Electronic Supplementary Material (ESI) for CrystEngComm.

Crystal engineering, optical properties and electron density distribution of polar multicomponent materials containing sulfanilamide

Supporting Information

Joanna Wojnarska, Marlena Gryl, Tomasz Seidler, K. Stadnicka*

Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland

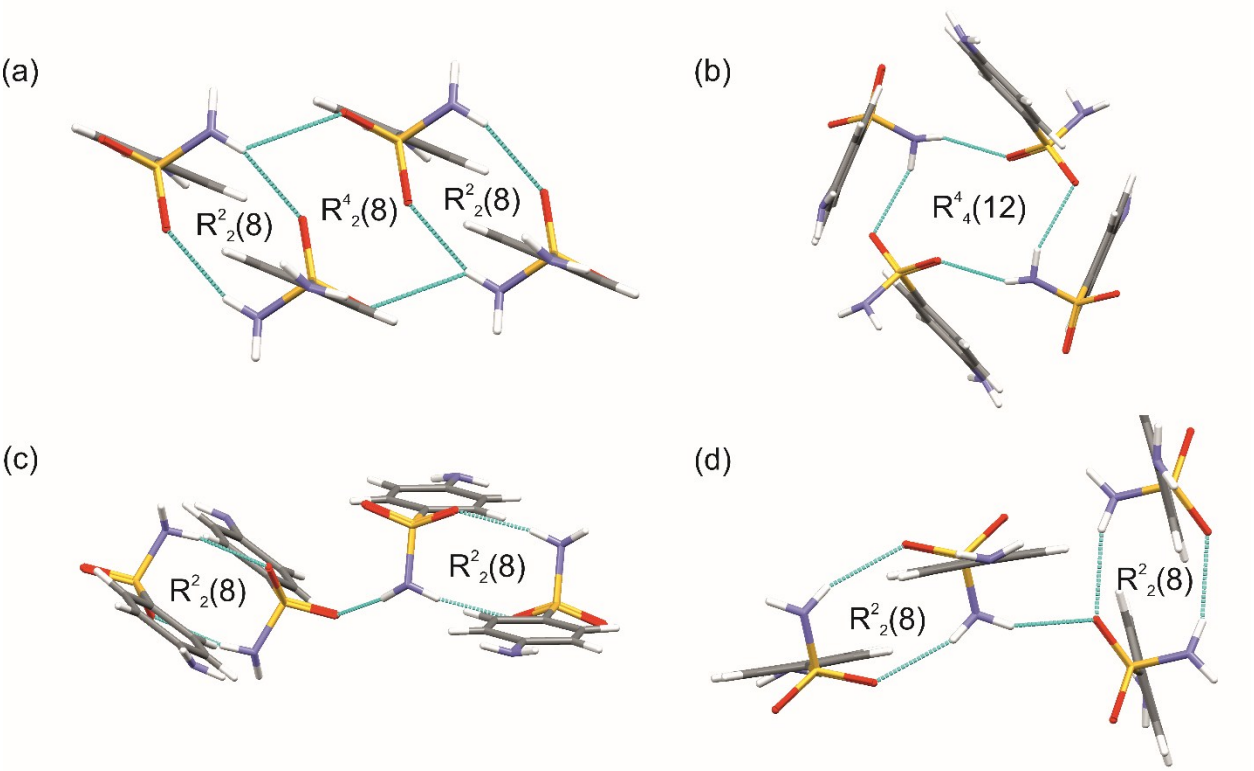

Fig. S1 Hydrogen bond motifs in (a) α-sulfanilamide - Pbca, (b) β-sulfanilamide - $P2_1/c$, (c) γ-sulfanilamide - $P2_1/c$, (d) δ-sulfanilamide - Pbca. Drawing were prepared in Mercury software. (C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek and P. A. Wood, *J. Appl. Cryst.,* 2008, **41**, 466-470.)

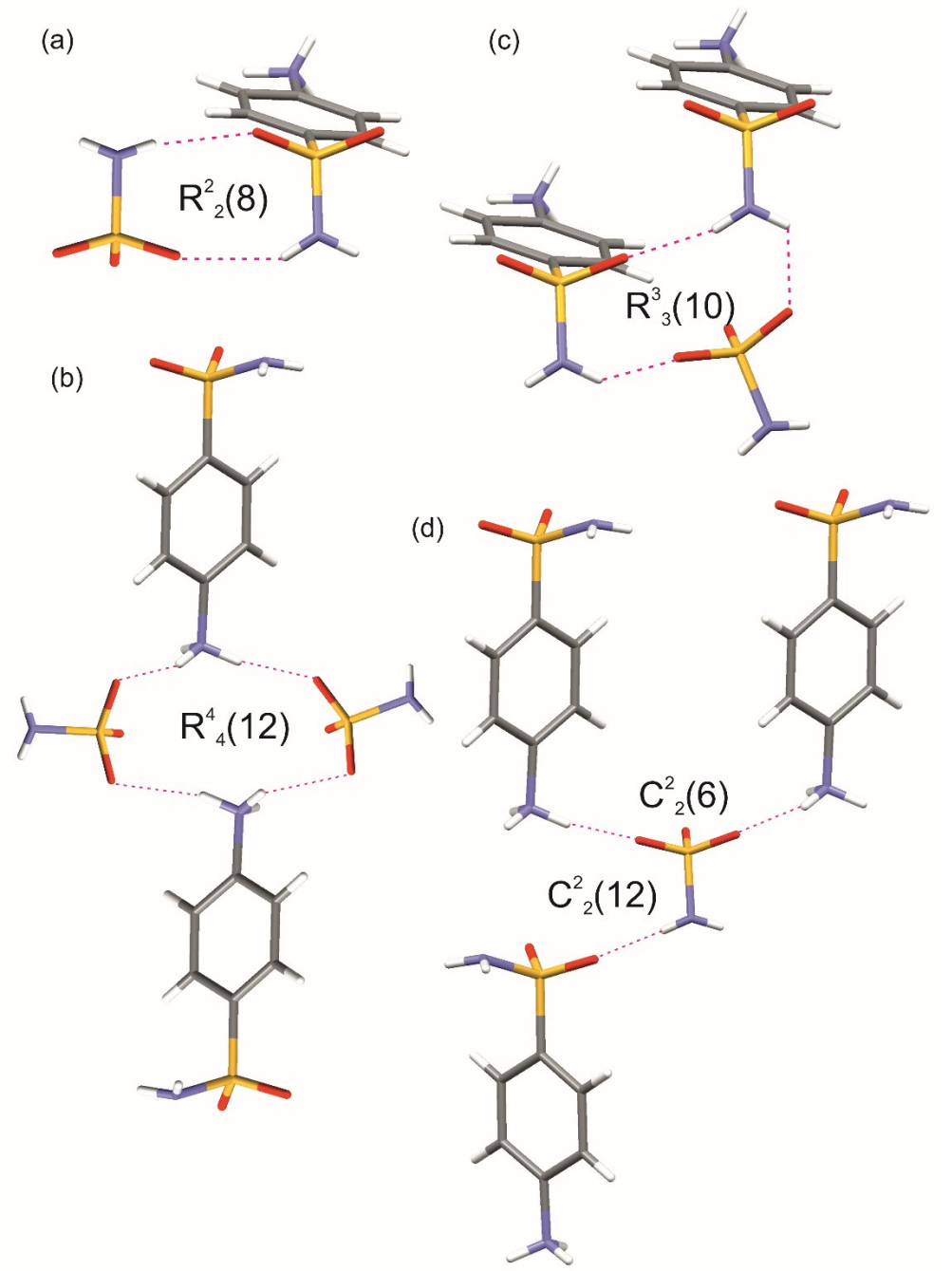

Fig. S2 Possible interactions between sulfanilamide cation and sulfamic acid anion.

