Table S1 Selected bond distances of **matc***

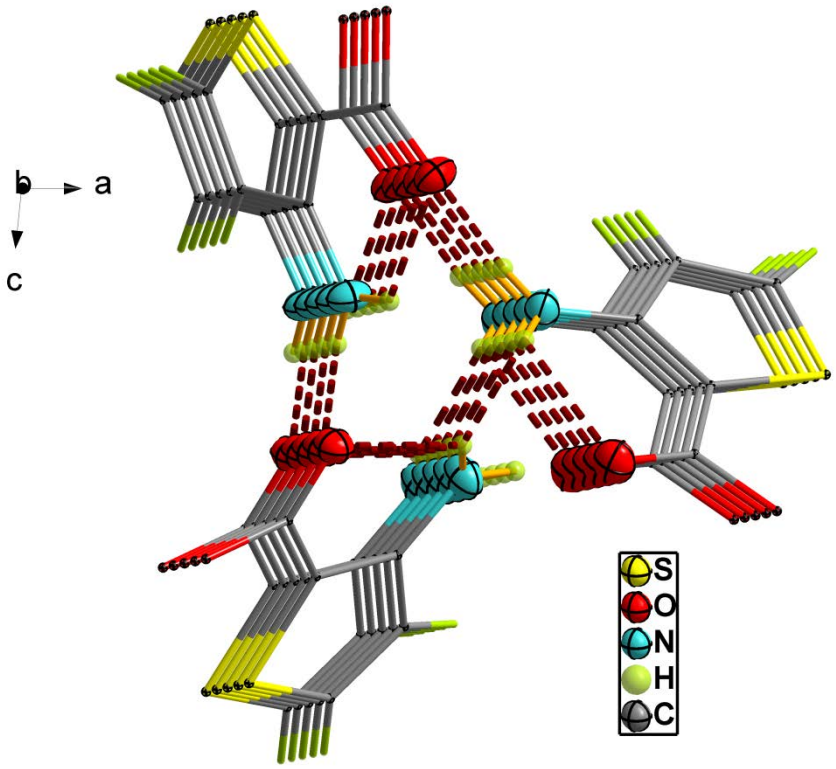
Molecule A		Molecule B		Molecule C	
Bond	**Distances /Å**	**Bond**	**Distances /Å**	**Bond**	**Distances /Å**
S3–C13	1.7383(17)	**S1–C1**	1.7348(17)	**S2–C7**	1.7395(16)
S3–C18	1.7121(19)	**S1–C6**	1.7118(18)	**S2–C12**	1.7113(19)
O6–C14	1.349(2)	**O1–C2**	1.350(2)	**O3–C8**	1.344(2)
O6–C15	1.446(2)	**O1–C3**	1.443(2)	**O3–C9**	1.446(2)
O5–C14	1.219(2)	**O2–C2**	1.226(2)	**O4–C8**	1.222(2)
N3-H3E	0.8630	**N1–H1A**	0.8526	**N2–H2A**	0.8916
N3-H3D	0.8249	**N1–H1B**	0.8358	**N2–H2B**	0.8009
N3–C16	1.347(2)	**N1–C4**	1.351(2)	**N2–C10**	1.354(2)
C14–C13	1.442(2)	**C1–C2**	1.432(2)	**C8–C7**	1.441(2)
C16–C13	1.390(2)	**C1–C4**	1.398(2)	**C7–C10**	1.392(2)
C16–C17	1.435(2)	**C4–C5**	1.429(2)	**C10–C11**	1.433(2)
C17–C18	1.357(3)	**C5–C6**	1.358(3)	**C11–C12**	1.358(3)

* For the different molecules, please refer to the Fig. 1.

