Electronic Supplementary Information

Supramolecular frameworks constructed by exclusion complexes of symmetric dicyclohexanocucurbit[6]uril with benzene ring-containing guests

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Figure S1. Titration ^{1}H NMR spectra (400 MHz, D_2O) of $CyH_2Q[6]$ (2 mM) with G2. (a) $CyH_2Q[6]$; (b) $n(CyH_2Q[6])$: n(G2) = 1.0 : 0.5; (c) $n(CyH_2Q[6])$: n(G2) = 1.0 : 0.9; (d) G2.

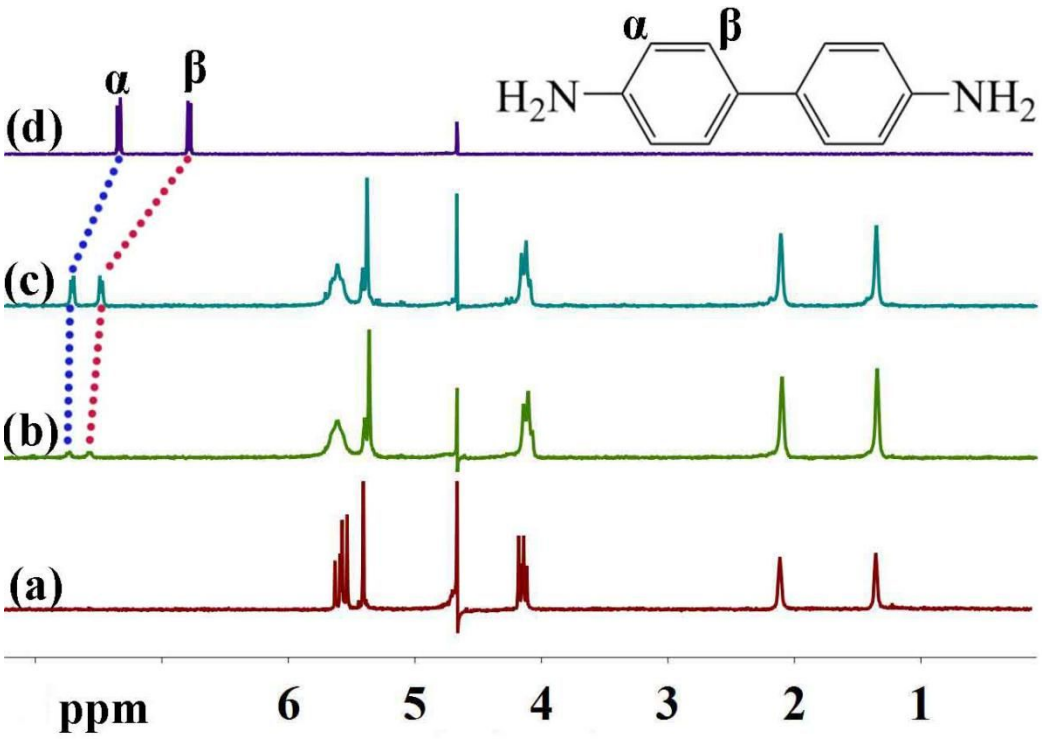

Figure S2. Titration ^{1}H NMR spectra (400 MHz, D_2O) of $CyH_2Q[6]$ (2 mM) with G3. (a) $CyH_2Q[6]$; (b) $n(CyH_2Q[6])$: n(G3) = 1.0 : 0.70; (c) $n(CyH_2Q[6])$:n(G3) = 1.0 : 1.3; (d) G3.

