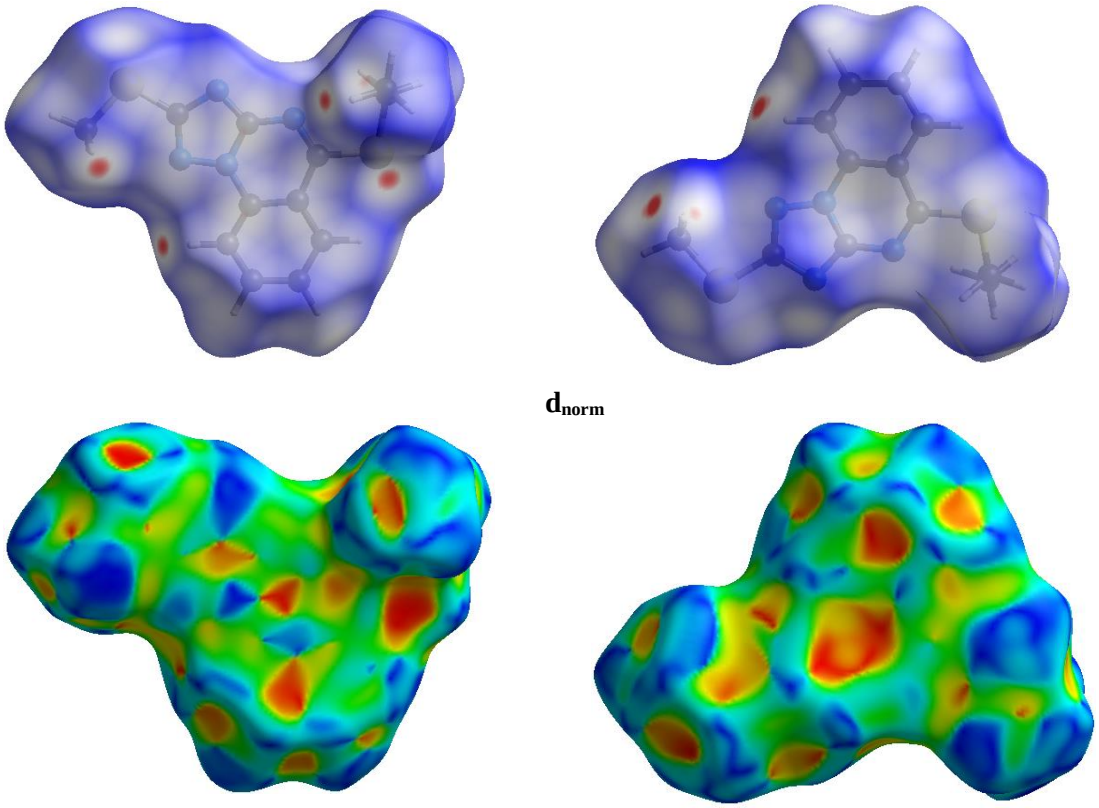
To Supplementary data



d_{norm}

Shape index

Curvedness

Figure S1. Hirshfeld analysis of CCDC 1827320.

