Supplementary Materials: Insights into Adsorption of Chlorobenzene in High Silica MFI and FAU Zeolites Gained from Chromatographic and Diffractometric Techniques

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Figure S1. Observed (dotted line), calculated (solid line) and difference (bottom) X-ray powder diffraction patterns of Y–CB (**a**) and ZSM-5–CB (**b**), respectively.

Table S1. Framework atomic fractional coordinates and thermal isotropic displacement factor of Y–CB.

Table S2. Framework atomic fractional coordinates and thermal isotropic displacement factor of ZSM-5–CB.

Table S3. Extraframework atomic fractional coordinates, thermal isotropic displacement factor and occupancy of Y–CB.

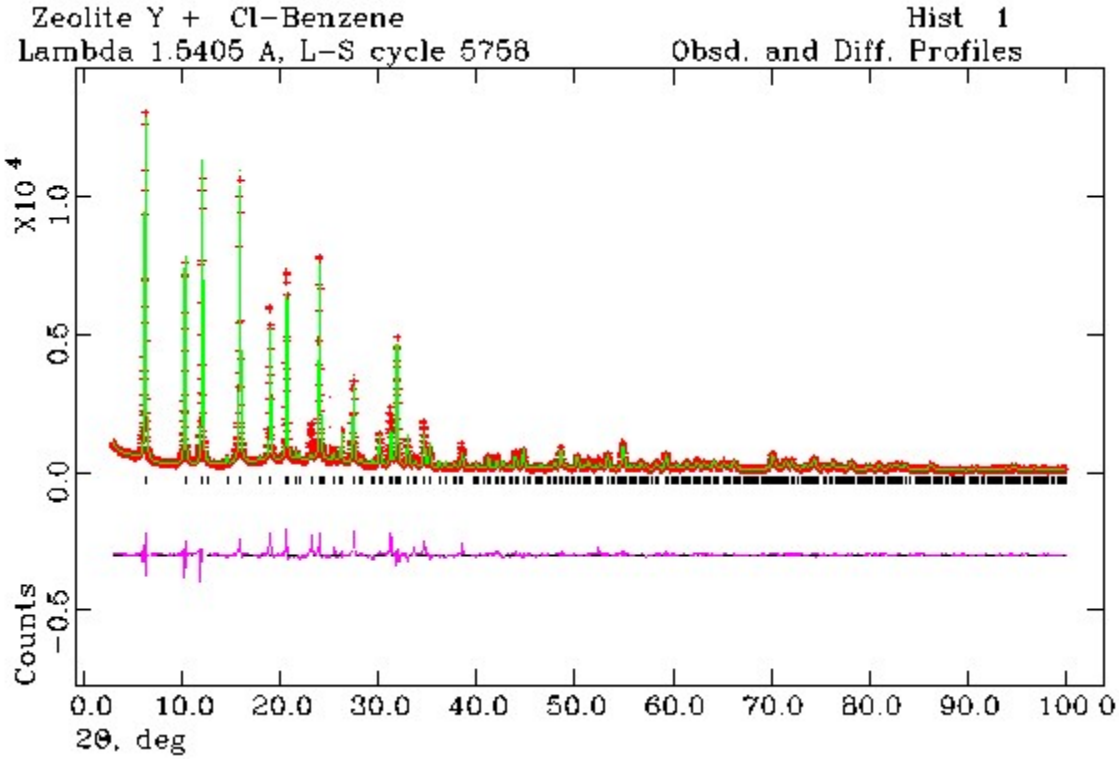
Table S4. Extraframework atomic fractional coordinates, thermal isotropic displacement factor and occupancy of ZSM-5–CB; *x/a* atomic fractional coordinates of CB2 molecule atoms have exactly the same values, in order to maintain the molecule planarity.

Table S5. Selected bond distances (Å) and angles (°) within both the Y–CB framework and extraframework atoms at T_{amb}.