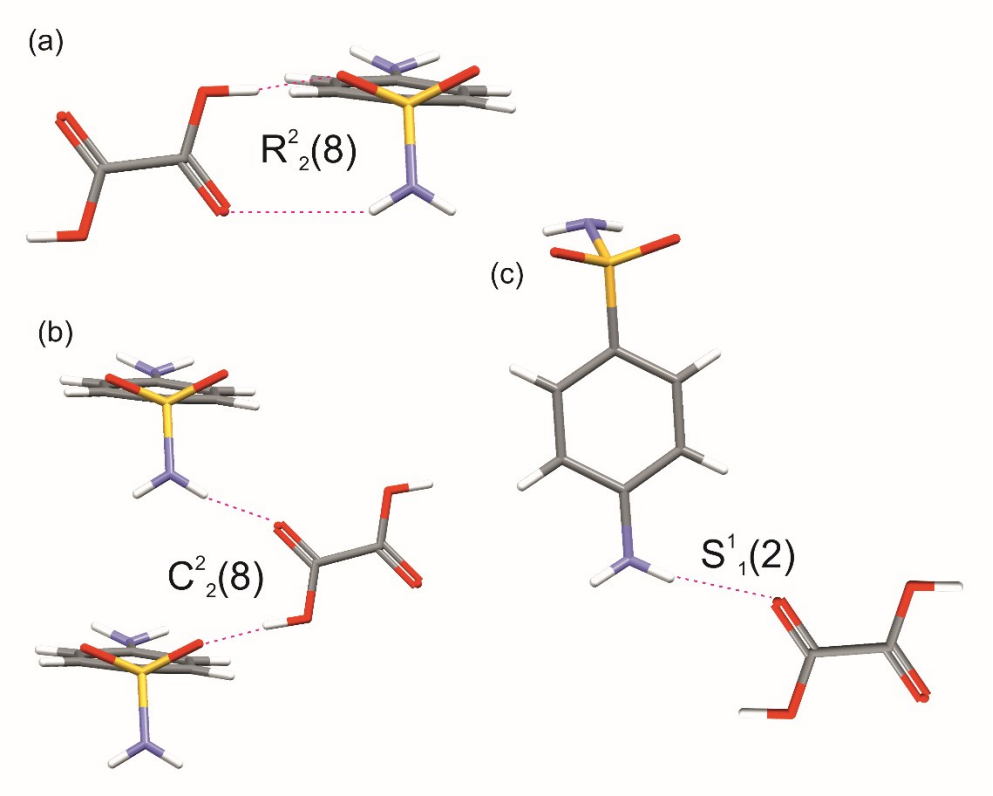

Fig. S3 Possible interactions between sulfanilamide and oxalic acid.

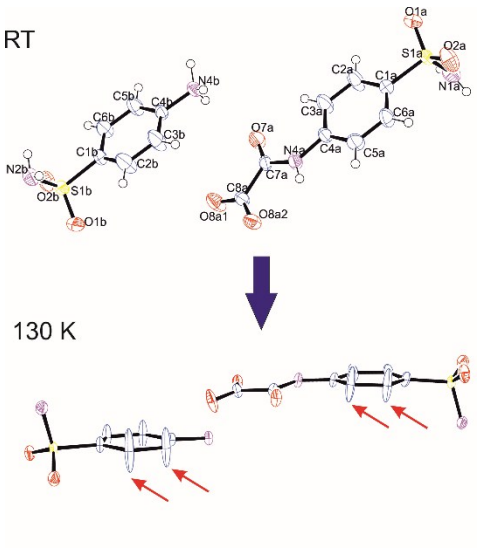

Fig. S4 Asymmetric unit of (I) at RT and disorder observed in 130 K.

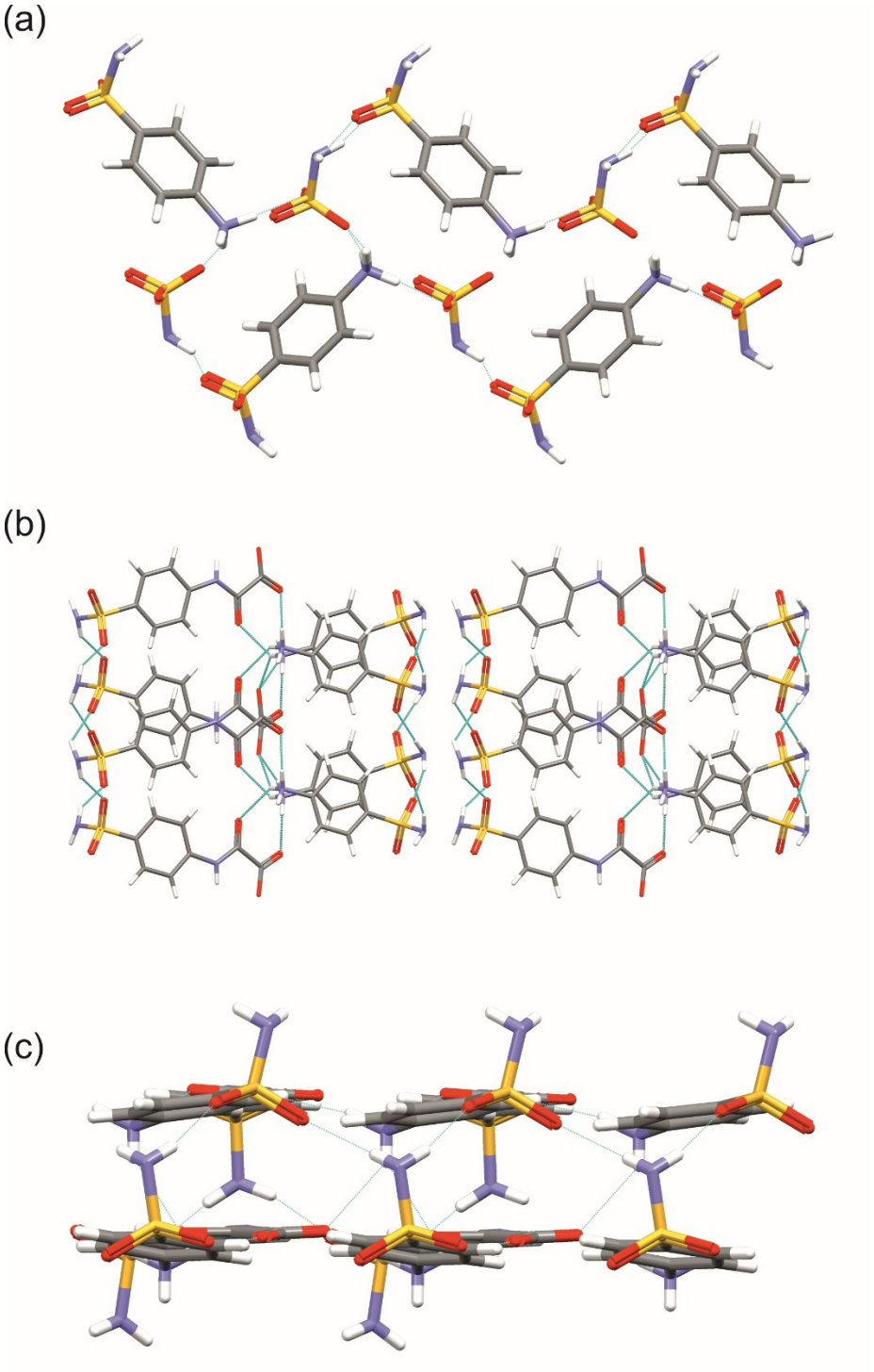

Fig. S5 Brick-wall motif in (I) (a), infinite layers in (II) (b) and brick wall-motif in (II) (c).