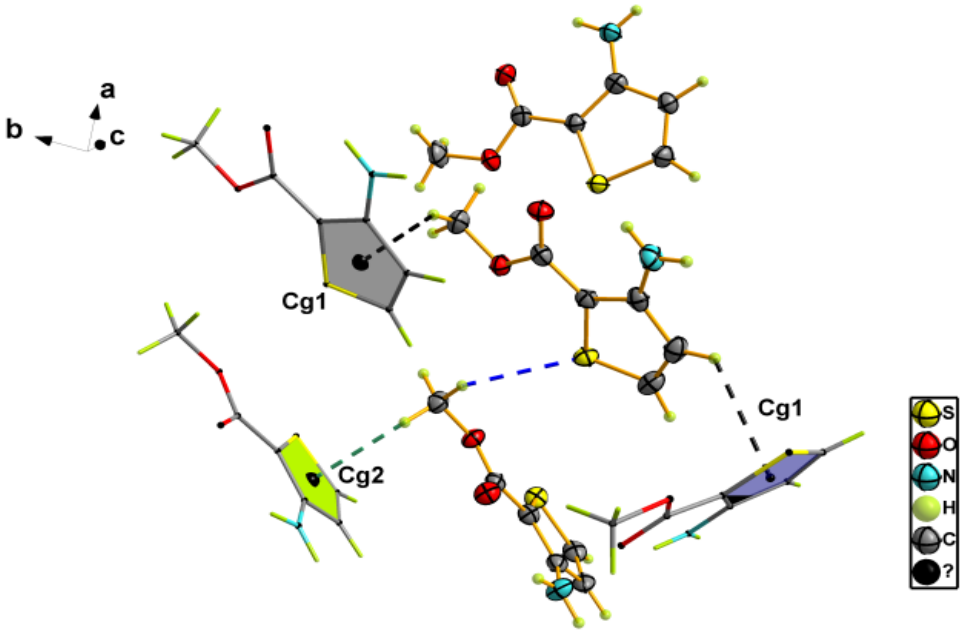
Table S2 Selected bond angles **of matc***

Molecule A		Molecule B		Molecule C	
Angles	/°	**Angles**	/°	**Angles**	/°
C6 – S1 – C1	91.10(8)	**C18 – S3 – C13**	90.83(8)	**C12 – S2 – C7**	90.93(9)
C2 – O1 – C3	115.03(14)	**C14 – O6 – C15**	115.67(15)	**C8 – O3 – C9**	115.98(13)
C2 – C1 – S1	123.44(12)	**C14 – C13 – S3**	123.39(13)	**C8 – C7 – S2**	122.37(12)
C4 – C1 – S1	111.61(12)	**C17– C18– S3**	113.65(14)	**C11 – C12 – S2**	113.49(13)
C5 – C6 – S1	113.34(14)	**C16 – C13 – S3**	111.81(12)	**C10 – C7 – S2**	111.73(12)
O2 – C2 – O1	122.65(15)	**O5 – C14 – O6**	122.83(15)	**O4 – C8 – O3**	123.43(15)
O2 – C2 – C1	124.19(15)	**O5 – C14 – C13**	124.04(16)	**O4 – C8 – C7**	123.79(15)
O1 – C2 – C1	113.14(14)	**O6 – C14 – C13**	113.13(15)	**O3 – C8 – C7**	112.78(14)
N1 – C4 – C1	125.21(16)	**N3 – C16 – C13**	125.38(16)	**N2 – C10 – C7**	125.37(16)
N1 – C4 – C5	123.45(16)	**N3 – C16 – C17**	123.15(16)	**N2 – C10 – C11**	123.24(16)
C4 – C1 – C2	124.94(15)	**C16 – C13 – C14**	124.80(15)	**C10 – C7 – C8**	125.90(15)
C1 – C4 – C5	111.31(15)	**C13 – C16 – C17**	111.47(15)	**C7 – C10 – C11**	111.39(15)
C6 – C5 – C4	112.63(16)	**C18 – C17 – C16**	112.24(16)	**C12 – C11 – C10**	112.45(16)

* For the different molecules, please refer to the Fig. 1.



a



b

Fig. S1 (a) A view of the strong hydrogen-bonds along the *b* axis in **matc**; (b): Weak interactions in the asymmetric unit of **matc**