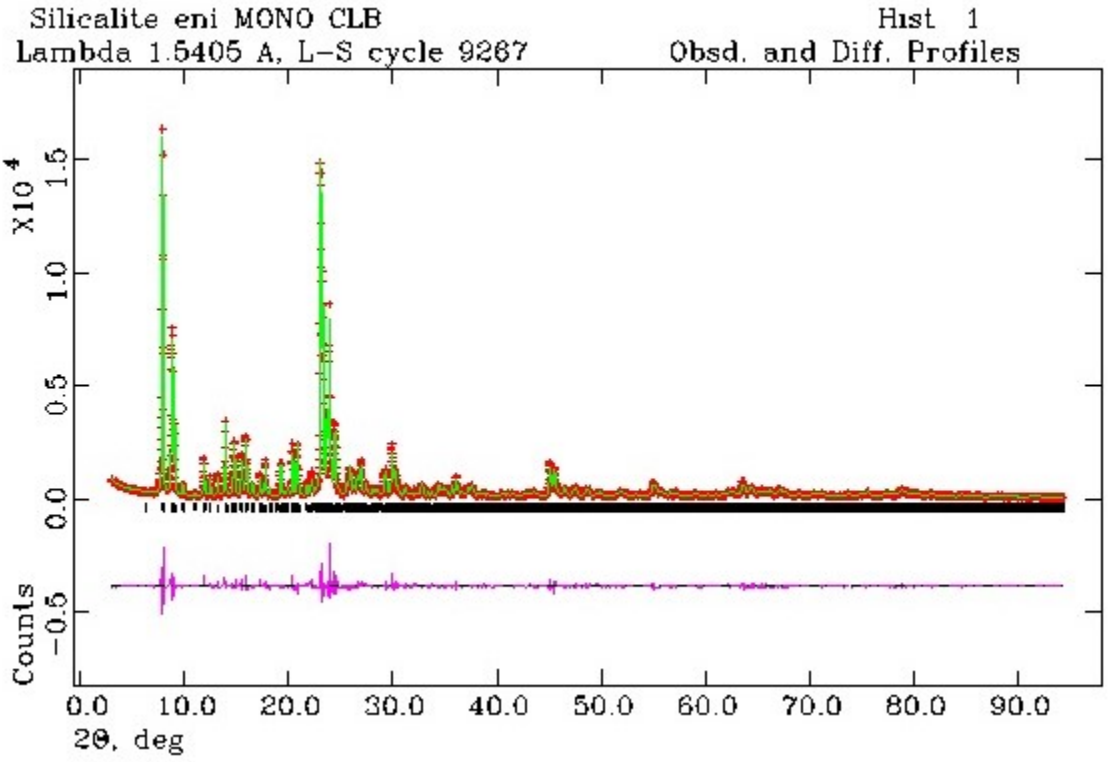
Table S6. Selected bond distances (Å) and angles (°) within both the ZSM-5–CB framework and extraframework atoms at T_{amb}.

Crystallographic Information File (CIF) of Y-CB

Crystallographic Information File (CIF) of ZSM-5-CB



(**a**)



(**b**)

Figure S1. Observed (dotted line), calculated (solid line) and difference (bottom) X-ray powder diffraction patterns of Y–CB (**a**) and ZSM-5–CB (**b**), respectively.

Table S1. Framework atomic fractional coordinates and thermal isotropic displacement factor of Y–CB.

Sites	*x/a*	*y/b*	*z/c*	U_{iso} (Å²)	Fraction
T1	−0.0536(1)	0.1178(2)	0.0380(1)	0.002(1)	1.00
T2	−0.0534(1)	0.0330(1)	0.1234(1)	0.002(1)	1.00
O1	−0.1080(3)	−0.0029(1)	0.1099(1)	0.005(1)	1.00
O2	−0.0053(7)	−0.0094(1)	0.1417(2)	0.005(1)	1.00
O3	−0.0333(1)	0.0607(1)	0.0660(1)	0.005(1)	1.00
O4	−0.0546(2)	0.0858(1)	0.1640(1)	0.005(1)	1.00

Table S2. Framework atomic fractional coordinates and thermal isotropic displacement factor of ZSM-5–CB.