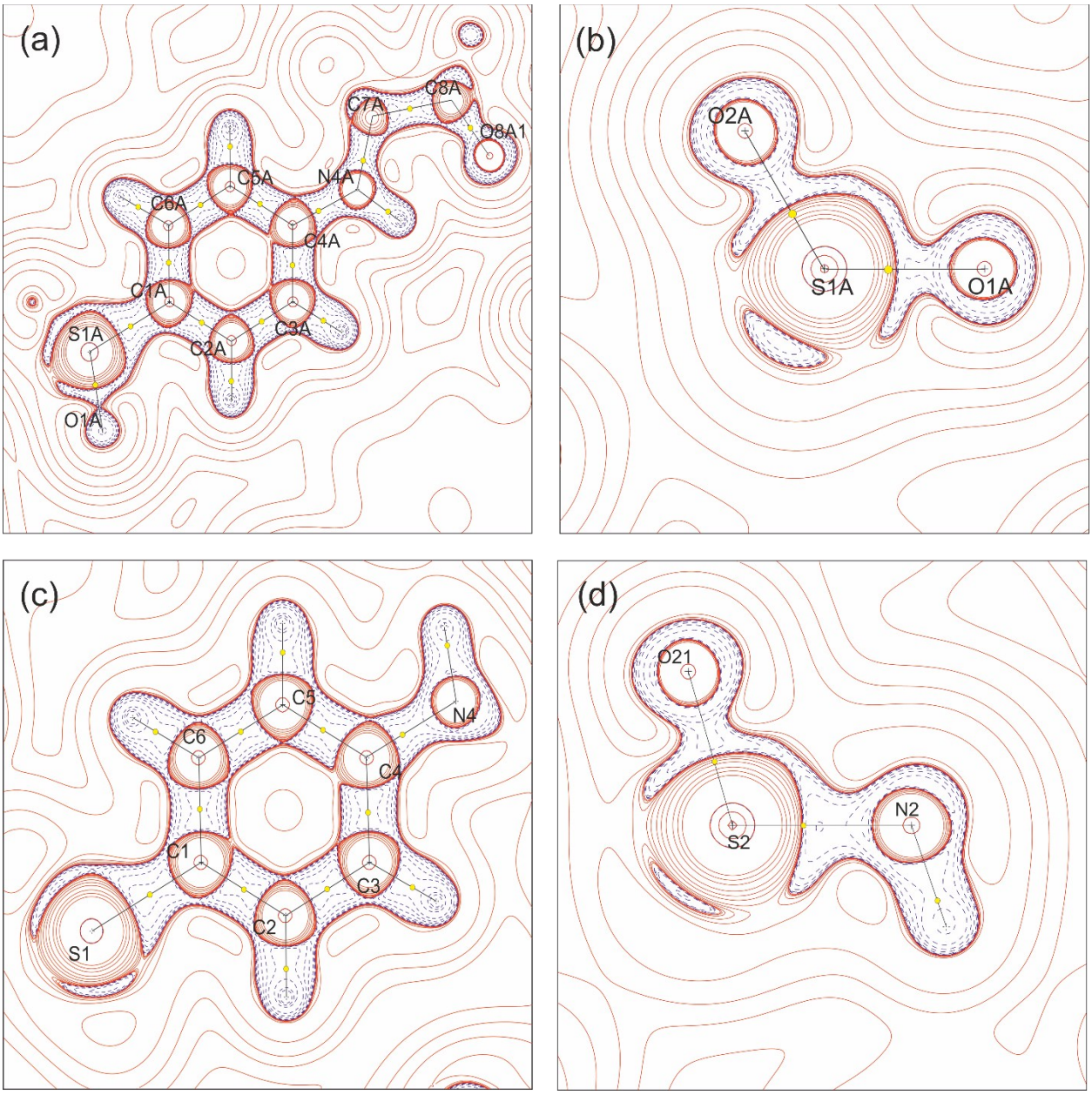

Fig. S6 Theoretical Laplacian maps for sulfoxamic anion plotted in C1A-C3A-C5A plane (a), sulfonamide group of sulfoxamic anion plotted in C1B-C3B-C5B (b) of (II), sulfanilamide cation plotted in C1-C3-C5 plane (c) and sulfamic acid anion plotted in S2-N2-O21 plane (d) of (I). Contours are at logarithmic intervals. Blue, dashed lines show positive contour and red solid lines show negative contour. Yellow dots represent BCPs

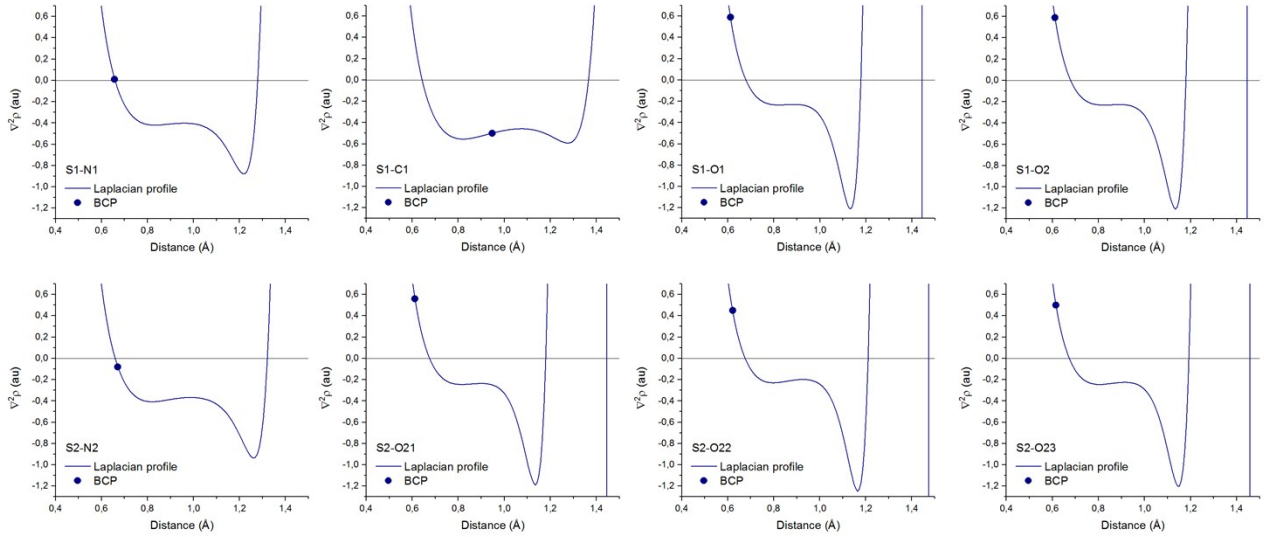

Fig. S7 Laplacian profiles along S-O, S-N and S-C bonds in (I).

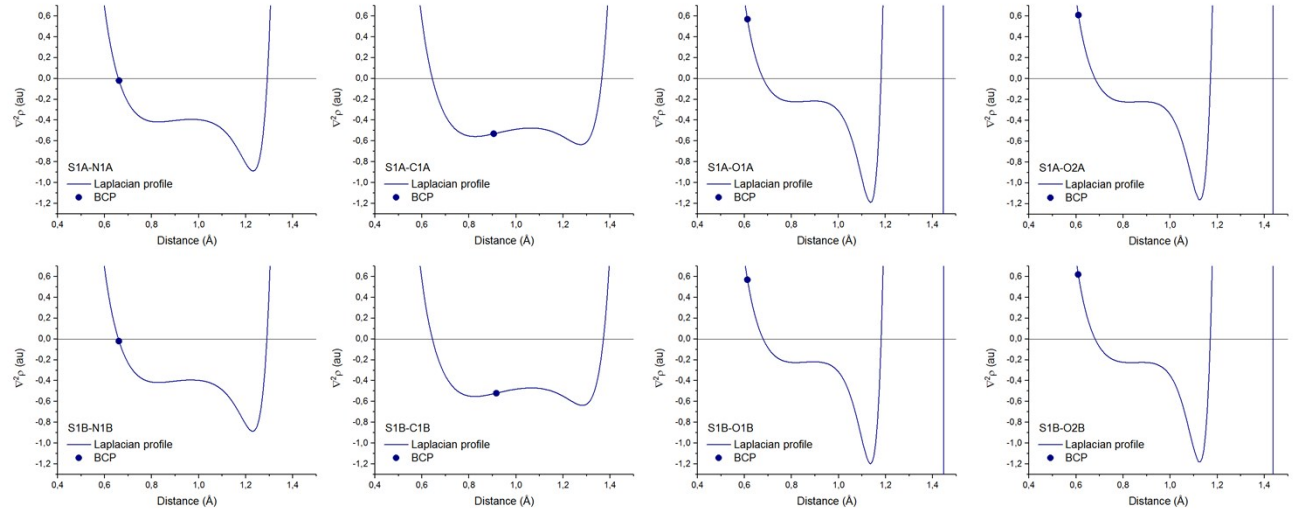

Fig. S8 Laplacian profiles along S-O, S-N and S-C bonds in (II).

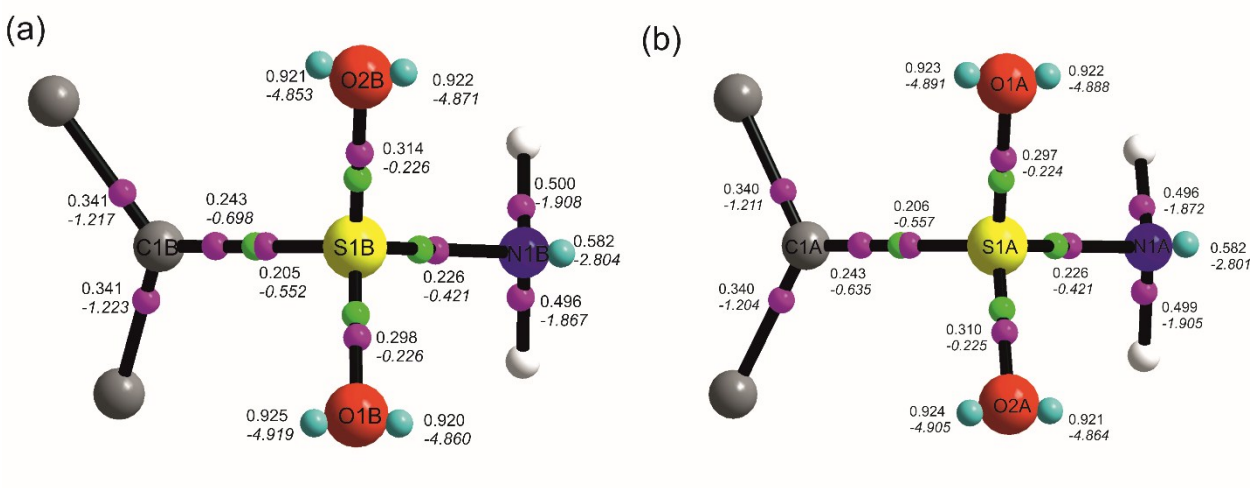

Fig. S9 VSCC analysis of sulfonamide group of sulfonamide (a) and sulfoxamic (b) in (II); small pink spheres represent BMs, small light blue spheres represent NBMs. The small green spheres represent BCPs. The values of ρ and Laplacian (italic) are given for all VSCC maxima.