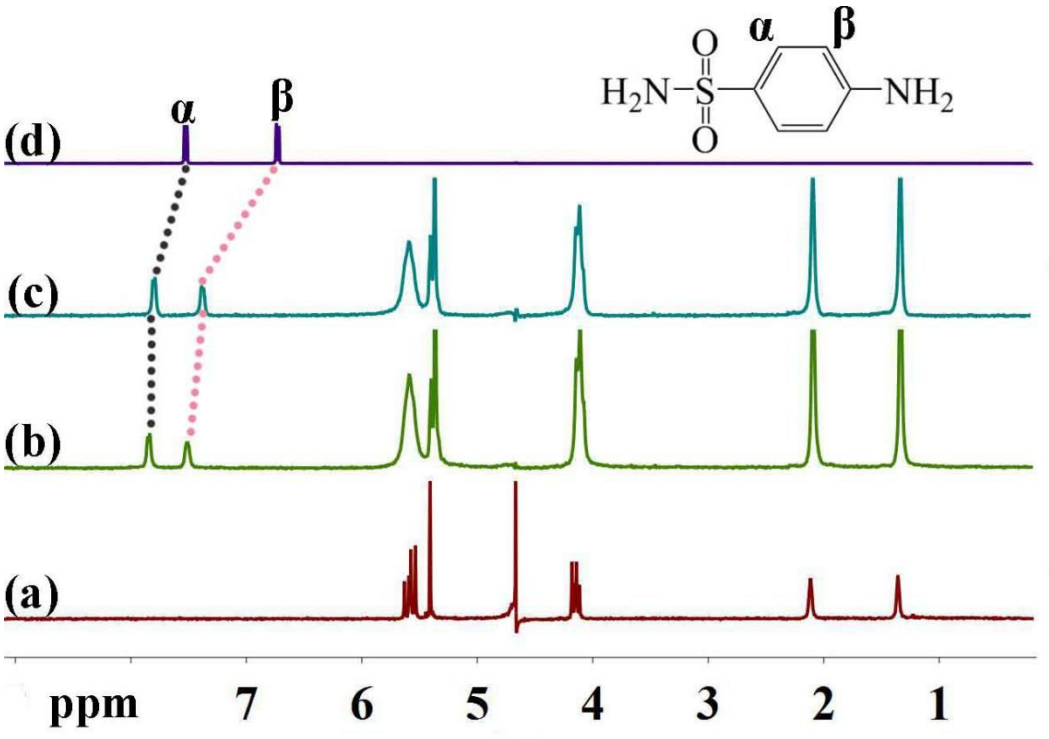

Figure S3. Titration ^{1}H NMR spectra (400 MHz, D_2O) of $CyH_2Q[6]$ (2 mM) with G4. (a) $CyH_2Q[6]$; (b) $n(CyH_2Q[6])$: n(G4) = 1.0 : 0.73; (c) $n(CyH_2Q[6])$:n(G4) = 1.0 : 1.4; (d) G4.

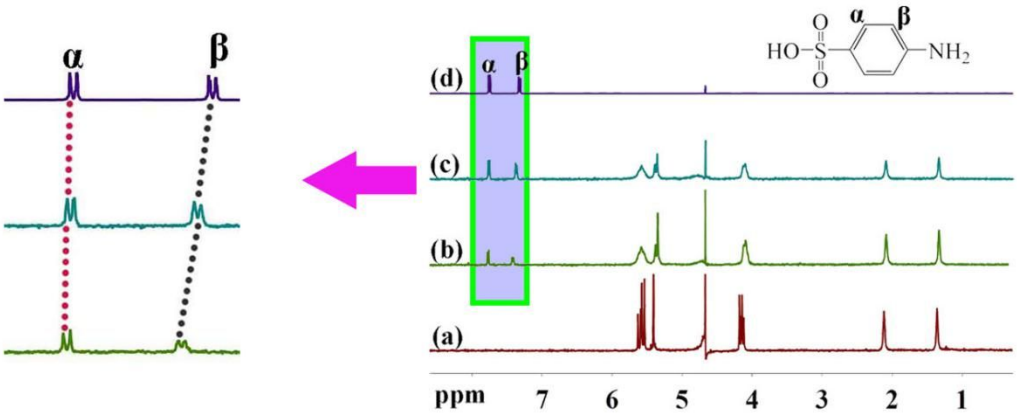

Figure S4. Titration ^{1}H NMR spectra (400 MHz, D_2O) of $CyH_2Q[6]$ (2 mM) with G5. (a) $CyH_2Q[6]$; (b) $n(CyH_2Q[6])$: n(G5) = 1.0 : 0.5; (c) $n(CyH_2Q[6])$:n(G5) = 1.0 : 1.2; (d) G5.

