Electronic Supporting Information

Complexation of triangular silver(I) or copper(I) nitropyrazolates with dibenzothiophenes having potential use in adsorptive desulfurization

Lin Yang[a], Lihong Wang[b], Xingpu Lv[a], Jing-Huo Chen[*a], Yang Wang[*b] and Guang Yang[a*]

[a]*Green Catalysis Center, and College of Chemistry, Zhengzhou University, Zhengzhou, Henan, 450001, China*

[b]*School of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou, Jiangsu 225002, China*

E-mail: yang@zzu.edu.cn; yangwang@yzu.edu.cn; jhchen@zzu.edu.cn

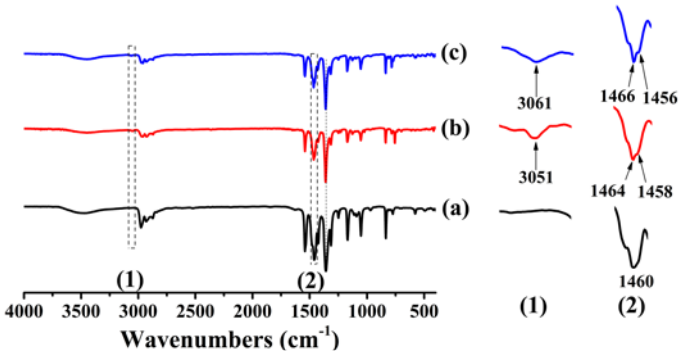

Fig. S1 IR spectra (KBr pellet) of (a) **Ag_3pz_3**, (b) **Ag_3pz_3**·DBT, (c) **Ag_3pz_3**·DMDBT, (1) peaks at 3010-3090 cm^{-1}, (2) peaks at 1430-1500 cm^{-1}.

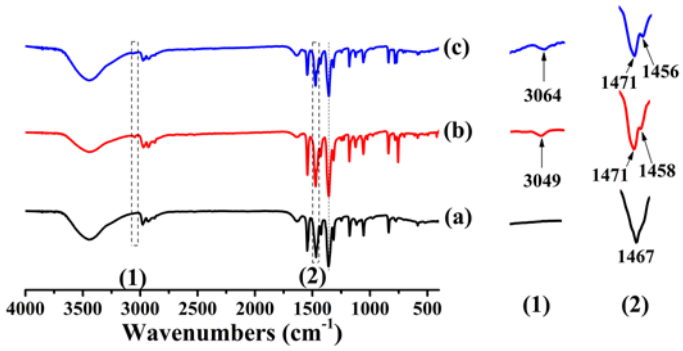

Fig. S2 IR spectra (KBr pellet) of (a) **Cu_3pz_3**, (b) **Cu_3pz_3**·DBT, (c) **Cu_3pz_3**·DMDBT, (1) peaks at 3010-3100 cm^{-1}, (2) peaks at 1440-1500 cm^{-1}.

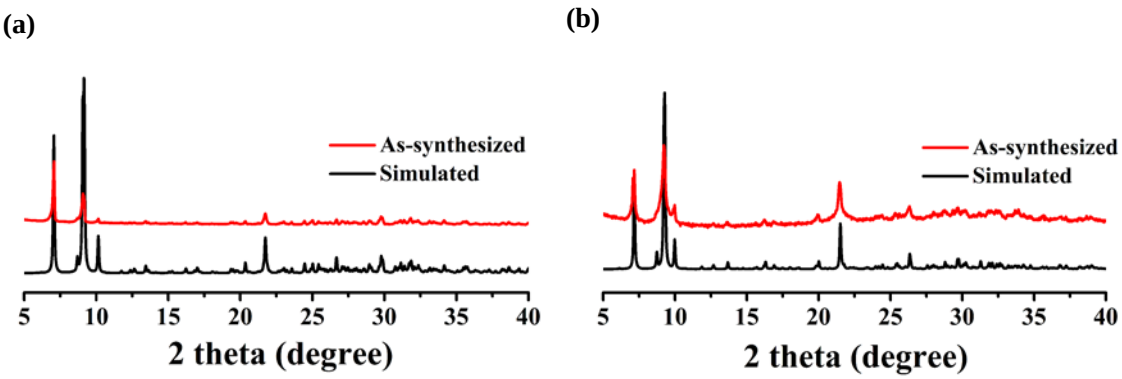

Fig. S3 Comparison of the PXRD pattern of the as-synthesized sample of **Ag_3pz_3** (a) and **Cu_3pz_3** (b) (red line) with the simulated pattern based on the crystal data (black line).

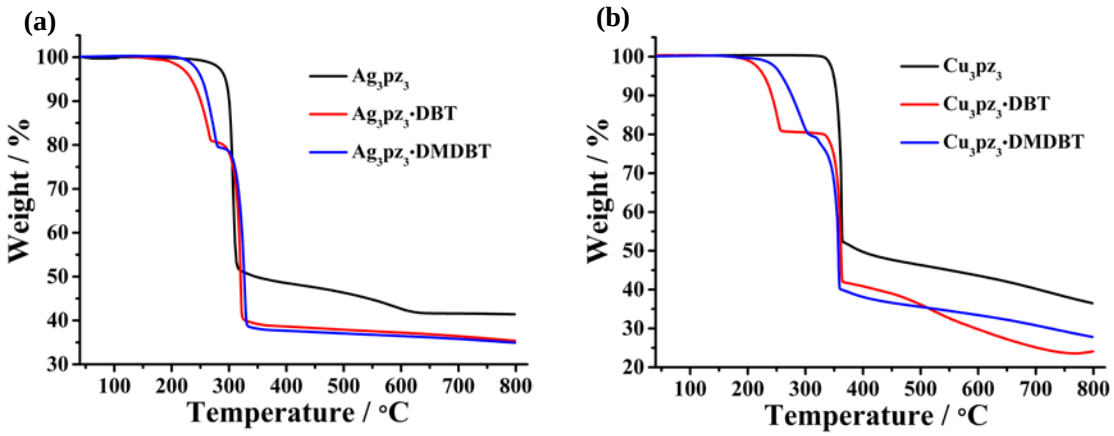

Fig. S4 Thermogravimetric curves of **Ag_3pz_3** (a), **Cu_3pz_3** (b) and their adducts with DBT/DMDBT.