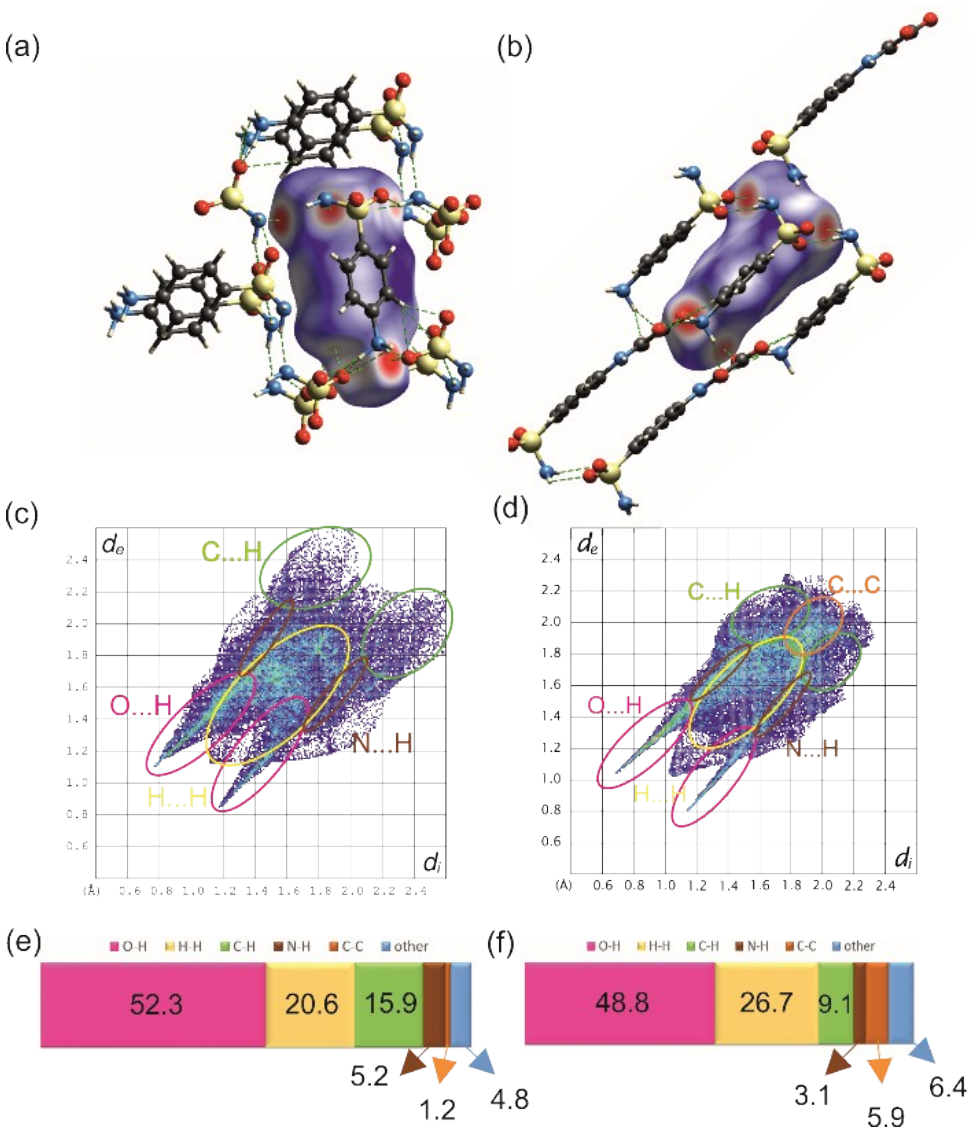

Fig. S10 Hirshfeld surface for sulfanilamide cations (a)(b), fingerprint plots for sulfanilamide cations (c)(d) and relative contribution of weak interactions to Hirshfeld surface area (e)(f). Figures on the left were obtained for sulfanilamide cation from crystal structure of (I) and on the right for the sulfanilamide cation from the crystal structure of (II).

The Hirshfeld surface (HS) for sulfanilamide cation in (II) is flattened over aromatic ring what can be correlated with the presence of π···π interactions in crystal structure of (II). This feature is not observed in sulfanilamide cation in (I) (Fig. S10a,b). Additionally, function of normalized contact distance (d_{norm}) was mapped on HS to visualize intermolecular interactions (marked as red spots). For more detailed comparison fingerprint plots and percentage contribution of interactions were determined (Fig. S10c-f). In both crystal structures the majority of contacts for sulfanilamide cation are O···H and H···H interactions. The significant difference in relative contribution of weak interactions to the HS is observed for C···H and C···C contacts.

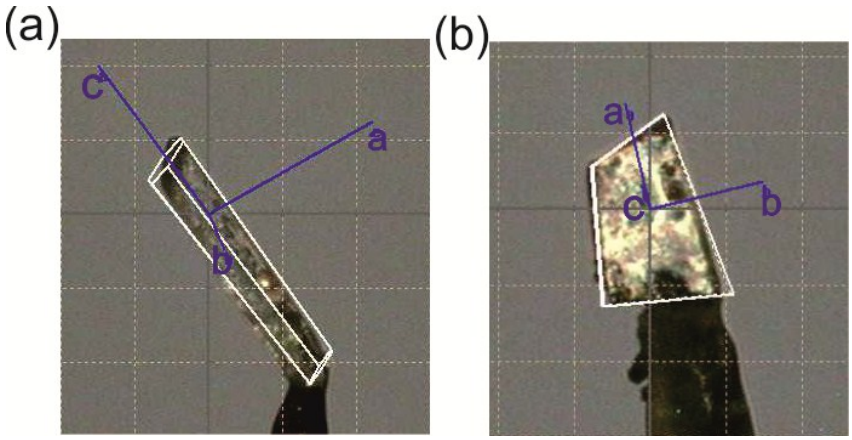

Fig. S11 Crystallographic directions for (I) (a) and (II) (b).

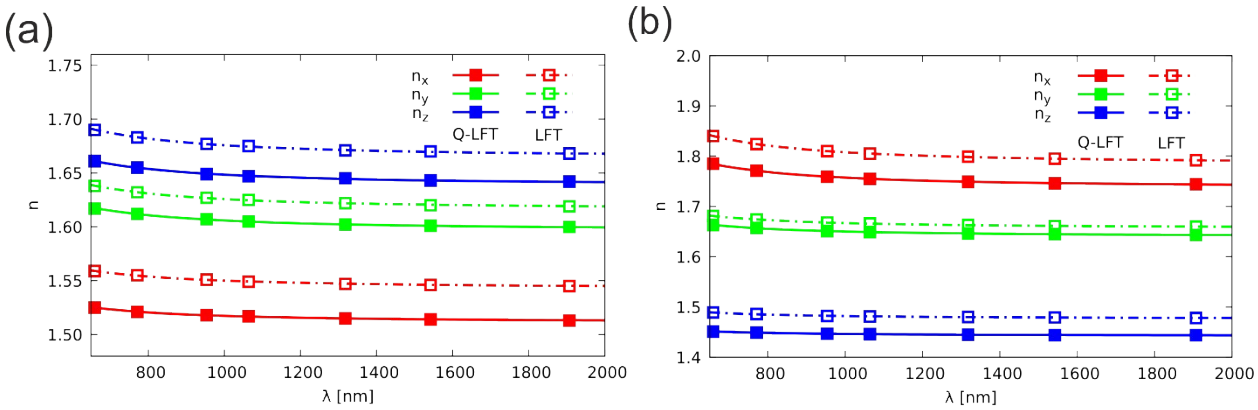

Fig. S12 Dispersion of refractive indices for (I) (a) and (II) (b).