Sites	*x/a*	*y/b*	*z/c*	U_{iso} (Å²)	Fraction
T1	0.0501(4)	0.4255(4)	−0.3339(5)	0.52(1)	1.00
T2	0.0303(4)	0.3159(4)	−0.1760(8)	0.52(1)	1.00
T3	0.0632(4)	0.2806(2)	0.0325(3)	0.52(1)	1.00
T4	0.0658(4)	0.1215(2)	0.0359(2)	0.52(1)	1.00
T5	0.0275(1)	0.0727(4)	−0.1785(5)	0.52(1)	1.00
T6	0.0590(4)	0.1914(4)	−0.3193(3)	0.52(1)	1.00
T7	−0.1748(3)	0.4261(1)	−0.3355(4)	0.52(1)	1.00
T8	−0.1296(3)	0.3149(1)	−0.1827(6)	0.52(1)	1.00
T9	−0.1757(3)	0.2712(1)	0.0337(6)	0.52(1)	1.00
T10	−0.1829(3)	0.1191(1)	0.0346(3)	0.52(1)	1.00
T11	−0.1309(2)	0.0698(4)	−0.1786(4)	0.52(1)	1.00
T12	−0.1638(5)	0.1882(2)	−0.3172(5)	0.52(1)	1.00
T13	0.4411(3)	0.4281(4)	−0.3370(4)	0.52(1)	1.00
T14	0.4721(2)	0.3179(4)	−0.1879(4)	0.52(1)	1.00
T15	0.4354(2)	0.2828(2)	0.0313(2)	0.52(1)	1.00
T16	0.4335(3)	0.1235(2)	0.0193(2)	0.52(1)	1.00
T17	0.4717(4)	0.0729(2)	−0.1960(2)	0.52(1)	1.00
T18	0.4361(4)	0.1930(4)	−0.3274(4)	0.52(1)	1.00
T19	0.6657(1)	0.4225(1)	−0.3232(2)	0.52(1)	1.00
T20	0.6305(2)	0.3069(4)	−0.1734(4)	0.52(1)	1.00
T21	0.6653(2)	0.2756(3)	0.0500(2)	0.52(1)	1.00
T22	0.6717(3)	0.1191(3)	0.0376(2)	0.52(1)	1.00
T23	0.6324(2)	0.0732(6)	−0.1837(4)	0.52(1)	1.00
T24	0.6815(4)	0.1911(4)	−0.3163(4)	0.52(1)	1.00
O1	0.0484(5)	0.3843(6)	−0.2314(4)	0.71(2)	1.00
O2	0.0738(3)	0.3144(2)	−0.0749(3)	0.71(2)	1.00
O3	0.0620(3)	0.2009(4)	0.0264(4)	0.71(2)	1.00
O4	0.0634(2)	0.1021(2)	−0.0803(3)	0.71(2)	1.00
O5	0.0453(6)	0.1197(4)	−0.2713(4)	0.71(2)	1.00
O6	0.0433(3)	0.2516(6)	−0.2444(4)	0.71(2)	1.00
O7	−0.1567(4)	0.3785(4)	−0.2429(3)	0.71(2)	1.00
O8	−0.1634(3)	0.3002(3)	−0.0765(4)	0.71(2)	1.00
O9	−0.1554(4)	0.1940(4)	0.0356(4)	0.71(2)	1.00
O10	−0.1594(3)	0.0884(4)	−0.0702(4)	0.71(2)	1.00