Table S1. Thermogravimetric data of **Ag_3pz_3**, **Cu_3pz_3** and their adducts

	Weight loss (found)	Temperature (°C)	Weight loss (Calc.)	Assignment
Ag_3pz_3·DMDBT	20.5%	141 – 281	20.1%	−DMDBT
Ag_3pz_3·DBT	19.0%	130 – 270	18.2%	−DBT
Cu_3pz_3·DMDBT	21.0%	141 –309	23.2%	−DMDBT
Cu_3pz_3·DBT	19.3%	132 – 260	20.8%	−DBT

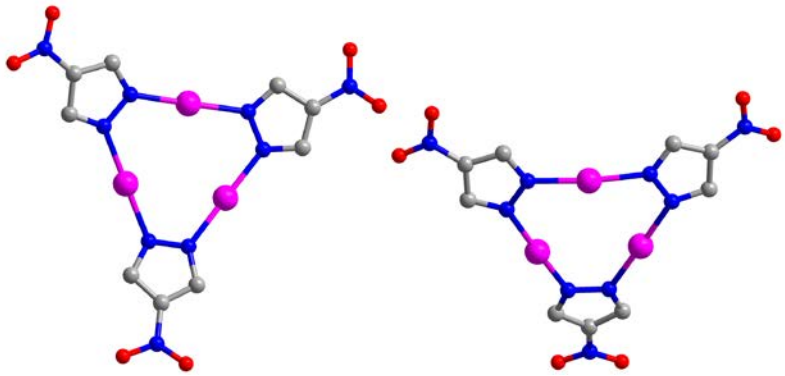

Fig. S5 The asymmetric unit of **Ag_3pz_3** showing two crystallographically independent molecules. Colour code: Ag, pink; N, blue; C, gray and O, red. The diethyl groups and hydrogen atoms of pyrazole have been omitted in this and the following figures for clarity.

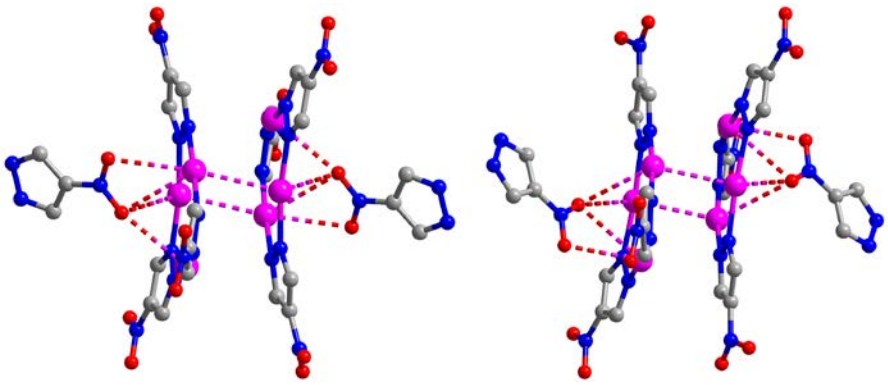

Fig. S6 The dimer of trimers of **Ag_3pz_3**. Colour code: Ag, pink; N, blue; C, gray and O, red.

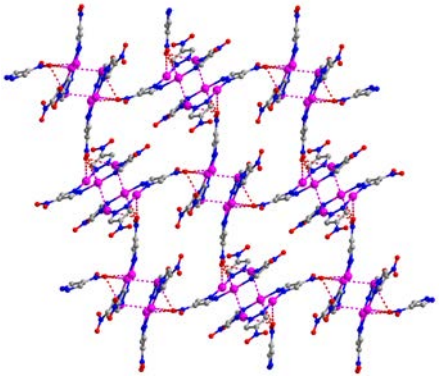

Fig. S7 A fragment of the 2D net in the crystal structure of **Ag_3pz_3**. Colour code: Ag, pink; N, blue; C, gray and O, red.

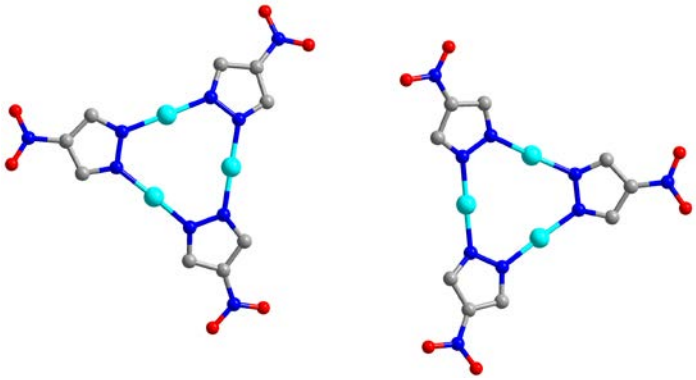

Fig. S8 The asymmetric unit of **Cu_3pz_3** showing two crystallographically independent molecules. Colour code: Cu, turquiose; N, blue; C, gray and O, red.

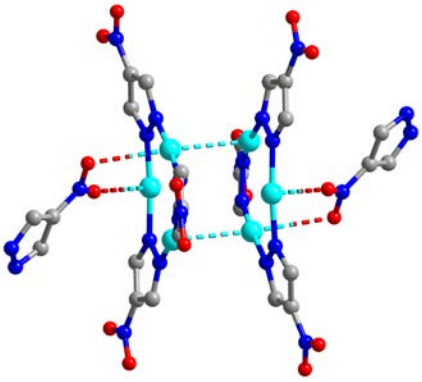

Fig. S9 The dimer of trimers of **Cu_3pz_3**. Colour code: Cu, turquiose; N, blue; C, gray and O, red.

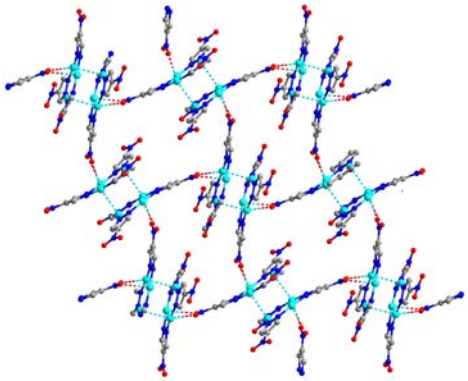

Fig. S10 A fragment of the 2D net in the crystal structure of **Cu_3pz_3**. Colour code: Cu, turquiose; N, blue; C, gray and O, red.

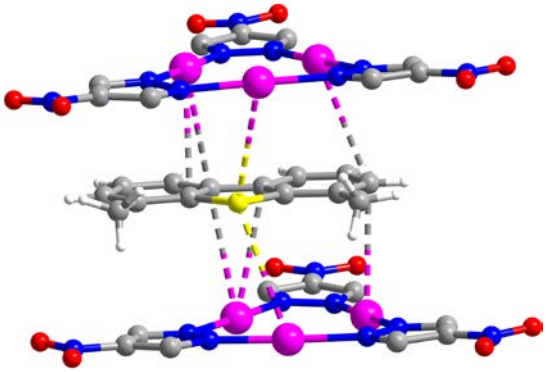

Fig. S11 A fragment of the columnar stacking of **Ag_3pz_3**·DMDBT, showing Ag···S and Ag···C contacts. Ag, pink; N, blue; C, gray; H, white; O, red and S, yellow. The diethyl group of pyrazole have been omitted in this and the following figures for clarity.