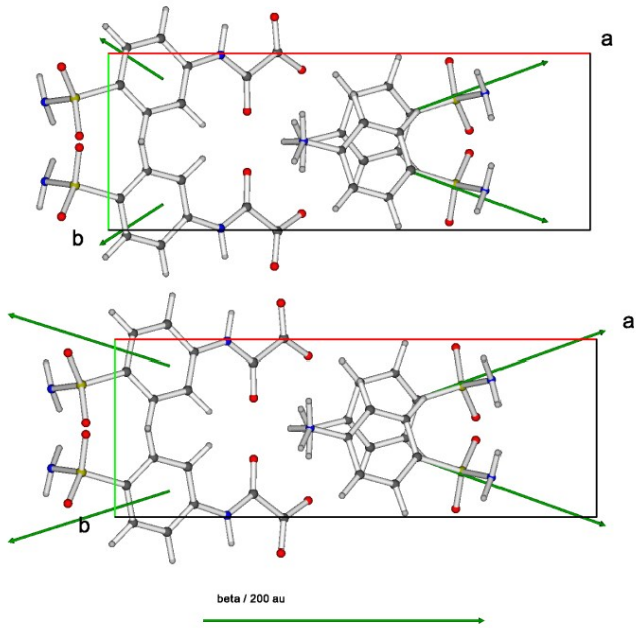

Fig. S13 Vectorial hyperpolarizabilities of the cations and anions in (II) as oriented in the unit cell (top picture shows results for the static limit, bottom for λ = 1064 nm; B3LYP/6-311++G(d,p) calculations results)

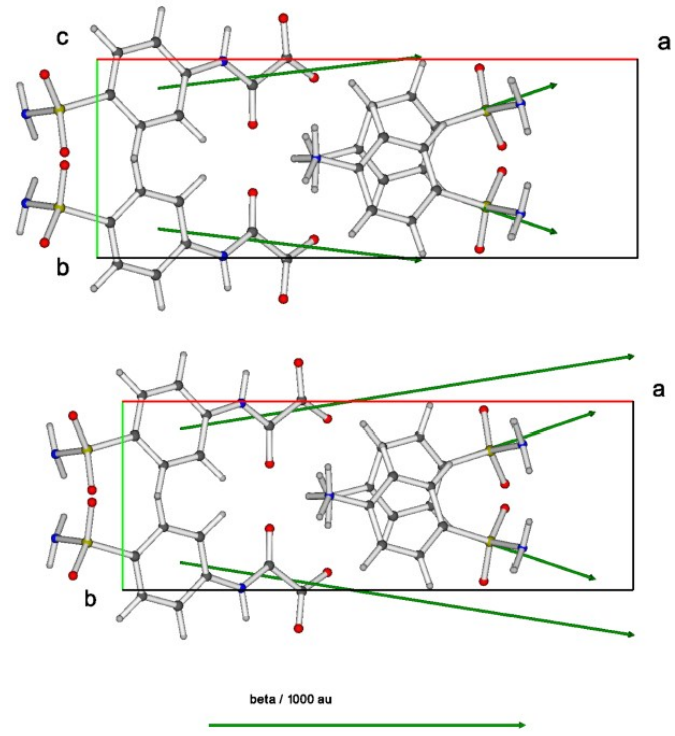

Fig. S14 Vectorial hyperpolarizabilities of of the cations and anions in (II) in the unit cell (ac projection, top picture shows results for the static limit, bottom for λ = 1064 nm; B3LYP/6-311++G(d,p) calculations results). Embedding field in the calculations is ignored.

For most of the cases, when embedding electric field forces are ignored hyperpolarizabilities of crystal building blocks sum up to much larger macroscopic values and the effect of the frequency dispersion forces typical increase of the properties together with incoming wave energy. However, taking into account embedding polarizing field of the isolated ions, the significant drop of property is observed. In the case of sulfoxamic anion in (II) the drop is so spectacular that the vectorial beta of sulfoxamic changes its orientation to the opposite one (compare Figures S13, S14). The effect of the frequency dispersion enhances vectorial hyperpolarizabilities of both crystal components resulting in the decrease of $\chi(2)$ selected components with smaller wavelength (Table 4). Further frequency dispersion should lead to an increase of the properties after crossing of the zero.

Table S1. Selected experimental single crystal X-ray diffraction data for (I) and (II).

Crystal data	(I)	(II)
Chemical formula	$C_6\ H_{11}\ N_3\ O_5\ S_2$	$C_{14}\ H_{16}\ N_4\ O_7\ S_2$
Mr	269.30	416.43
Crystal system, space group	monoclinic, *P2₁*	monoclinic, *Pc*
Lattice parameters (Å, °)	a = 4.81720(10)	a = 17.2685(4)
	b = 9.6864(3)	b = 6.2883(2)
	c = 11.2302(3)	c = 7.9171(2)
	α = 90	α = 90
	β = 96.724(3)	β = 97.627(3)
	γ = 90	γ = 90
T (K)	130(2)	298(2)
V (Å^3)	520.41(2)	852.11(4)
Z	2	2
Dx (g/cm^{-3})	1.719	1.623
Radiation type	MoKα	MoKα
μ (mm^{-1})	0.523	0.362
Crystal size (mm)	0.50 x 0.20 x 0.18	0.25 x 0.18 x 0.03
Data collection		
Diffractometer	Rigaku, SuperNova™	Rigaku, SuperNova™
Data collection method	ω-scan	ω-scan
Absorption correction	multi-scan	multi-scan
Tmin, Tmax	0.964, 0.998	0.963, 0.995
θ_{max}	31.805	29.684

Spherical Refinement

No. of measured reflections	15834	12463
No. of unique reflections	3370	3347
No. of reflections with I>2σ(I)	3014	2472
No. of parameters	166	270
R[I>2σ(I))]/wR(I)/S	0.0364/ 0.0766/1.058	0.0379/ 0.0921/ 0.970
ρ_{max}/ρ_{min}/rms (eÅ^{-3})	0.450/-0.345/ 0.082	0.235/-0.319/0.048
Flack parameter	-0.02(4)	0.23(9)

Table S2. Topological analysis of critical points for selected bonds in (I) (first row) and in isolated ions (second row).

Bond	d	d_1	d_2	$\rho(r)$	$\nabla^2\rho(r)$	λ_1	λ_2	λ_3	ε
S2-O21	1.513	0.611	0.902	0.244	0.56	-0.36	-0.35	1.28	0.02
	1.473	0.574	0.899	0.287	0.82	-0.50	-0.48	1.80	0.03
S2-O22	1.542	0.621	0.921	0.232	0.45	-0.34	-0.33	1.11	0.02
	1.482	0.577	0.905	0.283	0.75	-0.49	-0.47	1.70	0.04
S2-O23	1.525	0.615	0.910	0.239	0.50	-0.35	-0.34	1.20	0.03
	1.473	0.574	0.899	0.287	0.82	-0.50	-0.48	1.81	0.03
S2-N2	1.693	0.670	1.023	0.205	-0.08	-0.28	-0.26	0.45	0.08
	1.733	0.761	0.972	0.209	-0.52	-0.34	-0.32	0.14	0.05
S1-O1	1.510	0.611	0.899	0.243	0.59	-0.36	-0.35	1.30	0.02
	1.453	0.568	0.885	0.295	1.02	-0.51	-0.50	2.02	0.01
S1-O2	1.512	0.611	0.901	0.242	0.59	-0.36	-0.35	1.29	0.03
	1.453	0.568	0.885	0.295	1.02	-0.51	-0.50	2.02	0.01
S1-N1	1.655	0.656	0.999	0.214	0.01	-0.3	-0.26	0.58	0.17
	1.656	0.647	1.009	0.238	-0.41	-0.38	-0.35	0.32	0.09
C1-S1	1.801	0.854	0.947	0.204	-0.50	-0.31	-0.29	0.10	0.08
	1.795	0.953	1.002	0.206	-0.42	-0.36	-0.34	0.28	0.05
C2-C1	1.384	0.674	0.710	0.318	-0.92	-0.68	-0.57	0.32	0.19
	1.389	0.685	0.704	0.310	-0.87	-0.64	-0.54	0.31	0.18
C2-C3	1.384	0.697	0.687	0.319	-0.93	-0.68	-0.58	0.32	0.18
	1.391	0.682	0.709	0.308	-0.86	-0.64	-0.54	0.31	0.18
C3-C4	1.382	0.663	0.719	0.323	-0.97	-0.71	-0.58	0.32	0.21
	1.385	0.652	0.733	0.312	-0.88	-0.65	-0.53	0.30	0.24

C4-C5	1.385	0.719	0.666	0.323	-0.96	-0.70	-0.58	0.32	0.21
	1.385	0.733	0.652	0.312	-0.88	-0.65	-0.53	0.30	0.24
C5-C6	1.385	0.689	0.696	0.318	-0.93	-0.68	-0.57	0.32	0.19
	1.391	0.709	0.682	0.308	-0.87	-0.64	-0.54	0.31	0.19
C6-C1	1.388	0.677	0.711	0.316	-0.92	-0.67	-0.57	0.32	0.19
	1.390	0.686	0.704	0.310	-0.87	-0.64	-0.54	0.31	0.18
C4-N4	1.473	0.595	0.878	0.252	-0.61	-0.49	-0.49	0.37	0.01
	1.488	0.529	0.959	0.231	-0.48	-0.38	-0.37	0.27	0.01

d – intermolecular distance (Å); d_1, d_2 – distance between BCPs and interacting atoms (Å); $\rho(r)$ – charge density (a.u.); $\nabla^2\rho(r)$ – Laplacian of electron density (a.u.); λ_1, λ_2, λ_3 - eigenvalues of Hessian (a.u.); ε – bond ellipticity.

Table S3. Topological analysis of critical points for selected bonds in (I) (first row) and in isolated ions (second row).