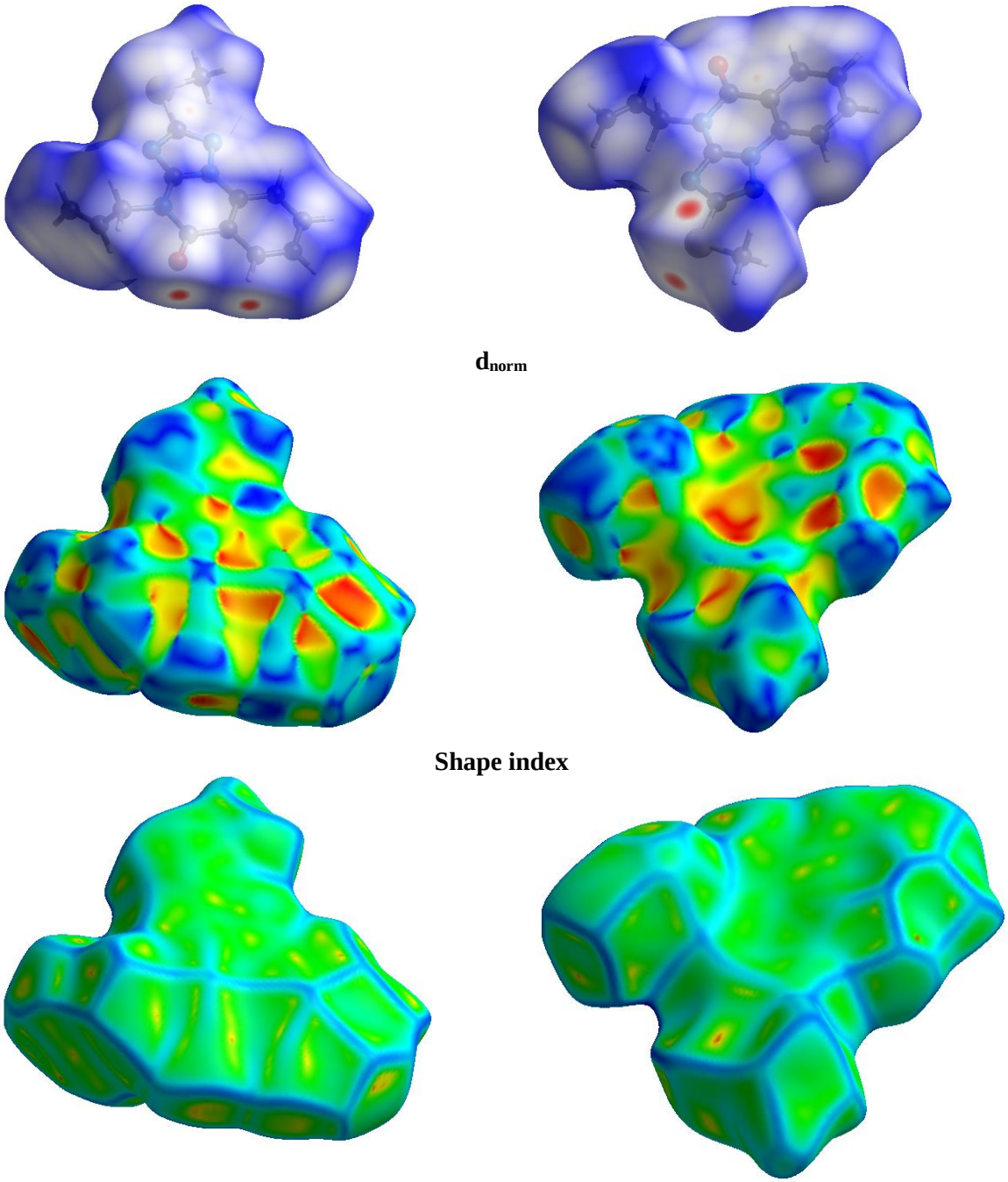


Figure S2. Hirshfeld analysis of **CCDC 1826859**.

Table S1 The calculated bond distances of **1** and **2**

Bond (s)	Calc.	Exp.	Bond(s)	Calc.	Exp.
	1			**2**	
R(1-22)	1.756	1.734	R(1-19)	1.757	1.741
R(1-23)	1.825	1.786	R(1-20)	1.825	1.789
R(2-20)	1.218	1.219	R(2-16)	1.776	1.751
R(3-20)	1.404	1.399	R(2-24)	1.838	1.809
R(3-21)	1.370	1.369	R(3-4)	1.363	1.379
R(3-27)	1.481	1.468	R(3-19)	1.333	1.325
R(4-21)	1.316	1.318	R(4-6)	1.377	1.383
R(4-22)	1.370	1.370	R(4-18)	1.38	1.369
R(5-6)	1.377	1.387	R(5-18)	1.324	1.314
R(5-22)	1.322	1.328	R(5-19)	1.358	1.363
R(6-10)	1.388	1.384	R(6-7)	1.401	1.324
R(6-21)	1.361	1.337	R(6-15)	1.416	1.407
R(7-30)	1.328	1.236	R(7-9)	1.381	1.317
R(10-11)	1.397	1.385	R(9-11)	1.405	1.39
R(10-19)	1.406	1.403	R(11-13)	1.381	1.371
R(11-13)	1.387	1.372	R(13-15)	1.409	1.395
R(13-15)	1.401	1.376	R(15-16)	1.457	1.451
R(15-17)	1.386	1.366	R(16-17)	1.304	1.305
R(17-19)	1.400	1.394	R(17-18)	1.353	1.363
R(19-20)	1.482	1.470	R(24-27)	1.524	1.51
R(27-30)	1.505	1.510			
A(22-1-23)	100.047	100.941	A(19-1-20)	100.259	101.765
A(1-22-4)	119.496	117.583	A(1-19-3)	123.661	123.903
A(1-22-5)	124.251	126.137	A(1-19-5)	119.811	119.094
A(2-20-3)	120.54	120.366	A(1-20-21)	105.664	109.5
A(2-20-19)	123.763	123.895	A(1-20-22)	110.652	109.485
A(20-3-21)	121.757	121.406	A(1-20-23)	110.708	109.498
A(20-3-27)	119.212	120.593	A(16-2-24)	101.742	101.655
A(3-20-19)	115.697	115.739	A(2-16-15)	117.68	116.74
A(21-3-27)	119.009	117.754	A(2-16-17)	118.752	119.663
A(3-21-4)	128.537	127.078	A(2-24-25)	103.413	109.058