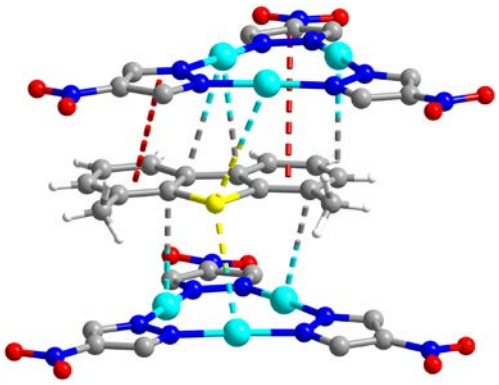

Fig. S12 A fragment of the columnar stacking of **Cu$_3$pz$_3$**·DMDBT, showing Cu···S, Cu···C contacts and π···π interactions. Colour code: Cu, turquiose; N, blue; C, gray; H, white; O, red and S, yellow.

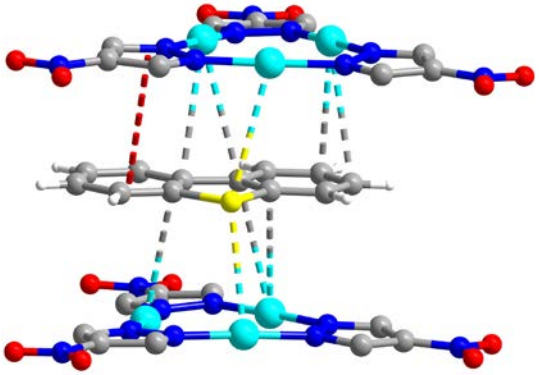

Fig. S13 A fragment of the columnar stacking of **Cu$_3$pz$_3$**·DBT showing Cu···S, Cu···C contacts and π···π stacking interactions. Colour code: Cu, turquiose; N, blue; C, gray; H, white; O, red and S, yellow.

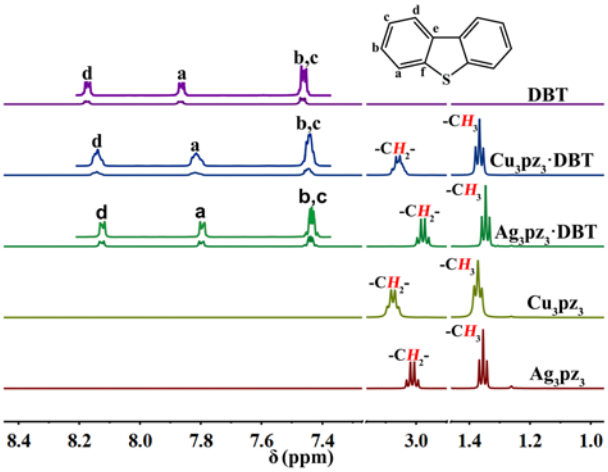

Fig. S14 Stack plot of ^{1}H NMR spectra for DBT, **Cu$_3$pz$_3$**·DBT, **Ag$_3$pz$_3$**·DBT, **Cu$_3$pz$_3$** and **Ag$_3$pz$_3$** in CD_2Cl_2.

Table S2. Comparison of ^{1}H NMR of DBT, **Cu$_3$pz$_3$**·DBT **Ag$_3$pz$_3$**·DBT, **Cu$_3$pz$_3$** and **Ag$_3$pz$_3$**

^{1}H NMR/ppm	d	a	b,c	C*H*$_2$	C*H*$_3$
DBT	8.19 (dd)	7.89 (dd)	7.48 (m)		
Cu$_3$pz$_3$				3.08 (q)	1.37 (t)
Cu$_3$pz$_3$·DBT	8.14 (t)	7.82 (dd)	7.45 (m)	3.07 (q)	1.37 (t)
Δ/ppm	0.05	0.07	0.03	0.01	0
Ag$_3$pz$_3$				3.01 (q)	1.36 (t)
Ag$_3$pz$_3$·DBT	8.13 (dd)	7.80 (dd)	7.44 (m)	2.98 (q)	1.35 (t)
Δ/ppm	0.06	0.09	0.04	0.03	0.01

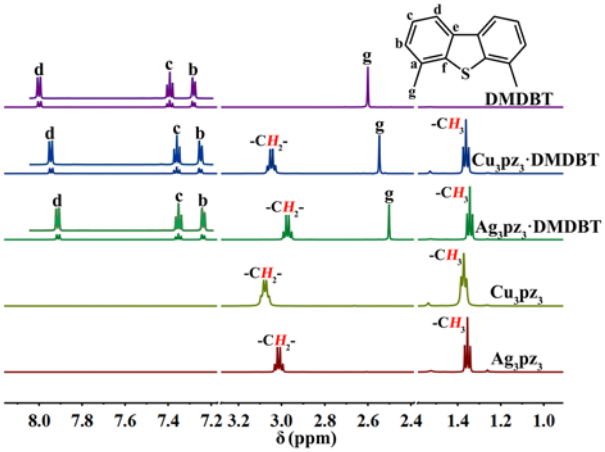

Fig. S15 Stack plot of ^{1}H NMR spectra for DMDBT, **Cu$_3$pz$_3$**·DMDBT, **Ag$_3$pz$_3$**·DMDBT, **Cu$_3$pz$_3$** and **Ag$_3$pz$_3$** in CD_2Cl_2.