Bond	$\rho(r)$	$\nabla^2\rho(r)$	G(r)	V(r)	E(r)	|V(r)|/G(r)	G(r)/ρ(r)	E(r)/ρ(r)
S2-O21	0.244	0.56	0.377	-0.614	-0.237	1.63	1.545	-0.971
	0.287	0.82	0.556	-0.906	-0.351	1.63	1.939	-1.223
S2-O22	0.232	0.45	0.336	-0.56	-0.224	1.67	1.448	-0.966
	0.283	0.75	0.534	-0.882	-0.348	1.65	1.889	-1.230
S2-O23	0.239	0.50	0.359	-0.592	-0.233	1.65	1.502	-0.975
	0.287	0.82	0.556	-0.906	-0.351	1.63	1.939	-1.223
S2-N2	0.205	-0.08	0.181	-0.382	-0.201	2.11	0.883	-0.980
	0.209	-0.52	0.092	-0.314	-0.222	3.42	0.438	-1.060
S1-O1	0.243	0.59	0.381	-0.616	-0.235	1.62	1.568	-0.967
	0.295	1.02	0.612	-0.970	-0.358	1.58	2.073	-1.211
S1-O2	0.242	0.59	0.379	-0.61	-0.231	1.61	1.566	-0.955
	0.295	1.02	0.612	-0.970	-0.358	1.58	2.073	-1.211
S1-N1	0.214	0.01	0.213	-0.422	-0.209	1.98	0.995	-0.977
	0.238	-0.41	0.212	-0.525	-0.314	2.48	0.889	-1.318
C1-S1	0.204	-0.50	0.047	-0.218	-0.171	4.64	0.230	-0.838
	0.206	-0.42	0.045	-0.194	-0.150	4.37	0.216	-0.729
C2-C1	0.318	-0.92	0.105	-0.441	-0.336	4.20	0.330	-1.057
	0.310	-0.87	0.102	-0.420	-0.319	4.14	0.328	-1.030
C3-C2	0.319	-0.93	0.103	-0.44	-0.337	4.27	0.323	-1.056
	0.308	-0.87	0.101	-0.419	-0.318	4.14	0.328	-1.031
C3-C4	0.323	-0.97	0.106	-0.453	-0.347	4.27	0.328	-1.074
	0.312	-0.88	0.108	-0.438	-0.329	4.03	0.348	-1.055

C5-C4	0.323	-0.96	0.105	-0.45	-0.345	4.29	0.325	-1.068
	0.312	-0.88	0.108	-0.438	-0.329	4.03	0.348	-1.055
C5-C6	0.318	-0.93	0.103	-0.438	-0.335	4.25	0.324	-1.053
	0.308	-0.87	0.101	-0.419	-0.318	4.14	0.328	-1.031
C6-C1	0.316	-0.92	0.104	-0.437	-0.333	4.20	0.329	-1.054
	0.310	-0.87	0.102	-0.420	-0.319	4.14	0.328	-1.030
C4-N4	0.252	-0.61	0.104	-0.36	-0.256	3.46	0.413	-1.016
	0.231	-0.48	0.161	-0.444	-0.282	2.75	0.698	-1.220

$\rho(r)$ – charge density (a.u.); $\nabla^2\rho(r)$ – Laplacian of electron density (a.u.); G(r), V(r), E(r) – local kinetic, potential and total energy density (a.u.)

Table S4. Topological analysis of critical points for selected bonds in (II) (first row) and in isolated ions (second row).

Bond	d	d_1	d_2	$\rho(r)$	$\nabla^2\rho(r)$	λ_1	λ_2	λ_3	ε
S1B-O2B	1.503	0.609	0.894	0.245	0.62	-0.36	-0.35	1.33	0.02
	1.453	0.568	0.885	0.295	1.02	-0.51	-0.50	2.02	0.01
S1B-O1B	1.513	0.612	0.901	0.241	0.57	-0.35	-0.35	1.27	0.02
	1.453	0.568	0.885	0.295	1.02	-0.51	-0.50	2.02	0.01
S1B-N2B	1.665	0.660	1.005	0.212	-0.02	-0.3	-0.26	0.54	0.17
	1.656	0.647	1.009	0.238	-0.41	-0.38	-0.35	0.32	0.09
C1B-S1B	1.802	0.886	0.916	0.204	-0.52	-0.31	-0.29	0.07	0.07
	1.795	0.953	1.002	0.206	-0.42	-0.36	-0.34	0.28	0.05
S1A-O2A	1.505	0.610	0.895	0.244	0.61	-0.36	-0.35	1.32	0.02
	1.458	0.569	0.889	0.292	0.97	-0.50	-0.50	1.97	0.00
S1A-O1A	1.515	0.613	0.902	0.241	0.57	-0.35	-0.35	1.27	0.02
	1.458	0.569	0.889	0.292	0.97	-0.50	-0.50	1.97	0.00
S1A-N1A	1.666	0.661	1.005	0.211	-0.02	-0.3	-0.26	0.53	0.17
	1.680	0.671	1.009	0.227	-0.49	-0.35	-0.33	0.20	0.07
C1A-S1A	1.796	0.891	0.905	0.206	-0.53	-0.31	-0.28	0.06	0.08
	1.760	0.790	0.970	0.215	-0.45	-0.38	-0.34	0.28	0.10
C7A-O7A	1.234	0.424	0.810	0.399	-0.63	-1.01	-0.94	1.31	0.07
	1.216	0.414	0.802	0.405	-0.15	-1.05	-1.02	1.92	0.03
C7A-N4A	1.350	0.514	0.836	0.328	-1.05	-0.75	-0.65	0.35	0.16
	1.388	0.529	0.859	0.297	-0.79	-0.59	-0.58	0.38	0.01
C8A-C7A	1.556	0.762	0.794	0.247	-0.64	-0.53	-0.48	0.37	0.10
	1.585	0.742	0.843	0.227	-0.49	-0.45	-0.41	0.38	0.10

C8A-O8A2	1.262	0.437	0.825	0.375	-0.76	-0.92	-0.86	1.02	0.07
	1.259	0.431	0.828	0.370	-0.42	-0.90	-0.87	1.35	0.03
C8A-O8A1	1.251	0.431	0.820	0.383	-0.69	-0.96	-0.89	1.16	0.08
	1.229	0.420	0.809	0.396	-0.31	-1.01	-0.96	1.66	0.06
C4A-N4A	1.408	0.545	0.863	0.283	-0.79	-0.58	-0.54	0.33	0.07
	1.368	0.509	0.859	0.311	-0.90	-0.64	-0.61	0.35	0.05
C4B-N4B	1.469	0.592	0.877	0.253	-0.62	-0.49	-0.49	0.36	0.01
	1.488	0.529	0.959	0.231	-0.48	-0.38	-0.37	0.27	0.01
C3A-C4A	1.395	0.667	0.728	0.315	-0.93	-0.68	-0.57	0.32	0.21
	1.410	0.677	0.733	0.300	-0.83	-0.62	-0.53	0.32	0.18
C5A-C4A	1.394	0.672	0.722	0.317	-0.94	-0.69	-0.57	0.32	0.21
	1.410	0.677	0.733	0.300	-0.83	-0.62	-0.53	0.32	0.18
C3A-C2A	1.383	0.688	0.695	0.319	-0.93	-0.68	-0.57	0.32	0.20
	1.382	0.681	0.701	0.311	-0.88	-0.65	-0.53	0.30	0.21
C2A-C1A	1.385	0.681	0.704	0.318	-0.92	-0.68	-0.57	0.32	0.19
	1.395	0.686	0.709	0.304	-0.83	-0.62	-0.52	0.31	0.19
C6A-C1A	1.385	0.679	0.706	0.318	-0.92	-0.68	-0.57	0.32	0.18
	1.395	0.686	0.709	0.304	-0.83	-0.62	-0.52	0.31	0.19
C6B-C1B	1.383	0.677	0.706	0.319	-0.93	-0.68	-0.57	0.32	0.19
	1.389	0.685	0.704	0.310	-0.87	-0.64	-0.54	0.31	0.18
C6B-C5B	1.389	0.693	0.696	0.316	-0.92	-0.67	-0.57	0.32	0.18
	1.391	0.709	0.682	0.308	-0.86	-0.64	-0.54	0.31	0.18
C6A-C5A	1.379	0.688	0.691	0.321	-0.94	-0.69	-0.57	0.32	0.20
	1.382	0.681	0.701	0.311	-0.88	-0.65	-0.53	0.30	0.21
C5B-C4B	1.384	0.668	0.716	0.323	-0.96	-0.71	-0.57	0.32	0.23
	1.385	0.652	0.733	0.312	-0.88	-0.65	-0.53	0.30	0.24

C2B-C1B	1.385	0.678	0.707	0.319	-0.93	-0.68	-0.57	0.32	0.18
	1.389	0.685	0.704	0.310	-0.87	-0.64	-0.54	0.31	0.18
C3B-C4B	1.385	0.665	0.720	0.322	-0.96	-0.7	-0.58	0.32	0.21
	1.385	0.652	0.733	0.312	-0.88	-0.65	-0.53	0.30	0.24
C3B-C2B	1.381	0.688	0.693	0.32	-0.94	-0.68	-0.58	0.32	0.18
	1.391	0.682	0.709	0.308	-0.86	-0.64	-0.54	0.31	0.18

d – intermolecular distance (Å); d_1, d_2 – distance between BCPs and interacting atoms (Å); $\rho(r)$ – charge density (a.u.); $\nabla^2\rho(r)$ – Laplacian of electron density (a.u.); λ_1, λ_2, λ_3 - eigenvalues of Hessian (a.u.); ε – bond ellipticity.