A(3-21-6)	120.565	120.946	A(2-24-26)	106.797	109.052
A(3-27-30)	112.158	110.664	A(2-24-27)	114.018	112.635
A(21-4-22)	102.094	101.508	A(4-3-19)	101.219	100.518
A(4-21-6)	110.894	111.964	A(3-4-6)	127.217	127.306
A(4-22-5)	116.253	116.256	A(3-4-18)	110.068	109.869
A(6-5-22)	101.49	100.883	A(3-19-5)	116.528	117.002
A(5-6-10)	126.83	126.562	A(6-4-18)	122.714	122.567
A(5-6-21)	109.269	109.38	A(4-6-7)	122.362	119.285
A(10-6-21)	123.892	123.987	A(4-6-15)	116.083	115.419
A(6-10-11)	122.435	122.625	A(4-18-5)	109.423	110.193
A(6-10-19)	116.304	116.255	A(4-18-17)	121.897	122.661
A(7-30-27)	123.581	125.554	A(18-5-19)	102.762	102.416
A(11-10-19)	121.262	121.119	A(5-18-17)	128.681	127.144
A(10-11-13)	118.649	118.969	A(7-6-15)	121.556	125.291
A(10-19-17)	118.816	118.041	A(6-7-9)	118.836	116.219
A(10-19-20)	121.779	121.607	A(6-15-13)	117.828	116.188
A(11-13-15)	121.007	120.75	A(6-15-16)	117.595	118.619
A(13-15-17)	119.905	120.698	A(7-9-11)	120.81	124.364
A(15-17-19)	120.361	120.422	A(9-11-13)	120.215	118.666
A(17-19-20)	119.404	120.337	A(11-13-15)	120.756	119.248
			A(13-15-16)	124.577	125.172
			A(15-16-17)	123.566	123.549
			A(16-17-18)	118.144	117.064

Table S2 Natural charge populations at the different atomic sites of the studied compounds.

Atom	Charge	Atom	Charge
1		**2**	
S 1	0.2773	S 1	0.2771
O 2	-0.6098	S 2	0.2477
N 3	-0.4489	N 3	-0.3809
N 4	-0.5709	N 4	-0.1986
N 5	-0.3800	N 5	-0.5299
N 6	-0.2105	C 6	0.2051
C 7	-0.3408	C 7	-0.2141
H 8	0.1869	H 8	0.2337
H 9	0.1884	C 9	-0.1545
C 10	0.1916	H 10	0.2081
C 11	-0.2191	C 11	-0.2064
H 12	0.2322	H 12	0.2094
C 13	-0.1537	C 13	-0.1537
H 14	0.2070	H 14	0.2195
C 15	-0.2120	C 15	-0.1445
H 16	0.2087	C 16	0.1579
C 17	-0.1350	N 17	-0.5208
H 18	0.2292	C 18	0.5649
C 19	-0.1653	C 19	0.2337
C 20	0.6855	C 20	-0.6846
C 21	0.6028	H 21	0.2132
C 22	0.2380	H 22	0.2092
C 23	-0.6828	H 23	0.2094
H 24	0.2141	C 24	-0.4678
H 25	0.2107	H 25	0.2089
H 26	0.2103	H 26	0.2288
C 27	-0.2036	C 27	-0.5773
H 28	0.2207	H 28	0.2021
H 29	0.2246	H 29	0.1938
C 30	-0.1942	H 30	0.2105
H 31	0.1988		

Table S3 The calculated and experimental chemical shifts (ppm) for **1** (according to figure 6)

Atom	$(C.S)_{calc}$	$(C.S)_{exp}$	Atom	$(C.S)_{calc}$	$(C.S)_{exp}$
C 7	126.000	112.25	H 24	2.370	2.65
C 10	141.687	138.14	H 25	2.752	2.65
C 11	119.810	131.33	H 26	2.752	2.65
C 13	142.130	129.21	H 8	5.864	5.31
C 15	131.393	117.23	H 9	5.595	5.31
C 17	135.594	127.60	H 12	8.173	8.26
C 19	120.973	114.90	H 14	8.097	7.75
C 20	164.484	167.32	H 16	7.746	7.51
C 21	156.463	145.72	H 18	8.574	7.77
C 22	173.225	154.43	H 28	4.489	4.80
C 23	20.181	13.90	H 29	5.173	5.31
C 27	51.554	45.50	H 31	6.346	6.00
C 30	140.334	133.17			

Table S4 The calculated and experimental chemical shifts (ppm) for **2** (according to the Fig. 6)

Atom	$(C.S)_{calc}$	$(C.S)_{exp}$	Atom	$(C.S)_{calc}$	$(C.S)_{exp}$
C 6	139.981	133.73	H 8	8.496	8.22
C 7	120.594	115.55	H 10	8.229	8.22
C 9	141.741	135.95	H 12	7.842	7.69
C 11	131.483	126.78	H 14	8.484	8.08
C 13	131.589	126.01	H 21	2.402	2.69
C 15	122.754	117.50	H 22	2.807	2.69
C 16	177.517	167.69	H 23	2.821	2.69
C 18	158.454	152.73	H 25	2.987	4.80
C 19	175.310	164.61	H 26	3.946	4.80
C 20	19.963	14.44	H 28	1.463	1.42
C 24	34.677	24.48	H 29	1.217	1.42
C 27	16.574	13.97	H 30	1.593	1.42