Table S3. Comparison of ^{1}H NMR of DMDBT, **Cu$_3$pz$_3$**·DMDBT **Ag$_3$pz$_3$**·DMDBT, **Cu$_3$pz$_3$** and **Ag$_3$pz$_3$**

`	d	c	b	g	C*H*$_2$	C*H*$_3$
DMDBT	8.02 (d)	7.41 (t)	7.30 (d)	2.62 (s)		
Cu$_3$pz$_3$					3.08 (q)	1.37 (t)
Cu$_3$pz$_3$·DMDBT	7.95 (d)	7.37 (t)	7.26 (d)	2.55 (s)	3.05 (q)	1.37 (t)
Δ/ppm	0.07	0.04	0.04	0.07	0.03	0
Ag$_3$pz$_3$					3.01 (q)	1.36 (t)
Ag$_3$pz$_3$·DMDBT	7.92 (d)	7.36 (t)	7.24 (d)	2.51 (s)	2.98 (q)	1.35 (t)
Δ/ppm	0.1	0.05	0.06	0.11	0.03	0.01

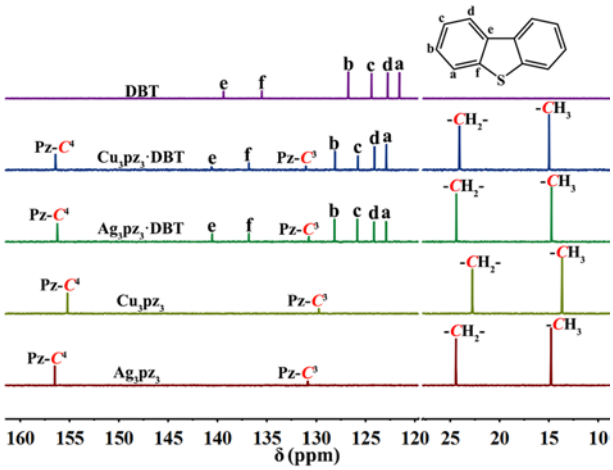

Fig. S16 Stack plot of ^{13}C NMR spectra for DBT, **Cu$_3$pz$_3$**·DBT, **Ag$_3$pz$_3$**·DBT, **Cu$_3$pz$_3$** and **Ag$_3$pz$_3$** in CD_2Cl_2.

Table S4. Comparison of ^{13}C NMR of DBT, **Cu$_3$pz$_3$**·DBT, **Ag$_3$pz$_3$**·DBT **Cu$_3$pz$_3$** and **Ag$_3$pz$_3$**.

^{13}C NMR/ppm	e	f	b	c	d	a	pz-*C*^{3}	pz-*C*^{4}	*C*H$_2$	*C*H$_3$
DBT	139.81	135.92	127.18	124.83	123.18	122.00				
Cu$_3$pz$_3$							130.17	155.64	23.19	14.09
Cu$_3$pz$_3$·DBT	139.71	135.91	127.21	124.87	123.19	121.99	130.14	155.52	23.17	14.08
Δ/ppm	0.1	0.01	-0.03	-0.04	-0.01	0.01	0.03	0.12	0.02	0.01
Ag$_3$pz$_3$							129.94	155.60	23.51	13.87
Ag$_3$pz$_3$·DBT	139.63	135.91	127.25	124.93	123.24	122.02	129.86	155.34	23.48	13.83
Δ/ppm	0.18	0.01	-0.07	-0.1	-0.06	-0.02	0.08	0.26	0.03	0.04

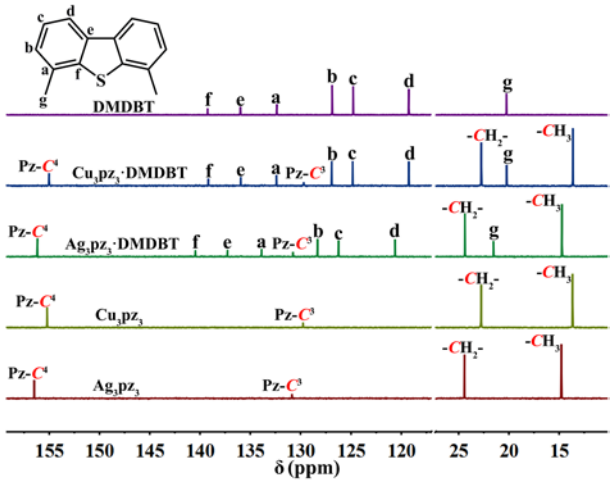

Fig. S17 Stack plot of ^{13}C NMR spectra for DMDBT, **Cu$_3$pz$_3$**·DMDBT, **Ag$_3$pz$_3$**·DMDBT, **Cu$_3$pz$_3$** and **Ag$_3$pz$_3$** in CD_2Cl_2.

Table S5. Comparison of ^{13}C NMR of DMDBT, **Cu_3pz_3**·DMDBT, **Ag_3pz_3**·DMDBT, **Cu_3pz_3** and **Ag_3pz_3**.

^{13}C NMR/ppm	f	e	a	b	c	d	g	pz-C^3	pz-C^4	CH_2	CH_3
DMDBT	139.67	136.40	132.78	127.32	125.22	119.69	20.67				
Cu_3pz_3								130.17	155.64	23.19	14.09
Cu_3pz_3·DMDBT	139.60	136.37	132.82	127.36	125.27	119.69	20.65	130.11	155.45	23.17	14.06
Δ/ppm	0.07	0.03	-0.04	-0.04	-0.05	0	0.02	0.06	0.19	0.02	0.03
Ag_3pz_3								129.94	155.60	23.51	13.87
Ag_3pz_3·DMDBT	139.56	136.36	132.97	127.44	125.35	119.72	20.63	129.84	155.27	23.47	13.82
Δ/ppm	0.11	0.04	-0.19	-0.12	-0.13	-0.03	0.04	0.1	0.33	0.04	0.05

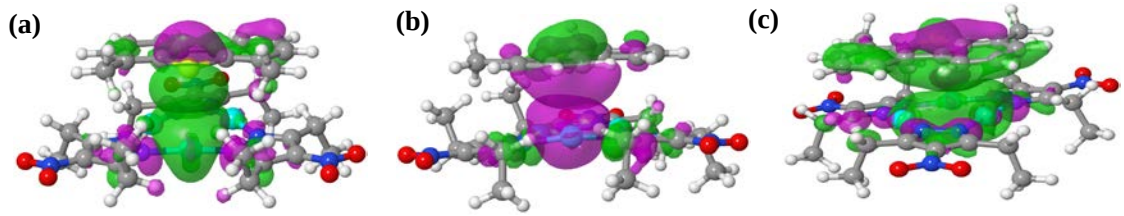

Fig. S18 The three most important MBFO pairs for the interactions between **Ag_3pz_3** and DMDBT. The bond order for the MBFO pair is 0.050, 0.019 and 0.015 in (a), (b) and (c), respectively. The orbitals are shown with an isovalue of 0.03.