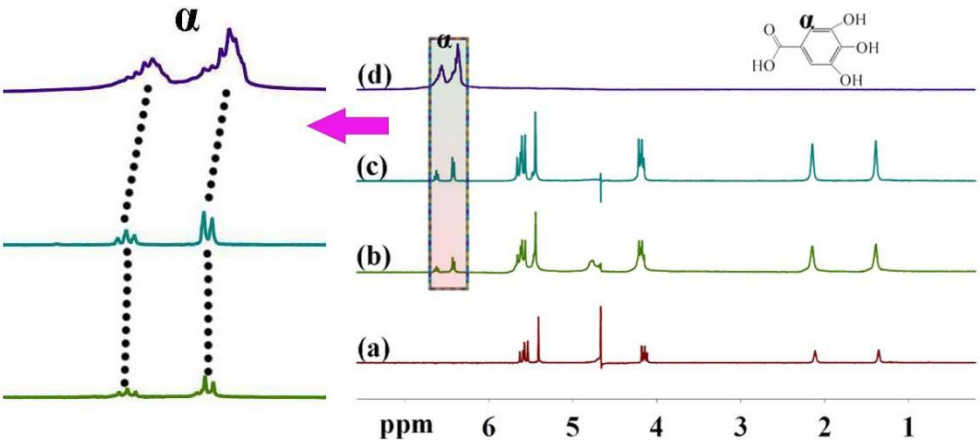

Figure S5. The ESI-TOF mass spectrometry for the exclusion complex $CyH_2Q[6]\cdot G1$. The peak found at *m*/*z* 1315.5095 corresponds to $[CyH_2Q[6]\cdot HG1]^+$ (calculated for $[CyH_2Q[6]\cdot HG1]^+$, 1315.5113).

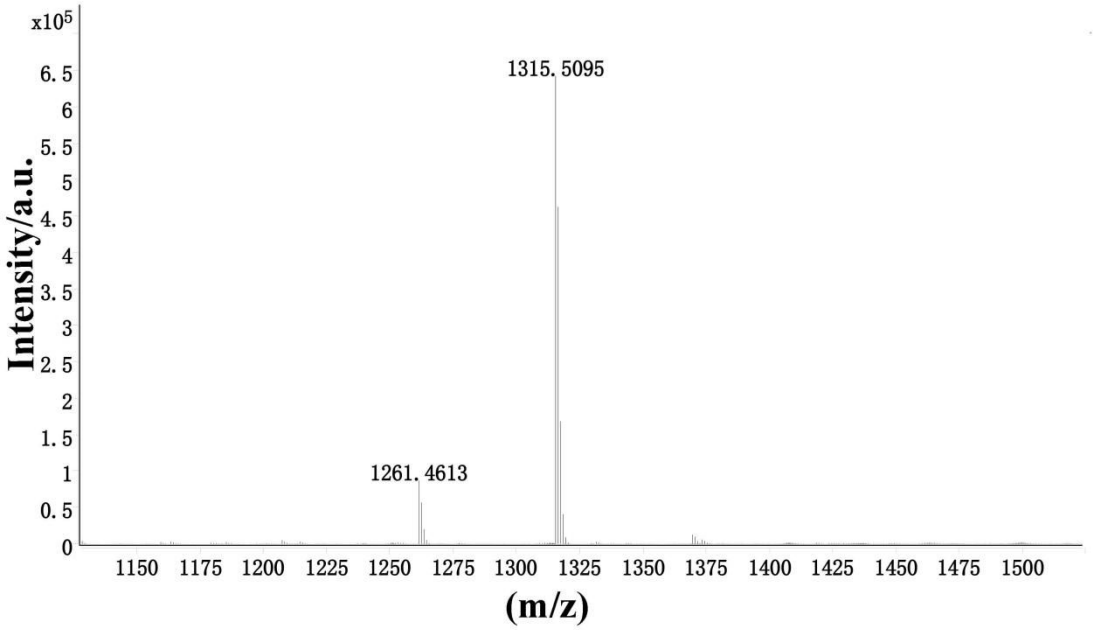

Figure S6. The ESI-TOF mass spectrometry for the exclusion complex $CyH_2Q[6]\cdot G2$. The peak found at *m/z* 1289.4936 corresponds to $[CyH_2Q[6]\cdot HG2]^+$ (calculated for $[CyH_2Q[6]\cdot HG]^+$, 1289.4957).