O11	−0.1567(5)	0.1152(4)	−0.2696(4)	0.71(2)	1.00
O12	−0.1385(4)	0.2480(3)	−0.2470(4)	0.71(2)	1.00
O13	−0.0498(5)	0.3216(4)	−0.1675(4)	0.71(2)	1.00
O14	−0.0516(3)	0.0682(4)	−0.1568(3)	0.71(2)	1.00
O15	0.1222(3)	0.4169(4)	−0.3852(4)	0.71(2)	1.00
O16	−0.0138(4)	0.4025(4)	−0.3986(4)	0.71(2)	1.00
O17	−0.1357(4)	0.4017(4)	−0.4332(4)	0.71(2)	1.00
O18	0.1338(4)	0.1817(4)	−0.3605(4)	0.71(2)	1.00
O19	−0.0011(3)	0.2057(4)	−0.3964(4)	0.71(2)	1.00
O20	−0.1322(3)	0.1841(4)	−0.4268(4)	0.71(2)	1.00
O21	0.0599(4)	0.0022(4)	−0.2069(4)	0.71(2)	1.00
O22	−0.1630(3)	−0.0006(3)	−0.2087(4)	0.71(2)	1.00
O23	−0.2552(4)	0.4281(3)	−0.3435(3)	0.71(2)	1.00
O24	−0.2411(3)	0.2009(3)	−0.3454(4)	0.71(2)	1.00
O25	−0.2543(3)	0.2769(3)	0.0577(3)	0.71(2)	1.00
O26	−0.2550(4)	0.1077(3)	0.0843(3)	0.71(2)	1.00
O27	0.4406(3)	0.3835(4)	−0.2378(4)	0.71(2)	1.00
O28	0.4396(3)	0.3142(3)	−0.0787(3)	0.71(2)	1.00
O29	0.4356(3)	0.2031(3)	0.0258(5)	0.71(2)	1.00
O30	0.4389(4)	0.0929(4)	−0.0910(3)	0.71(2)	1.00
O31	0.4357(3)	0.1213	−0.2750(3)	0.71(2)	1.00
O32	0.4574(3)	0.2530(4)	−0.2546(4)	0.71(2)	1.00
O33	0.6554(4)	0.3721(3)	−0.2317(3)	0.71(2)	1.00
O34	0.6562(3)	0.3066(4)	−0.0597(3)	0.71(2)	1.00
O35	0.6591(4)	0.1975(3)	0.0277(3)	0.71(2)	1.00
O36	0.6605(4)	0.0963(3)	−0.0764	0.71(2)	1.00
O37	0.6613(3)	0.1204(3)	−0.2698(3)	0.71(2)	1.00
O38	0.6620(4)	0.2454(4)	−0.2334	0.71(2)	1.00
O39	0.5503(4)	0.2996(3)	−0.1794(4)	0.71(2)	1.00
O40	0.5522(4)	0.0783(3)	−0.1942(3)	0.71(2)	1.00
O41	0.3779(4)	0.4188(4)	−0.4104(3)	0.71(2)	1.00
O42	0.5051(3)	0.4133(4)	−0.4057(3)	0.71(2)	1.00
O43	0.6415(3)	0.3911(3)	−0.4275(3)	0.71(2)	1.00
O44	0.3651(3)	0.1872(3)	−0.3836(3)	0.71(2)	1.00
O45	0.5017(3)	0.2017(3)	−0.3951(3)	0.71(2)	1.00
O46	0.6299(3)	0.1972(3)	−0.4084(3)	0.71(2)	1.00
O47	0.4484(3)	−0.0023(4)	−0.2169(3)	0.71(2)	1.00
O48	0.6539(4)	−0.0021(3)	−0.2070(4)	0.71(2)	1.00

Table S3. Extraframework atomic fractional coordinates, thermal isotropic displacement factor and occupancy of Y–CB.

Sites	*x/a*	*y/b*	*z/c*	U_{iso} (Å²)	Fraction
C	0.4768(1)	0.4768(1)	0.5463(3)	0.161(3)	0.34(6)
Cl	0.4496(1)	0.4496(1)	0.6008(1)	0.161(3)	0.34(6)
W1	0.3096(4)	0.3096(4)	0.3096(4)	0.113(1)	0.82(1)
W2	0.4176(2)	0.4176(2)	0.4176(2)	0.113(1)	0.80(8)
W3	0.6277(1)	0.2209(1)	0.0081(1)	0.113(1)	0.18(1)

Table S4. Extraframework atomic fractional coordinates, thermal isotropic displacement factor and occupancy of ZSM-5–CB; *x/a* atomic fractional coordinates of CB2 molecule atoms have exactly the same values, in order to maintain the molecule planarity.