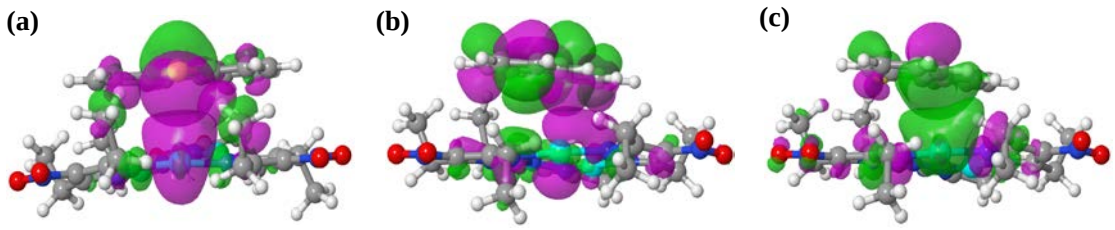

Fig. S19 The three most important MBFO pairs for the interactions between **Cu_3pz_3** and DBT. The bond order for the MBFO pair is 0.029, 0.024 and 0.023in (a), (b) and (c), respectively. The orbitals are shown with an isovalue of 0.03.

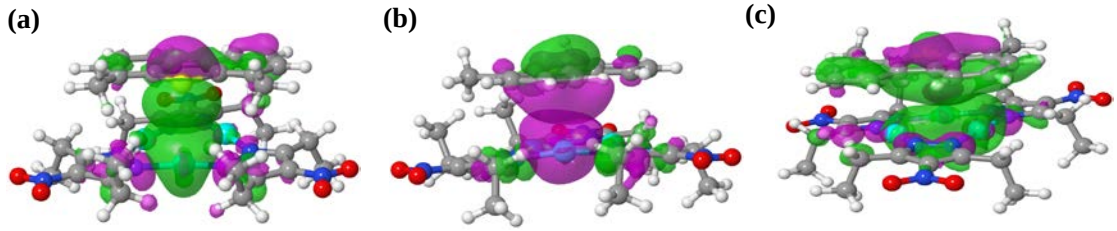

Fig. S20 The three most important MBFO pairs for the interactions between **Cu_3pz_3** and DMDBT. The bond order for the MBFO pair is 0.031, 0.017 and 0.014 in (a), (b) and (c), respectively. The orbitals are shown with an isovalue of 0.03.

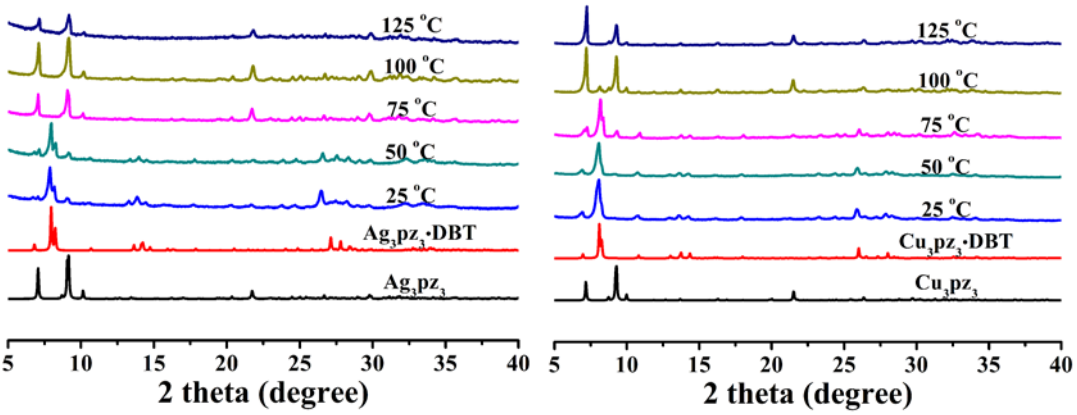

Fig. S21 Comparison of the PXRD patterns of DBT-adsorbed samples of **Ag_3pz_3**/**Cu_3pz_3** at different temperatures with those simulated from their crystal data (red and black line). (Experimental condition: 0.02 mmol M_3pz_3 in 10 mL of *n*-octane containing 1000 mg S/L of DBT with the molar ratio of S: M_3pz_3 = 15.6)

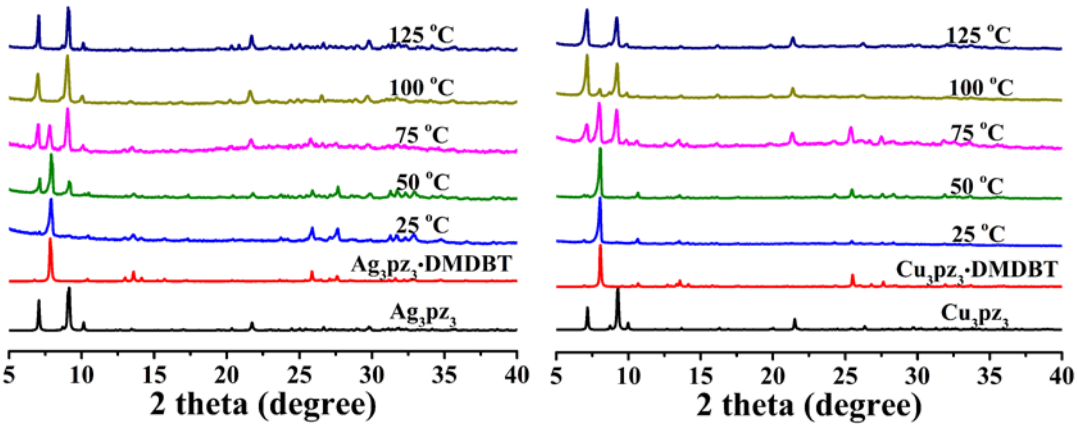

Fig. S22 Comparison of the PXRD patterns of DMDBT-adsorbed samples of **Ag_3pz_3**/**Cu_3pz_3** at different temperatures with those simulated from their crystal data (red and black line). (Experimental condition: 0.02 mmol M_3pz_3 in 10 mL of *n*-octane containing 800 mg S/L of DMDBT with the molar ratio of S: M_3pz_3 = 12.5)