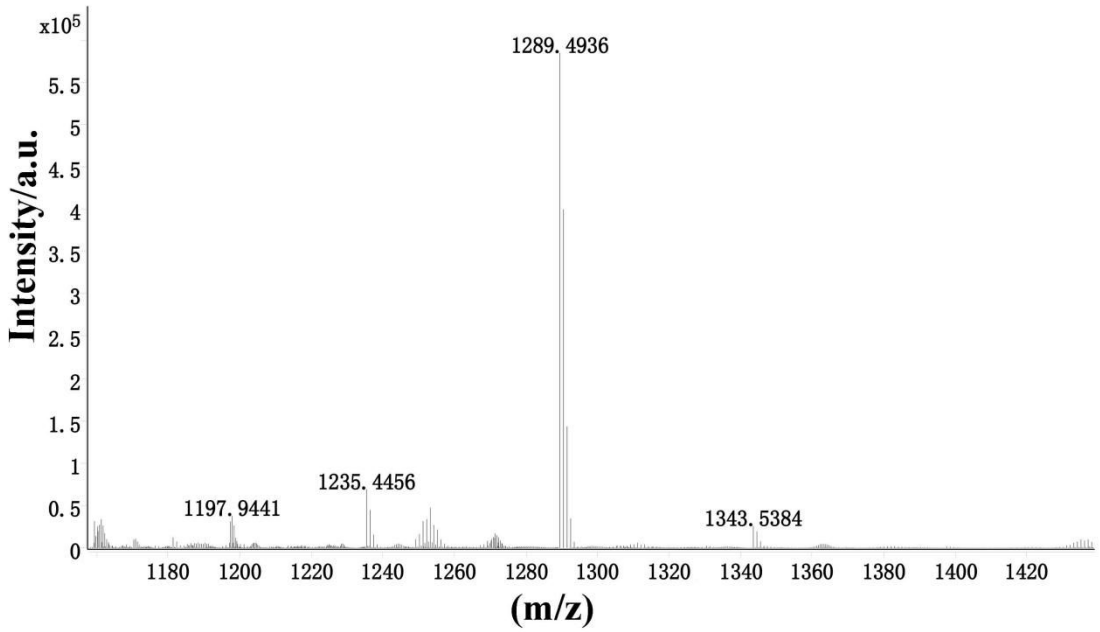

Figure S7. The ESI-TOF mass spectrometry for the exclusion complex $CyH_2Q[6]\cdot G3$. The peak found at *m*/*z* 1277.4226 corresponds to $[CyH_2Q[6]\cdot HG3]^+$ (calculated for $[CyH_2Q[6]\cdot HG3]^+$, 1277.4263).

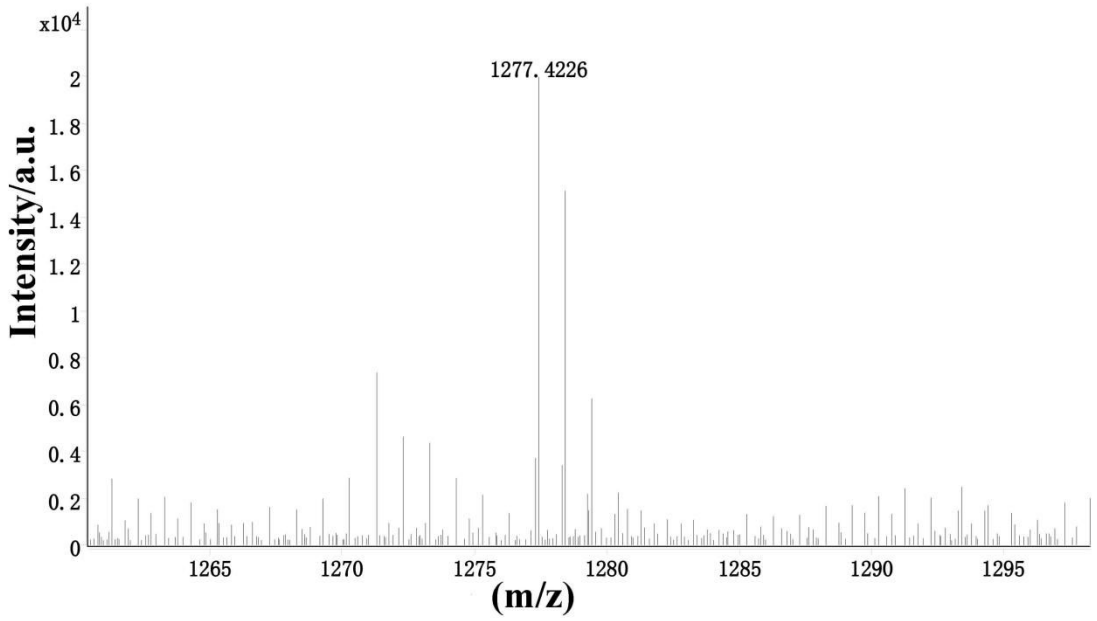

Figure S8. The ESI-TOF mass spectrometry for the exclusion complex $CyH_2Q[6]\cdot G4$. The peak found at *m/z* 1278.4509 corresponds to $[CyH_2Q[6]\cdot HG4]^+$ (calculated for $[CyH_2Q[6]\cdot HG4]^+$, 1278.4103).