Sites	*x/a*	*y/b*	*z/c*	U_{iso} (Å²)	Fraction
C1	0.7547(4)	0.5975(9)	0.0273(7)	0.211(7)	0.93(5)
C2	0.3017(5)	0.4444(9)	0.008(5)	0.211(7)	0.93(5)
C3	0.8151(8)	0.5686(7)	0.0564(6)	0.211(7)	0.93(5)
C4	0.8237(4)	0.5008(8)	0.0502(8)	0.211(7)	0.93(5)
C5	0.7110(7)	0.4899(6)	−0.0129(7)	0.211(7)	0.93(5)
C6	0.2285(7)	0.5386(9)	−0.0175(5)	0.211(7)	0.93(5)
Cl1	0.0991(2)	0.5357(2)	0.921(2)	0.211(7)	0.93(5)
C8	0.213(4)	0.1474(7)	0.7608(3)	0.285(2)	0.54(6)
C9	0.213(6)	0.0885(8)	0.7066(3)	0.285(2)	0.54(6)
C10	0.213(4)	0.0834(7)	0.9116(3)	0.285(2)	0.54(6)
C11	0.213(3)	0.1444(7)	0.8632(3)	0.285(2)	0.54(6)
C12	0.213(7)	0.0274(7)	0.8573(3)	0.285(2)	0.54(6)
C13	0.213(8)	0.0275(7)	0.7553(3)	0.285(2)	0.54(6)
Cl2	0.213(9)	−0.0544(7)	0.7127(3)	0.285(2)	0.54(6)
W1	0.7170(9)	0.7343(5)	0.1285(5)	0.193(3)	1.00(2)
W2	0.4209(7)	0.5034(5)	−0.0025(8)	0.193(3)	1.00(3)

Table S5. Selected bond distances (Å) and angles (°) within both the Y–CB framework and extraframework atoms at T_{amb}.

Distance	Value (Å)	Distance	Value (Å)
T1–O1	1.629	T2–O1	1.619
T1–O2	1.612	T2–O2	1.620
T1–O3	1.622	T2–O3	1.621
T1–O4	1.620	T2–O4	1.619
Mean Value	1.621	Mean Value	1.620
Angle	**Value (°)**	**Angle**	**Value (°)**
O1–T1–O2	105.6	O1–T2–O2	107.7
O1–T1–O3	110.5	O1–T2–O3	107.3
O1–T1–O4	117.7	O1–T2–O4	122.3
O2–T1–O3	112.3	O2–T2–O3	106.4
O2–T1–O4	103.3	O2–T2–O4	110.4
O3–T1–O4	107.3	O3–T2–O4	101.6
Mean value	109.45	Mean value	109.3
Angle	**Value (°)**	**Angle**	**Value (°)**
T1–O1–T2	124.7	O1–Cl	2.680
T1–O2–T2	142.7	O1–Cl	2.723
T1–O3–T2	128.6	O4–Cl	2.599

T1–O4–T2	171.4	C–C	1.379
Mean value	141.8	Mean value	1.620
Distance	**Value (Å)**	**Distance**	**Value (Å)**
W2–W2	2.926	W1–W3	2.201
W2–W1	2.737	W3–CL	2.454
W2–W3	2.421	W3–CL	3.211

Table S6. Selected bond distances (Å) and angles (°) within both the ZSM-5–CB framework and extraframework atoms at T_{amb}.

Distance	**Value (Å)**
T1–O1	1.604
T1–O15	1.606
T1–O16	1.602
T1–O47	1.604
Mean value	1.604
T2–O1	1.604
T2–O2	1.604
T2–O6	1.606
T2–O13	1.605
Mean value	1.605
T3–O2	1.606
T3–O3	1.605
T3–O45	1.607
T3–O46	1.606
Mean value	1.606
T4–O3	1.604
T4–O4	1.605
T4–O42	1.605
T4–O43	1.602
Mean value	1.604
T5–O4	1.606
T5–O5	1.603
T5–O14	1.606
T5–O21	1.604
Mean value	1.605
T6–O5	1.603
T6–O6	1.605
T6–O18	1.604
T6–O19	1.603
Mean value	1.604
T7–O7	1.605
T7–O17	1.605
T7–O23	1.604
T7–O48	1.605
Mean value	1.605
T8–O7	1.604
T8–O8	1.606
T8–O12	1.606
T8–O13	1.605
Mean value	1.605
T9–O8	1.609