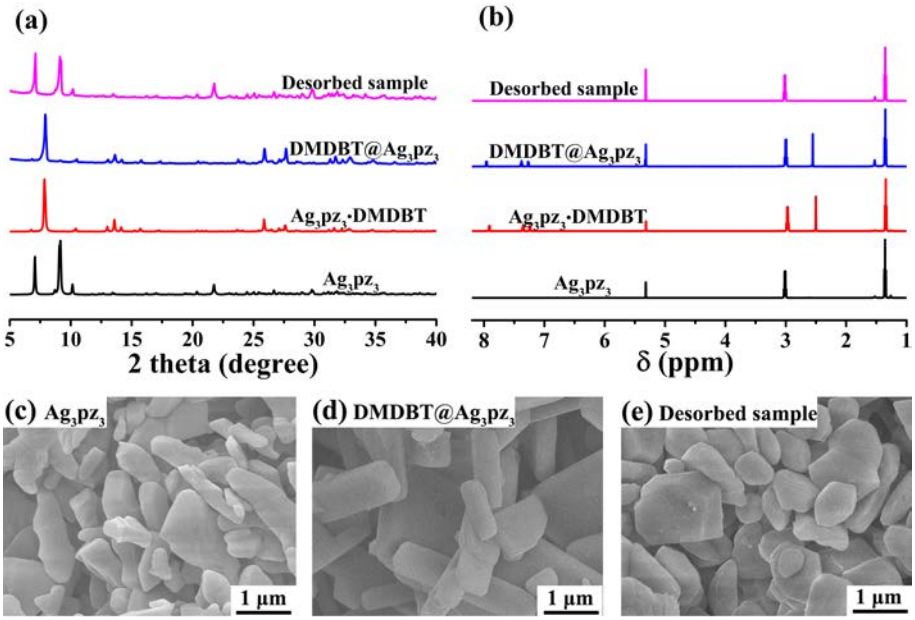

Fig. S23 PXRD patterns (a), ^{1}HNMR spectra (b) and SEM images (c,d,e) of the DMDBT-adsorbed and desorbed samples of **Ag_3pz_3** in comparison with those of **Ag_3pz_3** or **Ag_3pz_3**·DMDBT.

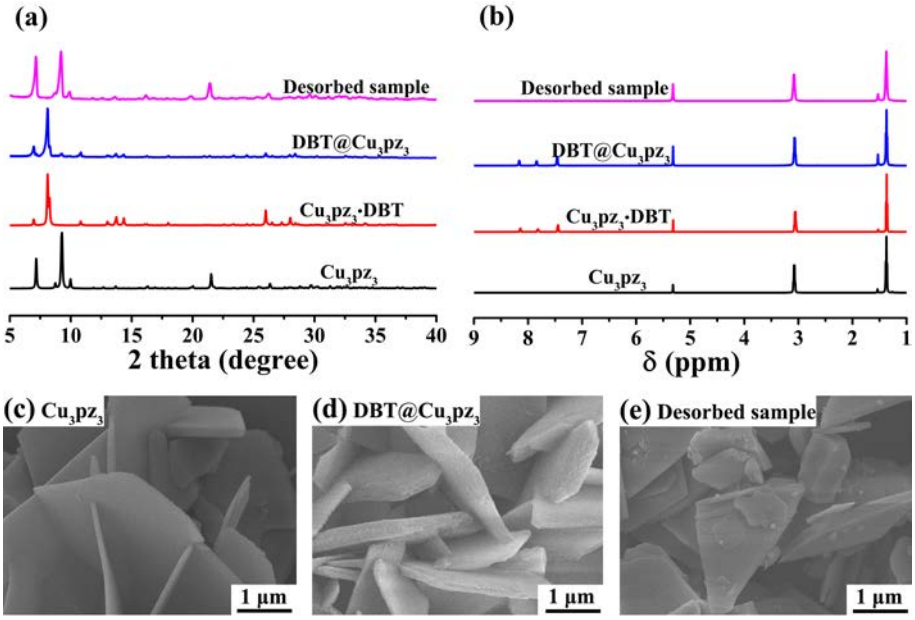

Fig. S24 PXRD patterns (a), ^{1}HNMR spectra (b) and SEM images (c,d,e) of the DBT-adsorbed and desorbed samples of **Cu_3pz_3** in comparison with those of **Cu_3pz_3** or **Cu_3pz_3**·DBT.

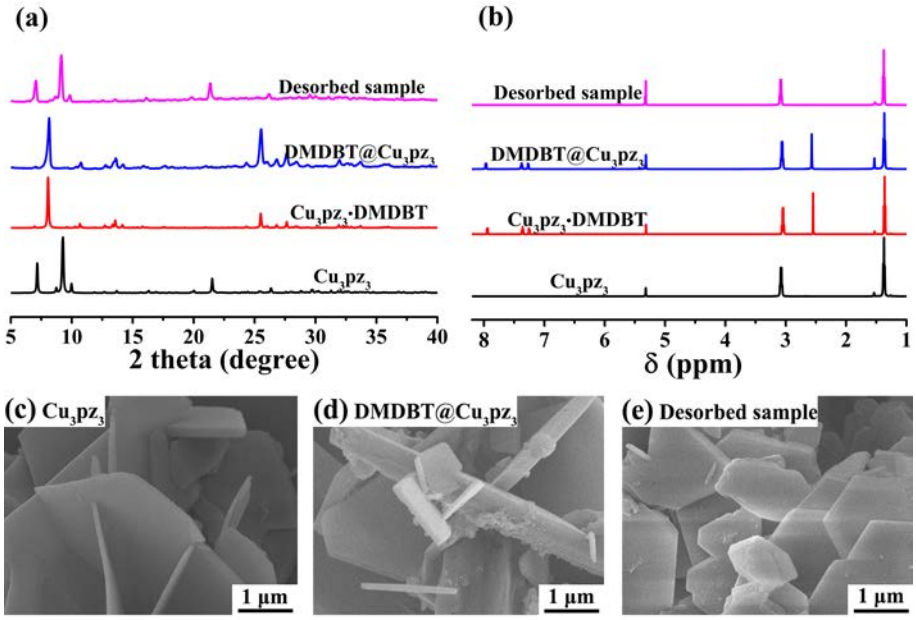

Fig. S25 PXRD patterns (a), ^{1}HNMR spectra (b) and SEM images (c,d,e) of the DMDBT-adsorbed and desorbed samples of **Cu_3pz_3** in comparison with those of **Cu_3pz_3** or **Cu_3pz_3**·DMDBT.