Table S5. Topological analysis of critical points for selected bonds in (I) (first row) and in isolated ions (second row)

Bond	ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	E(r)	|V(r)|/G(r)	G(r)/ρ(r)	E(r)/ρ(r)
S1B-O2B	0.245	0.62	0.390	-0.624	-0.234	1.6	1.592	-0.955
	0.295	1.02	0.612	-0.970	-0.358	1.58	2.073	-1.211
S1B-O1B	0.241	0.57	0.374	-0.605	-0.231	1.62	1.552	-0.959
	0.295	1.02	0.612	-0.970	-0.358	1.58	2.073	-1.211
S1B-N1B	0.212	-0.02	0.203	-0.411	-0.208	2.02	0.958	-0.981
	0.238	-0.41	0.212	-0.525	-0.314	2.48	0.889	-1.318
C1B-S1B	0.204	-0.52	0.047	-0.223	-0.177	4.84	0.225	-0.868
	0.206	-0.42	0.045	-0.194	-0.150	4.37	0.216	-0.729
S1A-O2A	0.244	0.61	0.388	-0.622	-0.234	1.60	1.59	-0.959
	0.292	0.97	0.597	-0.950	-0.353	1.59	2.040	-1.208
S1A-O1A	0.241	0.57	0.373	-0.603	-0.23	1.61	1.548	-0.954
	0.292	0.97	0.597	-0.950	-0.353	1.59	2.040	-1.208
S1A-N1A	0.211	-0.02	0.202	-0.409	-0.207	2.02	0.957	-0.981
	0.227	-0.49	0.167	-0.457	-0.290	2.73	0.737	-1.274
C1A-S1A	0.206	-0.53	0.048	-0.228	-0.18	4.75	0.233	-0.874
	0.215	-0.45	0.052	-0.216	-0.163	4.14	0.242	-0.760
C7A-O7A	0.399	-0.63	0.554	-1.265	-0.711	2.28	1.388	-1.782
	0.405	-0.15	0.639	-1.315	-0.676	2.06	1.580	-1.672
C7A-N4A	0.328	-1.05	0.204	-0.671	-0.467	3.28	0.622	-1.424
	0.297	-0.79	0.204	-0.607	-0.403	2.97	0.689	-1.357
C8A-C7A	0.247	-0.64	0.048	-0.256	-0.208	5.33	0.194	-0.842
	0.227	-0.49	0.052	-0.227	-0.175	4.35	0.229	-0.768

C8A-O8A2	0.375	-0.76	0.461	-1.112	-0.651	2.41	1.229	-1.736
	0.370	-0.42	0.490	-1.086	-0.596	2.22	1.324	-1.609
C8A-O8A1	0.383	-0.69	0.499	-1.17	-0.671	2.34	1.303	-1.752
	0.396	-0.31	0.578	-1.235	-0.657	2.14	1.462	-1.659
C4A-N4A	0.283	-0.79	0.151	-0.499	-0.348	3.30	0.534	-1.230
	0.311	-0.90	0.199	-0.623	-0.424	3.13	0.640	-1.361
C4B-N4B	0.253	-0.62	0.105	-0.364	-0.259	3.46	0.415	-1.024
	0.231	-0.48	0.161	-0.444	-0.282	2.75	0.698	-1.220
C3A-C4A	0.315	-0.93	0.100	-0.433	-0.333	4.33	0.317	-1.057
	0.301	-0.83	0.092	-0.393	-0.300	4.26	0.306	-0.997
C5A-C4A	0.317	-0.94	0.100	-0.434	-0.334	4.34	0.315	-1.054
	0.301	-0.83	0.092	-0.393	-0.300	4.26	0.306	-0.997
C3A-C2A	0.319	-0.93	0.104	-0.441	-0.337	4.24	0.326	-1.056
	0.313	-0.88	0.106	-0.433	-0.327	4.08	0.339	-1.044
C2A-C1A	0.318	-0.92	0.105	-0.441	-0.336	4.20	0.33	-1.057
	0.304	-0.83	0.100	-0.409	-0.309	4.08	0.330	-1.017
C6A-C1A	0.318	-0.92	0.104	-0.44	-0.336	4.23	0.327	-1.057
	0.304	-0.83	0.100	-0.409	-0.309	4.08	0.330	-1.017
C6B-C1B	0.319	-0.93	0.106	-0.444	-0.338	4.18	0.332	-1.060
	0.310	-0.87	0.102	-0.420	-0.319	4.14	0.328	-1.030
C6B-C5B	0.316	-0.92	0.101	-0.432	-0.331	4.27	0.32	-1.047
	0.308	-0.87	0.101	-0.419	-0.318	4.14	0.328	-1.031
C6A-C5A	0.321	-0.94	0.106	-0.448	-0.342	4.22	0.33	-1.065
	0.313	-0.88	0.106	-0.433	-0.327	4.08	0.339	-1.044
C5B-C4B	0.323	-0.96	0.105	-0.45	-0.345	4.28	0.325	-1.068
	0.312	-0.88	0.108	-0.438	-0.329	4.03	0.348	-1.055

C2B-C1B	0.319	-0.93	0.105	-0.442	-0.337	4.21	0.329	-1.056
	0.310	-0.87	0.102	-0.420	-0.319	4.14	0.328	-1.030
C3B-C4B	0.322	-0.96	0.105	-0.45	-0.345	4.28	0.326	-1.071
	0.312	-0.88	0.108	-0.438	-0.329	4.03	0.348	-1.055
C3B-C2B	0.320	-0.94	0.104	-0.444	-0.34	4.26	0.325	-1.062
	0.308	-0.87	0.101	-0.419	-0.318	4.14	0.328	-1.031

$\rho(r)$ – charge density (a.u.); $\nabla^2\rho(r)$ – Laplacian of electron density (a.u.); G(r), V(r), E(r) – local kinetic, potential and total energy density (a.u.)

Table S6. Percent Source Function (%SF) contribution to S-X bond critical points within sulfamic acid anion in (I).

Bond	ρ(r)	S2	O21	O22	O23	N2	Total
S2-O21	0.244	33.38	47.87	6.54	5.91	3.18	96.88
S2-O22	0.232	33.52	6.20	48.42	5.72	3.09	96.95
S2-O23	0.239	32.83	6.68	6.79	47.09	3.33	96.72
S2-N2	0.205	33.72	6.72	6.89	6.19	40.56	94.08

Table S7. Percent Source Function (%SF) contribution to S-X bond critical points within sulfanilamide cation in (I).

Bond	ρ(r)	S1	O1	O2	C1	N1	Total
S1-O1	0.243	35.28	48.45	6.31	0.88	3.97	94.89
S1-O2	0.242	35.66	6.11	48.47	0.85	3.87	94.96
S1-C1	0.204	34.21	5.54	5.58	36.51	3.08	84.92
S1-N1	0.214	36.67	6.89	6.94	0.74	41.36	92.60

Table S8. Percent Source Function (%SF) contribution to S-X bond critical points within sulfoxamic anion in (II).

Bond	ρ	S1A	O1A	O2A	C1A	N1A	Total
S1A-O1A	0.268	35.73	48.55	6.32	0.75	3.69	95.04
S1A-O2A	0.272	35.56	6.16	48.83	0.74	3.72	95.01
S1A-C1A	0.236	34.28	5.48	5.52	36.34	2.97	84.59
S1A-N1A	0.200	36.41	7.05	7.25	0.68	40.79	92.18

Table S9. Percent Source Function (%SF) contribution to S-X bond critical points within sulfanilamide cation in (II).

Bond	ρ	S1B	O1B	O2B	C1B	N1B	Total
S1B-O1B	0.268	35.62	48.61	6.40	0.81	3.67	95.11
S1A-O2A	0.273	35.78	6.10	48.93	0.83	3.57	95.21
S1B-O2B	0.241	34.20	5.70	5.83	30.69	3.07	79.49
S1A-N1A	0.200	37.19	6.75	6.86	0.71	40.68	92.19

Table S10. QTAIM atomic charges for selected atoms in (I) and (II).