T9–O9	1.603
T9–O25	1.605
T9–O44	1.604
Mean value	1.605
T10–O9	1.603
T10–O10	1.607
T10–O26	1.604
T10–O41	1.605
Mean value	1.605
T11–O10	1.606
T11–O11	1.605
T11–O14	1.606
T11–O22	1.604
Mean value	1.605
T12–O11	1.605
T12–O12	1.607
T12–O20	1.604
T12–O24	1.604
Mean value	1.605
T13–O21	1.603
T13–O27	1.604
T13–O41	1.603
T13–O42	1.605
Mean value	1.604
T14–O27	1.605
T14–O28	1.606
T14–O32	1.608
T14–O39	1.605
Mean value	1.606
T15–O19	1.605
T15–O20	1.605
T15–O28	1.606
T15–O29	1.604
Mean value	1.605
T16–O16	1.603
T16–O17	1.605
T16–O29	1.603
T16–O30	1.605
Mean value	1.604
T17–O30	1.606
T17–O31	1.604
T17–O40	1.607
Mean value	1.605
T18–O31	1.603
T18–O32	1.606
T18–O44	1.603
T18–O45	1.605
Mean value	1.604
T19–O22	1.605
T19–O23	1.604
T19–O33	1.605
T19–O43	1.604

Mean value	1.605
T20–O33	1.605
T20–O34	1.603
T20–O38	1.607
T20–O39	1.605
Mean value	1.605
T21–O18	1.605
T21–O25	1.606
T21–O34	1.605
T21–O35	1.603
Mean value	1.605
T22–O15	1.606
T22–O26	1.602
T22–O35	1.602
T22–O36	1.608
Mean value	1.605
T23–O36	1.607
T23–O37	1.605
T23–O40	1.607
T23–O48	1.605
Mean value	1.606
T24–O24	1.605
T24–O37	1.605
T24–O38	1.606
T24–O46	1.605
Mean value	1.605
Angle	**Value (°)**
O1–T1–O15	109.6
O1–T1–O16	107
O1–T1–O47	96.1
O15–T1–O16	116.6
O15–T1–O47	105.3
O16–T1–O47	120.2
Mean value	109.1
O1–T2–O2	106.6
O1–T2–O6	112.8
O1–T2–O13	101.5
O2–T2–O6	112.2
O2–T2–O13	118.2
O6–T2–O13	105.1
Mean value	109.4
O2–T3–O3	112.3
O2–T3–O45	123.5
O2–T3–O46	102.1
O3–T3–O45	103.9
O3–T3–O46	108.3
O45–T3–O46	105.8
Mean value	109.3
O3–T4–O4	99.5
O3–T4–O42	116
O3–T4–O43	103.1
O4–T4–O42	110.4

O4–T4–O43	106.2
O42–T4–O43	119.5
Mean value	109.1
O4–T5–O5	108.6
O4–T5–O14	107.7
O4–T5–O21	109.9
O5–T5–O14	113.4
O5–T5–O21	104.2
O14–T5–O21	113
Mean value	109.5
O5–T6–O6	113.2
O5–T6–O18	100.9
O5–T6–O19	107
O6–T6–O18	119.6
O6–T6–O19	96.8
O18–T6–O19	119.4
Mean value	109.5
O7–T7–O17	109.9
O7–T7–O23	106.5
O7–T7–O48	101.8
O17–T7–O23	116.3
O17–T7–O48	115.9
O23–T7–O48	105
Mean value	109.3
O7–T8–O8	116.7
O7–T8–O12	111.3
O7–T8–O13	109.1
O8–T8–O12	105.9
O8–T8–O13	108.9
O12–T8–O13	104.1
Mean value	109.3
O8–T9–O9	109
O8–T9–O25	108.2
O8–T9–O44	111.4
O9–T9–O25	108.2
O9–T9–O44	111.6
O25–T9–O44	108.3
Mean value	109.5
O9–T10–O10	105.5
O9–T10–O26	115.9
O9–T10–O41	100.8
O10–T10–O26	125.1
O10–T10–O41	89.7
O26–T10–O41	114.6
Mean value	108.6
O10–T11–O11	116.2
O10–T11–O14	101.2
O10–T11–O22	106.9
O11–T11–O14	117.3
O11–T11–O22	100.7
O14–T11–O22	114.7
Mean value	109.5