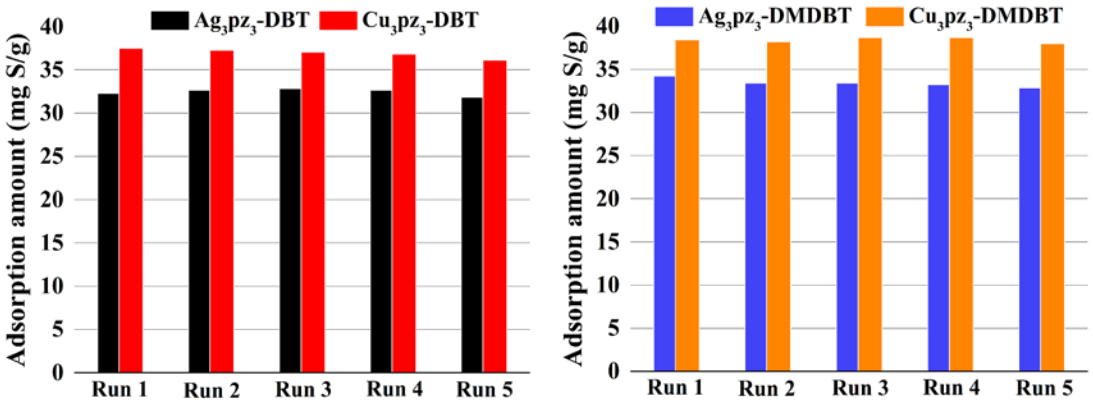

Fig. S26 Recycling test of **Ag_3pz_3** (0.02 mmol) and **Cu_3pz_3** (0.02 mmol) for the adsorption of DBT and DMDBT from *n*-octane containing 1000 mg S/L of DBT or 800 mg S/L of DMDBT (10 mL).

Table S6 Crystallographic data and structure refinements

	Ag$_3$pz$_3$	**Ag$_3$pz$_3$**·DBT	**Ag$_3$pz$_3$**·DMDBT	(**Ag$_3$pz$_3$**)$_2$·BT
Formula	$C_{42}H_{60}Ag_6N_{18}O_{12}$	$C_{33}H_{38}Ag_3N_9O_6S$	$C_{35}H_{42}Ag_3N_9O_6S$	$C_{50}H_{66}Ag_6N_{18}O_{12}S$
Mol. wt.	1656.30	1012.39	1040.44	1790.48
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$C2/c$
a (Å)	25.0348(10)	13.1758(2)	13.2738(6)	19.2517(4)
b (Å)	17.4283(7)	21.4602(4)	22.3282(7)	24.1571(5)
c (Å)	13.2012(5)	13.1785(3)	13.8197(6)	14.3647(3)
α (deg)				
β (deg)	91.0170(10)	100.0406(18)	100.078(4)	105.5782(8)
γ (deg)				
V (Å^3)	5759.0(4)	3669.21(13)	4032.7(3)	6435.1(2)
Z	4	4	4	4
T (K)	298.15(10)	120(10)	298.15(10)	298.15(10)
$\rho_{calcd.}$ (Mg/m^3)	1.910	1.833	1.714	1.848
μ (mm^{-1})	2.071	1.699	1.549	1.893
Reflns collected	73119	27145	28415	41721
Reflns unique	10151	6466	7123	5677
	(R_{int} = 0.0723)	(R_{int} = 0.0964)	(R_{int} = 0.0532)	(R_{int} = 0.0757)
Final R indices [I> 2σ(I)]	R_1 = 0.0404	R_1 = 0.0366	R_1 = 0.0626	R_1 = 0.0480
	wR_2 = 0.0825	wR_2 = 0.0797	wR_2 = 0.1762	wR_2 = 0.1056
S	1.026	1.030	1.067	1.062
$\Delta\rho_{max}$(eÅ^{-3})	1.20	1.10	0.79	0.69
$\Delta\rho_{min}$(eÅ^{-3})	-0.88	-1.35	-0.93	-0.66

Table S7 Crystallographic data and structure refinements

	Cu_3pz_3	**Cu_3pz_3**·DBT	**Cu_3pz_3**·DMDBT
Formula	$C_{21}H_{30}Cu_3N_9O_6$	$C_{33}H_{38}Cu_3N_9O_6S$	$C_{35}H_{42}Cu_3N_9O_6S$
Mol. wt.	695.16	879.40	907.45
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	24.6486(15)	12.8446(18)	12.8398(6)
b (Å)	17.7157(10)	21.390(3)	21.8537(10)
c (Å)	12.7565(7)	13.7791(19)	14.0702(6)
α (deg)			
β (deg)	90.671(2)	99.202(4)	98.4970(10)
γ (deg)			
V (Å^3)	5570.0(6)	3737.0(9)	3904.7(3)
Z	8	4	4
T (K)	298.15(10)	298.15(10)	298.15(10)
$\rho_{calcd.}$ (Mg/m^3)	1.658	1.563	1.544
μ (mm^{-1})	2.323	1.803	1.728
Reflns collected	69497	45165	61638
Reflns unique	9813	6597	6899
	(R_{int} = 0.0426)	(R_{int} = 0.0466)	(R_{int} = 0.0352)
Final R indices	R_1 = 0.0519	R_1 = 0.0500	R_1 = 0.0357
[I> 2σ(I)]	wR_2 = 0.1267	wR_2 = 0.1300	wR_2 = 0.0844
S	1.059	1.022	1.019
$\Delta\rho_{max}$(eÅ^{-3})	0.97	0.62	0.67
$\Delta\rho_{min}$(eÅ^{-3})	-0.65	-0.47	-0.52

Table S8 Selected bond distances (Å) and bond angles (º).

