-01	1.5786	2.8401e+02
4.28225e-01	2.0462	2.9285e+02
4.14905e-01	4.0859	1.3886e+02
3.43753e-01	3.4352	1.2201e+02
2.72522e-01	2.7598	1.0861e+02
2.05162e-01	2.1003	9.8331e+01
1.33722e-01	1.3647	9.0500e+01
6.11880e-02	0.5203	1.0022e+02

BET summary
Slope = 250.341
Intercept = 1.207e+02
Correlation coefficient, r = 0.382359
C constant= 3.074

Surface Area = 9.385 ml/g