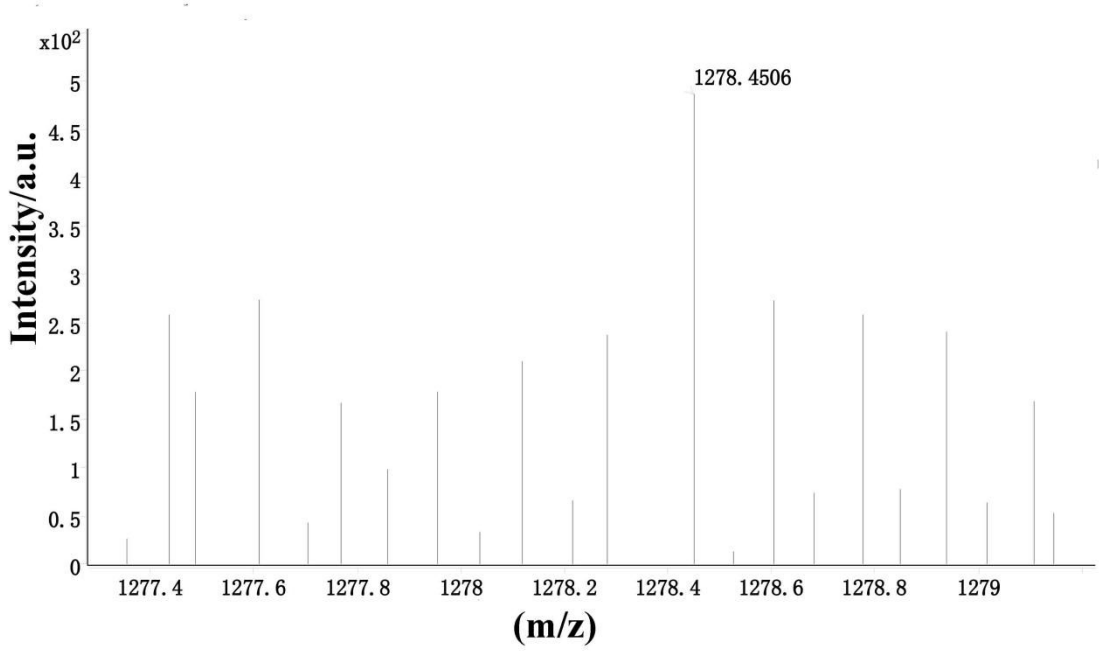

Figure S9. The ESI-TOF mass spectrometry for the exclusion complex $CyH_2Q[6]\cdot G5$. The peak found at *m*/*z* 1275.4107 corresponds to $[CyH_2Q[6]\cdot HG5]^+$ (calculated for $[CyH_2Q[6]\cdot HG5]^+$, 1275.4172).