O11–T12–O12	115.2
O11–T12–O20	106.5
O11–T12–O24	108.7
O12–T12–O20	116.8
O12–T12–O24	108.3
O20–T12–O24	100.1
Mean value	109.3
O21–T13–O27	102.5
O21–T13–O41	108.8
O21–T13–O42	113.2
O27–T13–O41	115.7
O27–T13–O42	112.4
O41–T13–O42	104.5
Mean value	109.5
O27–T14–O28	104.9
O27–T14–O32	111.5
O27–T14–O39	126.5
O28–T14–O32	113.4
O28–T14–O39	108.8
O32–T14–O39	91.6
Mean value	109.4
O19–T15–O20	112.9
O19–T15–O28	116.8
O19–T15–O29	99.7
O20–T15–O28	101.9
O20–T15–O29	115.6
O28–T15–O29	110.5
Mean value	109.6
O16–T16–O17	100.6
O16–T16–O29	105.8
O16–T16–O30	117.3
O17–T16–O29	108.4
O17–T16–O30	107.9
O29–T16–O30	115.6
Mean value	109.3
O30–T17–O31	104
O30–T17–O40	112.4
O30–T17–O47	105.6
O31–T17–O40	114.3
O31–T17–O47	109.1
O40–T17–O47	110.8
Mean value	109.4
O31–T18–O32	114.3
O31–T18–O44	97.6
O31–T18–O45	110.7
O32–T18–O44	124.6
O32–T18–O45	92.8
O44–T18–O45	117.6
Mean value	109.6
O22–T19–O23	90.7
O22–T19–O33	113.6
O22–T19–O43	126.9

O23–T19–O33	107.7
O23–T19–O43	99.9
O33–T19–O43	112.2
Mean value	108.5
O33–T20–O34	111.5
O33–T20–O38	105.2
O33–T20–O39	111.2
O34–T20–O38	110.4
O34–T20–O39	111
O38–T20–O39	107.2
Mean value	109.4
O18–T21–O25	109.7
O18–T21–O34	115.7
O18–T21–O35	129.3
O25–T21–O34	99.1
O25–T21–O35	95.9
O34–T21–O35	101.6
Mean value	108.6
O15–T22–O26	104.2
O15–T22–O35	113.7
O15–T22–O36	113.7
O26–T22–O35	108.3
O26–T22–O36	116.8
O35–T22–O36	100.4
Mean value	109.5
O36–T23–O37	110.3
O36–T23–O40	113.5
O36–T23–O48	110.9
O37–T23–O40	105.1
O37–T23–O48	108.7
O40–T23–O48	108.1
Mean value	109.4
O24–T24–O37	116.5
O24–T24–O38	108.8
O24–T24–O46	114.5
O37–T24–O38	105.7
O37–T24–O46	101.9
O38–T24–O46	108.9
Mean value	109.4
T1–O1–T2	147.7
T2–O2–T3	133.7
T3–O3–T4	171.7
T4–O4–T5	153.4
T5–O5–T6	151.7
T2–O6–T6	175.3
T7–O7–T8	159.5
T8–O8–T9	161.3
T9–O9–T10	145.5
T10–O10–T11	170.5
T11–O11–T12	148.0
T8–O12–T12	167.0
T2–O13–T8	165.6

T5–O14–T11	158.6
T1–O15–T22	151.5
T1–O16–T16	168.2
T7–O17–T16	147.6
T6–O18–T21	124.0
T6–O19–T15	176.0
T12–O20–T15	129.3
T5–O21–T13	136.7
T11–O22–T19	142.9
T7–O23–T19	165.4
T12–O24–T24	147.8
T9–O25–T21	163.9
T10–O26–T22	129.4
T13–O27–T14	143.2
T14–O28–T15	151.4
T15–O29–T16	178.3
T16–O30–T17	158.8
T17–O31–T18	146.1
T14–O32–T18	173.5
T19–O33–T20	158.2
T20–O34–T21	154.7
T21–O35–T22	159.6
T22–O36–T23	167.5
T23–O37–T24	153.6
T20–O38–T24	165.2
T14–O39–T20	161.5
T17–O40–T23	171.3
T10–O41–T13	157.4
T4–O42–T13	164.6
T4–O43–T19	127.3
T9–O44–T18	136.6
T3–O45–T18	172.6
T3–O46–T24	157.5
T1–O47–T17	140.7
T7–O48–T23	148.0