Ag_3pz_3			
Ag(1)-N(1)	2.095(5)	Ag(1)-N(6)	2.091(5)
Ag(2)-N(2)	2.097(5)	Ag(2)-N(3)	2.084(5)
Ag(3)-N(4)	2.073(5)	Ag(3)-N(5)	2.082(5)
Ag(4)-N(10)	2.058(5)	Ag(4)-N(15)	2.067(5)
Ag(5)-N(11)	2.085(5)	Ag(5)-N(12)	2.087(5)
Ag(6)-N(13)	2.093(5)	Ag(6)-N(14)	2.077(5)
Ag(1)···Ag(3) [#1]	3.0950(7)	Ag(4)···Ag(6) [#2]	3.1172(7)
Ag(1)···O(1) [#1]	3.0346(53)	Ag(1)···O(2) [#1]	3.0583(62)
Ag(2)···O(2) [#1]	2.9467(58)	Ag(3)···O(2) [#1]	3.1832(67)
Ag(4)···O(10)	3.1947(69)	Ag(5)···O(10)	3.0791(71)
Ag(5)···O(9)	2.9765(53)	Ag(6)···O(10)	2.9633(71)
N(6)-Ag(1)-N(1)	177.41(18)	N(3)-Ag(2)-N(2)	173.7(2)
N(4)-Ag(3)-N(5)	172.7(2)	N(10)-Ag(4)-N(15)	174.4(2)
N(11)-Ag(5)-N(12)	176.1(2)	N(14)-Ag(6)-N(13)	175.4(2)
[#1] 1-x, 1-y, -z; [#2] -x, 2-y, -z			
Ag_3pz_3·DBT			
Ag(1)-N(1)	2.084(3)	Ag(1)-N(6)	2.087(3)
Ag(2)-N(2)	2.104(3)	Ag(2)-N(3)	2.082(3)
Ag(3)-N(4)	2.068(3)	Ag(3)-N(5)	2.073(3)
Ag(1)···S(1) [#]	3.3752(11)	Ag(3)···S(1)	3.4064(11)
Ag(1)···C(28)	3.3284(40)	Ag(2)···C(26)	3.3155(39)
Ag(2)···C(26) [#]	3.6627(41)	Ag(2)···C(25) [#]	3.5113(39)
Ag(2)···C(25)	3.2411(42)	Ag(3)···C(28)	3.2855(40)
N(1)-Ag(1)-N(6)	175.42(11)	N(3)-Ag(2)-N(2)	177.15(11)
N(4)-Ag(3)-N(5)	179.48(11)		
[#] x, 1.5-y, -0.5+z			
Ag_3pz_3·DMDBT			
Ag(1)-N(1)	2.081(6)	Ag(1)-N(6)	2.075(6)
Ag(2)-N(2)	2.076(6)	Ag(2)-N(3)	2.076(6)
Ag(3)-N(4)	2.076(6)	Ag(3)-N(5)	2.076(6)
Ag(1)···S(1)	3.8077(21)	Ag(2)···S(1)	3.6251(21)
Ag(1)···C(27)	3.5101(70)	Ag(1)···C(22)	3.3629(74)
Ag(2)···C(27) [#]	3.4680(71)	Ag(2)···C(28) [#]	3.5070(77)
Ag(3)···C(31)	3.5654(95)	Ag(3)···C(31) [#]	3.4990(103)
N(6)-Ag(1)-N(1)	177.9(2)	N(3)-Ag(1)-N(2)	176.6(2)
N(4)-Ag(3)-N(5)	178.8(3)		
[#] x, 0.5-y, 0.5+z			
(**Ag_3pz_3**)$_2$·BT			

Ag(1)-N(1)	2.071(5)	Ag(1)-N(6)	2.067(5)
Ag(2)-N(2)	2.068(5)	Ag(2)-N(3)	2.076(6)
Ag(3)-N(4)	2.092(5)	Ag(3)-N(5)	2.086(5)
Ag(1)···Ag(2)[#]	3.091(7)	Ag(2)···C(23A)	3.468(273)
Ag(2)···C(24A)	3.400(311)	Ag(1)···C(25A)	3.467(263)
Ag(1)···C(26A)	3.481(274)	Ag(3)···C(28B)	3.534(228)
Ag(3)···C(27B)	3.395(170)	Ag(2)···C(23B)	3.390(221)
Ag(1)···C(25B)	3.153(225)	Ag(2)···S(1A)	3.468(273)
Ag(1)···C(28A)	3.322(329)	Ag(3)···C(26A)	3.482(321)
Ag(2)···S(1B)	3.326(175)	Ag(1)···C(28B)	3.412(240)
Ag(3)···C(25B)	3.701(218)	Ag(3)···C(24B)	3.717(221)
N(6)-Ag(1)-N(1)	175.9(2)	N(2)-Ag(2)-N(3)	177.3(2)
N(5)-Ag(3)-N(4)	177.9(2)		
[#] 0.5-x, 0.5-y, 1-z			
Cu_3pz_3			
Cu(1)-N(1)	1.858(4)	Cu(1)-N(6)	1.855(4)
Cu(2)-N(2)	1.870(5)	Cu(2)-N(3)	1.861(5)
Cu(3)-N(4)	1.850(5)	Cu(3)-N(5)	1.850(4)
Cu(4)-N(10)	1.854(4)	Cu(4)-N(15)	1.854(4)
Cu(5)-N(11)	1.861(4)	Cu(5)-N(13)	1.867(4)
Cu(6)-N(13)	1.862(4)	Cu(6)-N(14)	1.869(4)
Cu(2)···Cu(3)[#1]	3.0199(11)	Cu(4)···Cu(6)[#2]	2.9349(10)
Cu(1)···O(1)	2.9699(53)	Cu(2)···O(2)	2.9529(79)
Cu(5)···O(9)	2.8145(78)	Cu(6)···O(10)	3.0976(53)
N(6)-Cu(1)-N(1)	176.5(2)	N(3)-Cu(2)-N(2)	174.5(2)
N(5)-Cu(3)-N(4)	173.4(2)	N(15)-Cu(4)-N(10)	171.8(2)
N(11)-Cu(5)-N(12)	175.6(2)	N(13)-Cu(6)-N(14)	174.61(19)
[#1]1-x, 1-y, -z; [#2]-x, 1-y, -1-z			
Cu_3pz_3·DBT			
Cu(1)-N(1)	1.861(4)	Cu(1)-N(6)	1.855(4)
Cu(2)-N(2)	1.859(4)	Cu(2)-N(3)	1.854(3)
Cu(3)-N(4)	1.854(4)	Cu(3)-N(5)	1.854(4)
Cu(2)···S(1)[#]	3.2871(19)	Cu(3)···S(1)	3.5658(18)
Cu(1)···C(24)	3.5669(43)	Cu(1)···C(25)	3.5136(42)
Cu(1)···C(22)[#]	3.5040(34)	Cu(1)···C(27)[#]	3.4207(33)
Cu(2)···C(27)	3.5889(33)	Cu(2)···C(28)	3.5128(42)
Cu(3)···C(33)[#]	3.4782(43)	N(6)-Cu(1)-N(1)	178.16(18)
N(3)-Cu(2)-N(2)	176.16(16)	N(5)-Cu(3)-N(4)	178.88(18)
[#] x, 0.5-y, -0.5+z			
Cu_3pz_3·DMDBT			
Cu(1)-N(6)	1.854(2)	Cu(1)-N(1)	1.852(2)

Cu(2)-N(2)	1.854(2)	Cu(2)-N(3)	1.854(3)
Cu(3)-N(4)	1.845(3)	Cu(3)-N(5)	1.851(3)
Cu(1)···S(1)	3.5872(10)	Cu(3)···S(1)[#]	3.9414(10)
Cu(1)···C(27)[#]	3.4863(32)	Cu(1)···C(28)[#]	3.6231(29)
Cu(2)···C(24)[#]	3.5847(44)	Cu(2)···C(23)	3.4631(31)
Cu(3)···C(29)	3.3329(29)	N(1)-Cu(1)-N(6)	176.98(11)
N(2)-Cu(2)-N(3)	177.20(12)	N(4)-Cu(3)-N(5)	177.93(11)

[#] x, 0.5-y, 0.5+z