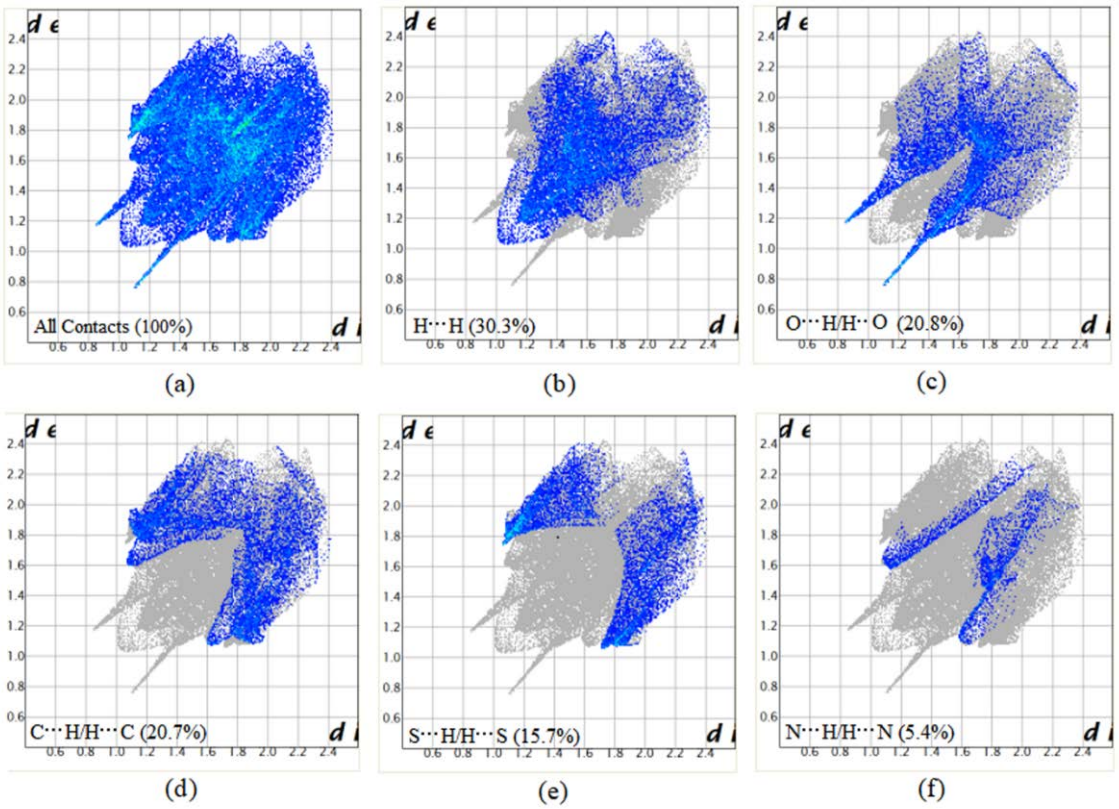


Fig. S2. Two-dimensional fingerprint plots with decomposition of each intermolecular contacts in **matc**.

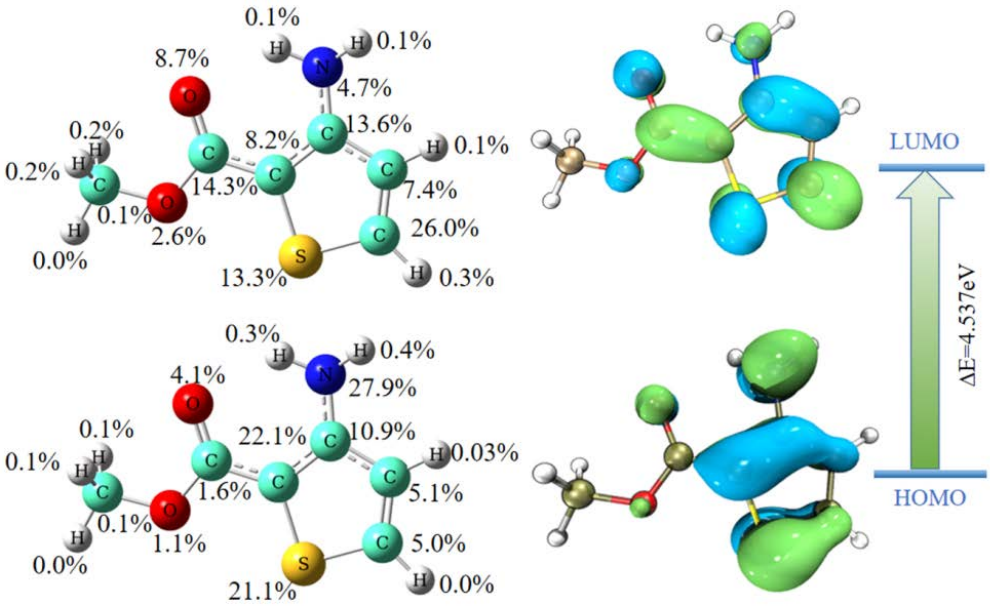


Fig.S3. Contour plots and energies of HOMO and LUMO of **matc**.