Distance	**Value (Å)**
C5–C6	1.39
C5–C4	2.40
C5–C2	1.35
C5–C3	2.76
C5–C1	2.39
C5–W2	2.64
C6–C5	1.39
C6–C4	1.38
C6–C2	2.41
C6–C3	2.38
C6–C1	2.76
C6–Cl1	2.70
C4–C5	2.40
C4–C6	1.38
C4–C2	2.83
C4–C3	1.38

C4–C1	2.40
C4–Cl1	1.75
C2–O20	3.03
C2–C5	1.35
C2–C6	2.41
C2–C4	2.83
C2–C3	2.49
C2–C1	1.48
C2–W2	2.66
C2–C14	2.97
C3–C5	2.76
C3–C6	2.38
C3–C4	1.38
C3–C2	2.49
C3–C1	1.39
C3–Cl2	2.94
C3–C7	2.72
C1–O24	3.21
C1–C5	2.39
C1–C6	2.76
C1–C4	2.40
C1–C2	1.48
C1–C3	1.39
C1–W1	3.16
C1–C14	2.76
C8–O18	2.36
C8–O25	3.19
C8–C9	1.39
C8–C10	2.40
C8–C11	1.37
C8–C12	2.74
C8–C13	2.41
C8–W1	3.13
C9–O18	2.61
C9–C8	1.39
C9–C10	2.75
C9–C11	2.38
C9–C12	2.36
C9–C13	1.39
C9–Cl2	2.87
C10–O4	3.01
C10–O43	2.64
C10–C8	2.40
C10–C9	2.75
C10–C11	1.39
C10–C12	1.34
C10–C13	2.38
C11–O4	3.19
C11–C8	1.37
C11–C9	2.38
C11–C10	1.39
C11–C12	2.35

C11–C13	2.76
C11–W1	2.81
C12–O21	3.20
C12–O26	2.95
C12–O41	2.93
C12–C8	2.74
C12–C9	2.36
C12–C10	1.34
C12–C11	2.35
C12–C13	1.37
C12–C14	2.54
C13–O21	3.14
C13–C8	2.41
C13–C9	1.39
C13–C10	2.38
C13–C11	2.76
C13–C12	1.37
C13–Cl2	1.74
W1–O20	3.33
W1–O28	3.33
W1–C1	3.16
W1–C8	3.13
W1–C11	2.81
W2–C5	2.64
W2–C2	2.66
W2–W2	3.15
CL2–O21	3.44
CL2–O26	3.03
CL2–O27	3.32
CL2–O41	3.26
CL2–C2	2.97
CL2–C3	2.94
CL2–C1	2.76
CL2–C9	2.87
CL2–C12	2.54
CL2–C13	1.74
Cl1–O31	2.69
Cl1–O44	3.17
Cl1–O47	2.99
Cl1–C6	2.70
Cl1–C4	1.75
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Crystallographic Information File (CIF) of Y-CB*Y–CB*

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O2 O −0.00534 −0.00939 0.14171 0.394783509124 1.00000
O3 O −0.03333 0.06065 0.06604 0.394783509124 1.00000
O4 O −0.05463 0.08582 0.16401 0.394783509124 1.00000
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w1 O 0.30959 0.30959 0.30959 9.04496393424 0.82154
C1 C 0.47678 0.47678 0.54634 12.7041333236 0.33590
w3 O 0.62774 0.22086 0.00814 9.04496393424 0.18780
CL1 CL 0.44958 0.44958 0.60084 12.7041333236 0.33590

Crystallographic Information File (CIF) of ZSM-5-CB

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SI4 SI 0.06578 0.12149 0.03589 0.41452268458 1.00000
SI5 SI 0.02748 0.07270 −0.17852 0.41452268458 1.00000
SI6 SI 0.05904 0.19140 −0.31926 0.41452268458 1.00000
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