Supplementary Material (ESI) for CrystEngComm

Supporting Information

Synthesis, crystal structures and nonlinear optical properties of three TCF-based chromophores

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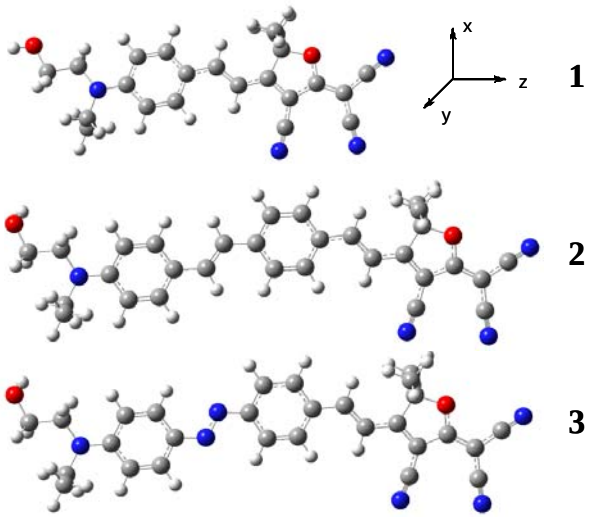
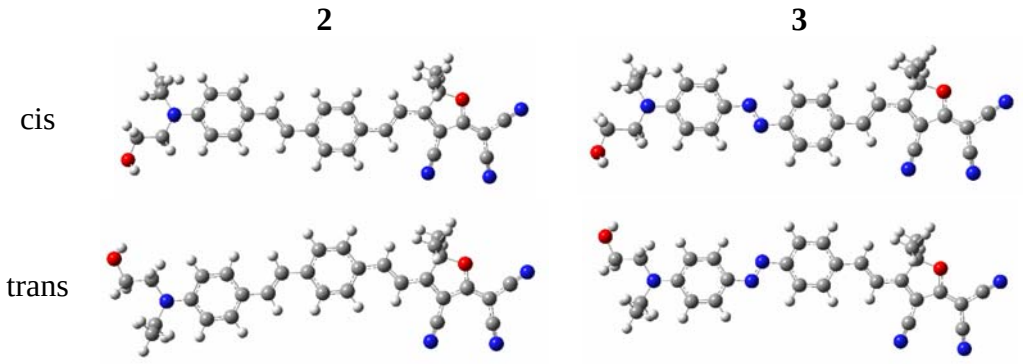


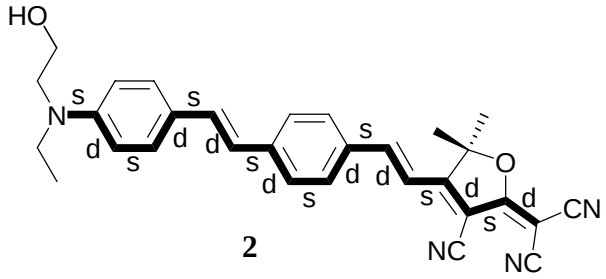
Fig. S1. Calculated geometries of **1**–**3**

Table S1 Comparison of the cis and trans conformations of **2** and **3**



Compound	E / kcal·mol^{-1}		μ / Debye		β_{tot} /10^{-30} esu	
	cis	trans	cis	trans	cis	trans
2	-959974.870	-959975.267	19.95	19.02	1061.7	1065.0
3	-980093.937	-980094.336	19.68	18.67	754.3	760.7

Table S2 Experimental and DFT calculated bond length (Å) used to calculate BLA (Å) of chromophores (Bonds used for calculating BLA are highlighted with label "s" for single bonds and "d" for double bonds.)



2

	1			**2**			**3**		
	cryst.	calc.		cryst.	calc.		cryst.-I [a)]	cryst.-II [a)]	calc.
N(4)-C(16)	1.359(4)	1.382	N(4)-C(26)	1.387(3)	1.391	N(6)-C(22)	1.377(14)	1.359(14)	1.385
C(16)-C(15)	1.409(4)	1.424	C(26)-C(24)	1.402(4)	1.416	C(22)-C(21)	1.432(16)	1.412(15)	1.420
C(15)-C(14)	1.362(4)	1.380	C(24)-C(22)	1.350(4)	1.396	C(21)-C(20)	1.363(16)	1.356(16)	1.383
C(14)-C(13)	1.395(4)	1.414	C(22)-C(21)	1.373(4)	1.407	C(20)-C(19)	1.427(16)	1.403(10)	1.406
C(13)-C(12)	1.425(4)	1.442	C(21)-C(20)	1.474(4)	1.453	C(19)-N(5)	1.390(10)	1.380(17)	1.394
C(12)-C(11)	1.362(4)	1.367	C(20)-C(19)	1.299(4)	1.356	N(5)-N(4)	1.299(7)	1.299(7)	1.272
C(11)-C(7)	1.408(4)	1.425	C(19)-C(18)	1.470(4)	1.454	N(4)-C(16)	1.415(5)	1.415(5)	1.408
C(7)-C(5)	1.383(3)	1.383	C(18)-C(16)	1.399(4)	1.417	C(16)-C(15)	1.356(7)	1.356(7)	1.409
C(5)-C(4)	1.427(4)	1.446	C(16)-C(14)	1.388(4)	1.392	C(15)-C(14)	1.374(7)	1.374(7)	1.383
C(4)-C(2)	1.373(4)	1.379	C(14)-C(13)	1.402(4)	1.416	C(14)-C(13)	1.314(8)	1.314(8)	1.415
BLA	0.012	0.022	C(13)-C(12)	1.433(4)	1.446	C(13)-C(12)	1.459(6)	1.459(6)	1.449
			C(12)-C(11)	1.348(4)	1.365	C(12)-C(11)	1.368(7)	1.368(7)	1.363
			C(11)-C(7)	1.416(4)	1.429	C(11)-C(3)	1.439(6)	1.439(6)	1.429
			C(7)-C(6)	1.373(4)	1.382	C(3)-C(2)	1.366(5)	1.366(5)	1.380
			C(6)-C(4)	1.426(4)	1.447	C(2)-C(1)	1.441(5)	1.441(5)	1.448
			C(4)-C(2)	1.364(4)	1.378	C(1)-C(5)	1.374(5)	1.374(5)	1.377
			BLA	0.048	0.034	BLA	0.040	0.041	0.030

[a)] Bond length values of **3** in two different sites because of disorder.

Table S3 BLA Values and calculated β of **1-3**

Compound	BLA (Å)		calculated β ($\times 10^{-30}$ esu)	
	crystal	calculated	β_{zzz}	β_{tot}
1	0.012	0.022	184.4	182.0
2	0.048	0.033	1073.1	1065.0
3	0.040	0.031	768.8	760.7