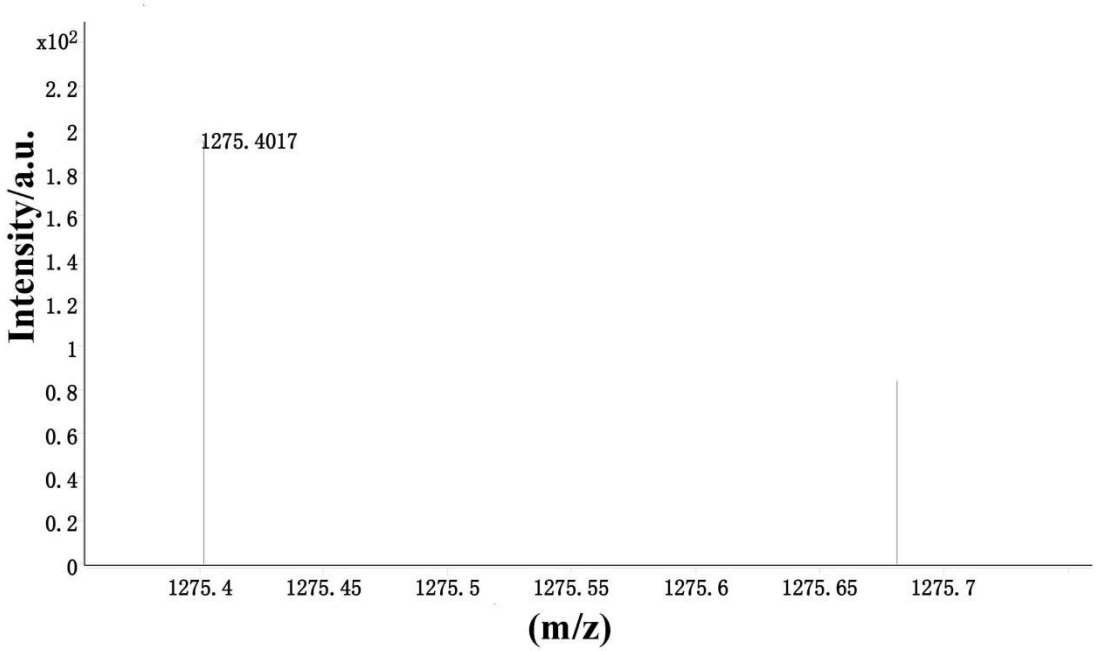

Table S1 Energy comparison of guests inside and outside the $CyH_2Q[6]$. $\Delta E = E$ (inclusion)-E (outer surface).

structure	**inclusion-energy (a.u.)**	**outer wall-energy (a.u.)**	**ΔE (kcal/mol)**
$CyH_2Q[6]$ + G5	-4569.062549	-4569.088718	16.42
$CyH_2Q[6]$ + G2	-4496.605411	-4496.618599	8.28
$CyH_2Q[6]$ + G3	-4814.127223	-4814.145359	11.38
$CyH_2Q[6]$ + G1	-4574.015697	-4574.025285	6.02
$CyH_2Q[6]$ + G4	-4833.993141	-4834.016489	14.65

Table S2. Crystal data as well as details of data collection and refinement for complexes **1**-**5**.

	1	**2**	**3**	**4**	**5**
Formula	$C_{72}H_{108}N_{28}O_{26}Cd_2Cl_8$	$C_{112}H_{164}N_{52}O_{44}Cd_2Cl_8$	$C_{56}H_{96}N_{28}O_{30}CdCl_6S_2$	$C_{56}H_{86}N_{26}O_{30}S_2$	$C_{58}H_{84}Cl_2N_{24}O_{33}$
M_r	2290.28	3451.35	2030.83	1667.63	1716.39
crystal system	triclinic	triclinic	monoclinic	monoclinic	triclinic
space group	*P*-1	*P*-1	*C*2/*c*	$P2_1/c$	*P*-1
a (Å)	11.5924(12)	14.487(2)	31.141(8)	12.3139(8)	11.9454(16)
b (Å)	14.8706(17)	16.686(2)	16.092(3)	22.6477(14)	12.2541(18)
c (Å)	15.7294(18)	16.724(2)	16.818(3)	12.6956(8)	14.643(2)
α (deg)	98.390(4)	73.331(5)	90	90	67.292(5)
β (deg)	103.391(4)	72.632(6)	94.338(12)	91.974(2)	73.031(5)
γ (deg)	109.103(4)	72.657(6)	90	90	71.375(5)
V (Å^3)	2419.0(5)	3595.0(9)	8404(3)	3538.5(4)	1838.6(4)
Z	1	1	4	2	1
*D*c (g·cm^{-3})	1.572	1.594	1.605	1.565	1.550
μ (mm^{-1})	0.747	0.546	0.597	0.183	0.197
F(000)	1176	1784	4200	1752	898
Data/params	9527 /550	13764/955	8260/493	6936/488	7171/487
θ (deg)	1.96-26.00	2.04-26.00	1.90-26.00	2.41-26.00	1.90-26.00
GOF(F^2)	1.006	1.010	1.004	1.007	1.006
$R_1[I>2\sigma(I)]$	0.0409	0.0859	0.0969	0.0668	0.0739
wR_2(all data)	0.1292	0.2595	0.2887	0.2078	0.2506
CCDC No.	2011169	2011170	2011172	2011164	2015547