(I)		(II)	
Atom	Q	Atom	Q
S2	3.60	S1A	2.99
O21	-1.34	O1A	-1.32
O22	-1.33	O2A	-1.31
O23	-1.34	C1A	-0.18
N2	-1.34	N1A	-1.36
S1	2.94	S1B	2.99
O1	-1.32	O1B	-1.32
O2	-1.33	O2B	-1.31
C1	-0.15	C1B	-0.16
N1	-1.39	N2B	-1.37

Table S11. Topological analysis of intermolecular interactions in (I).

	d	d_1	d_2	ρ(r)	$\nabla^2\rho(r)$	λ_1	λ_2	λ_3	ε
H21···O1i	2.127	0.798	1.329	0.017	0.07	-0.02	-0.02	0.11	0.0
H22···O2i	2.583	1.038	1.545	0.007	0.03	-0.01	-0.01	0.04	0.18
H11···O2i	1.904	0.691	1.213	0.025	0.10	-0.03	-0.03	0.17	0.04
H22···O1	2.057	0.767	1.29	0.018	0.08	-0.02	-0.02	0.12	0.07
H12···N2ii	1.906	0.638	1.268	0.033	0.09	-0.05	-0.05	0.18	0.03
H42···O23iii	1.879	0.644	1.235	0.030	0.10	-0.04	-0.04	0.19	0.05
H43···O22iv	1.795	0.61	1.185	0.036	0.12	-0.06	-0.05	0.23	0.05
H3···O21v	2.312	0.891	1.421	0.013	0.05	-0.01	-0.01	0.07	0.05
H5···O21vi	2.442	0.982	1.46	0.010	0.04	-0.01	-0.01	0.05	0.08
H3···O22v	2.457	0.972	1.485	0.010	0.04	-0.01	-0.01	0.06	0.18
H41···O22v	1.989	0.707	1.282	0.021	0.08	-0.03	-0.03	0.14	0.02
H21···O23vii	2.386	0.942	1.444	0.009	0.04	-0.01	-0.01	0.05	0.17

Symmetry codes: i[x+1,y,z]; ii[-x+1,y-1/2,-z]; iii[x,y-1,z]; iv[-x+1,y-1/2,-z+1]; v[-x+2,y-1/2;-z+1]; vi[x-1,y-1,z]; vii[-x,y-1/2,-z];

d – intermolecular distance (Å); d_1, d_2 – distance between BCPs and interacting atoms (Å); ρ(r) – charge density (a.u.); $\nabla^2\rho(r)$ – Laplacian of electron density (a.u.); λ_1, λ_2, λ_3 - eigenvalues of Hessian (a.u.); ε – bond ellipticity.

Table S12. Topological analysis of intermolecular interactions in (I).

	d	ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	E(r)	|V(r)|/ G(r)	G(r)/ρ(r)	E(r)/ ρ(r)
H21···O1^{i}	2.127	0.017	0.07	0.014	-0.012	0.002	0.86	0.823	0.118
H22···O2^{i}	2.583	0.007	0.03	0.005	-0.004	0.002	0.67	0.857	0.286
H11···O2^{i}	1.904	0.025	0.10	0.022	-0.020	0.003	0.87	0.92	0.120
H22···O1	2.057	0.018	0.08	0.016	-0.012	0.004	0.75	0.889	0.222
H12···N2^{ii}	1.906	0.033	0.09	0.023	-0.024	-0.001	1.04	0.697	-0.030
H42···O23^{iii}	1.879	0.030	0.10	0.024	-0.024	0.000	1.00	0.800	0.000
H43···O22^{iv}	1.795	0.036	0.12	0.030	-0.032	-0.002	1.07	0.833	-0.056
H3···O21^{v}	2.312	0.013	0.05	0.009	-0.008	0.002	0.80	0.769	0.154
H5···O21^{vi}	2.442	0.010	0.04	0.007	-0.005	0.002	0.71	0.700	0.200
H3···O22^{v}	2.457	0.010	0.04	0.007	-0.006	0.002	0.75	0.800	0.200
H41···O22^{v}	1.989	0.021	0.08	0.017	-0.014	0.003	0.82	0.81	0.143
H21···O23^{vii}	2.386	0.009	0.04	0.007	-0.005	0.002	0.71	0.778	0.222

Symmetry codes: i[x+1,y,z]; ii[-x+1,y-1/2,-z]; iii[x,y-1,z]; iv[-x+1,y-1/2,-z+1]; v[-x+2,y-1/2;-z+1]; vi[x-1,y-1,z]; vii[-x,y-1/2,-z];

d – intermolecular distance (Å); ρ(r) – charge density (a.u.); $\nabla^2\rho(r)$ – Laplacian of electron density (a.u.); G(r), V(r), E(r) – local kinetic, potential and total energy density (a.u.)

Table S13. Topological analysis of intermolecular interactions in (II).

	d	d_1	d_2	$\rho(r)$	$\nabla^2\rho(r)$	λ_1	λ_2	λ_3	ε
H4B3···O7A	1.98	0.723	1.257	0.023	0.09	-0.03	-0.03	0.15	0.01
H4B1···O8A2iii	1.729	0.577	1.152	0.042	0.13	-0.07	-0.07	0.27	0.02
H4B2···O8A1i	1.673	0.549	1.124	0.048	0.14	-0.08	-0.08	0.3	0.01
H4B3···O8A2ii	2.453	1.004	1.449	0.009	0.04	-0.01	-0.01	0.06	0.20
H2B2···O2Bi	2.002	0.75	1.252	0.02	0.09	-0.03	-0.02	0.14	0.06
H2B1···O1Biii	2.056	0.753	1.303	0.017	0.07	-0.02	-0.02	0.12	0.08
H1A1···O1Aiv	1.953	0.703	1.250	0.022	0.09	-0.03	-0.03	0.15	0.06
H1A2···O2A	2.091	0.794	1.297	0.016	0.07	-0.02	-0.02	0.11	0.06
H3A···O7A	2.287	0.923	1.364	0.017	0.06	-0.02	-0.01	0.1	0.17
H4A···O8A2	2.097	0.823	1.274	0.025	0.10	-0.03	-0.02	0.15	0.44

Symmetry codes: i[x,-y+1,z-1/2]; ii[x,y+1,z]; iii[x,-y,z-1/2]; iv[x,-y+1,z+1/2]

d – intermolecular distance (Å); d_1, d_2 – distance between BCPs and interacting atoms (Å); $\rho(r)$ – charge density (a.u.); $\nabla^2\rho(r)$ – Laplacian of electron density (a.u.); λ_1, λ_2, λ_3 - eigenvalues of Hessian (a.u.); ε – bond ellipticity.

Table S14. Topological analysis of intermolecular interactions in (II).

	d	ρ(r)	$\nabla^2\rho(r)$	G(r)	V(r)	E(r)	|V(r)|/ G(r)	G(r)/ ρ(r)	E(r)/ρ(r)
H4B3···O7A	1.980	0.023	0.09	0.020	-0.017	0.003	0.85	0.870	0.130
H4B1···O8A2^{iii}	1.729	0.042	0.13	0.035	-0.039	-0.004	1.114	0.833	-0.095
H4B2···O8A1^{i}	1.673	0.048	0.14	0.041	-0.047	-0.006	1.146	0.854	-0.125
H4B3···O8A2^{ii}	2.453	0.009	0.04	0.008	-0.005	0.003	0.625	0.889	0.333
H2B2···O2B^{i}	2.002	0.020	0.09	0.018	-0.015	0.003	0.833	0.900	0.150
H2B1···O1B^{iii}	2.056	0.017	0.07	0.015	-0.011	0.004	0.733	0.882	0.235
H1A1···O1A^{iv}	1.953	0.022	0.09	0.019	-0.016	0.003	0.842	0.864	0.136
H1A2···O2A	2.091	0.016	0.07	0.015	-0.011	0.003	0.786	0.875	0.188
H3A···O7A	2.287	0.017	0.06	0.014	-0.012	0.002	0.857	0.824	0.118
H4A···O8A2	2.097	0.025	0.10	0.024	-0.023	0.001	0.958	0.960	0.040

Symmetry codes: i[x,-y+1,z-1/2]; ii[x,y+1,z]; iii[x,-y,z-1/2]; iv[x,-y+1,z+1/2];

d – intermolecular distance (Å); ρ(r) – charge density (a.u.); $\nabla^2\rho$(r) – Laplacian of electron density (a.u.); *G*(r), *V*(r), *E*(r) – local kinetic, potential and total energy density (a.u.)

Table S15. Mixtures of immersion liquids used for refractive indices determination.

(I)		(II)	
n_α =1.56	Mixture of bromoform and xylene isomers	n_α=1.54	Mixture of bromoform and xylene isomers
n_β= 1.65	Mixture of methylene iodide and xylene isomers	n_β = 1.68	Mixture of methylene iodide and xylene isomers
n_γ = 1.69	Mixture of methylene iodide and xylene isomers	n_γ	None