Supporting Information

Encapsulation of Cation in Sulphate and Anion in Methyl Sulphate Salt of Sulphathiazole

Abhinav Hazarika, Abhay Pratap Singh, and Jubaraj B. Baruah*

Table of contents:

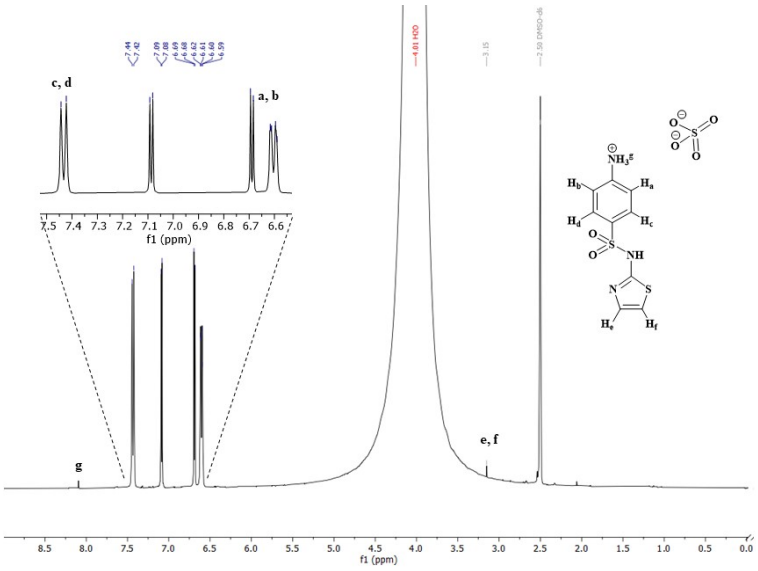


Figure S1: ^{1}HNMR (400 MHz, DMSO-d^{6}) spectra of sulphate salt of sulphathiazole (broad peak is from water in solvent).

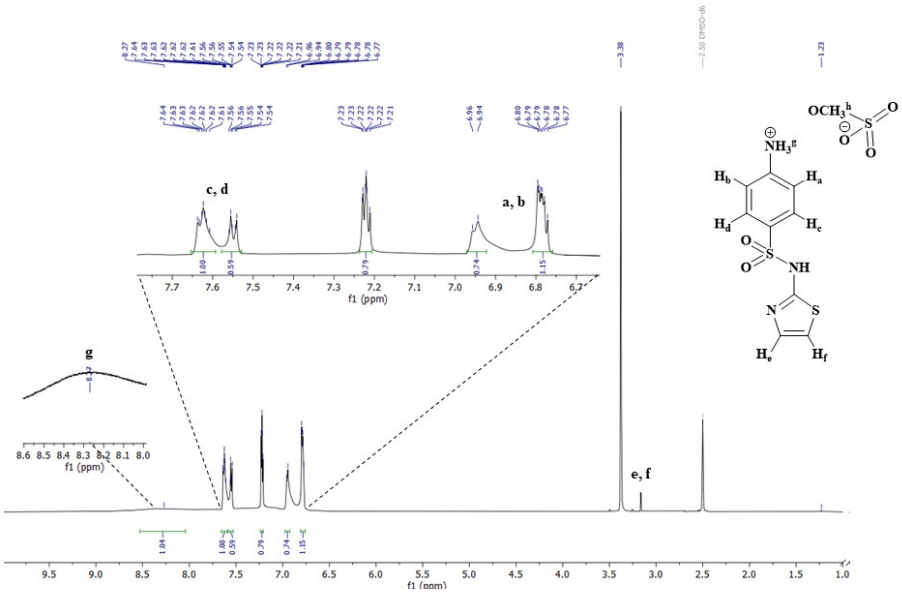
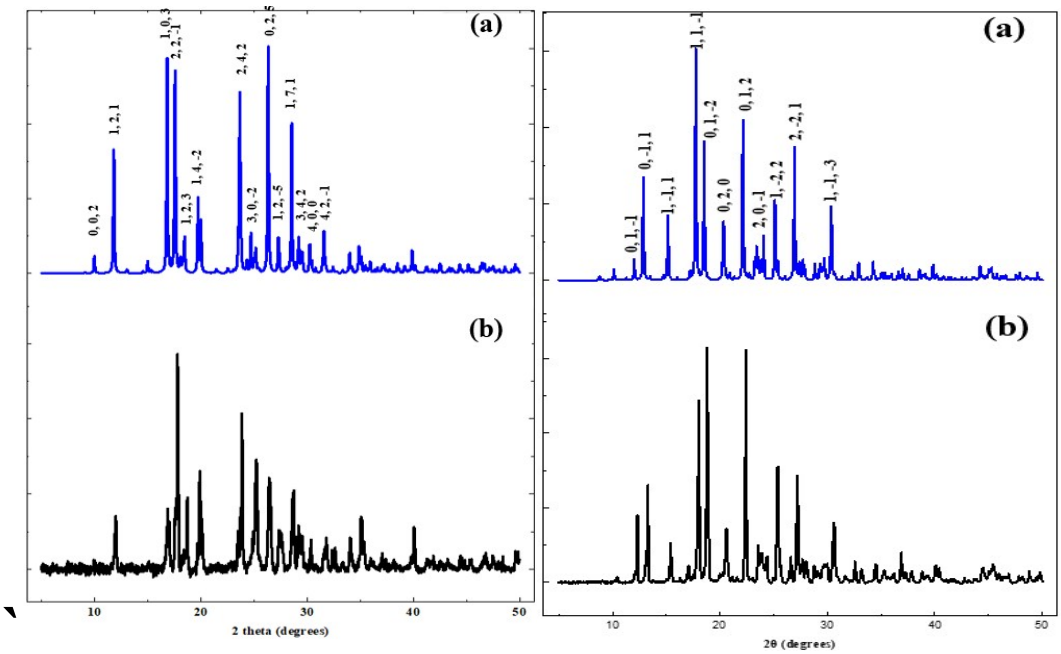


Figure S2: ^{1}HNMR (600 MHz, DMSO-d^{6}) spectra of methyl sulphate salt of sulphathiazole (broad peak is from water in solvent).



(i) (ii)

Figure S3: (a) Experimental and (b) Simulated from crystallographic information file of the (i) sulphate salt and (ii) methylsulphate salt of Sulphathiazole

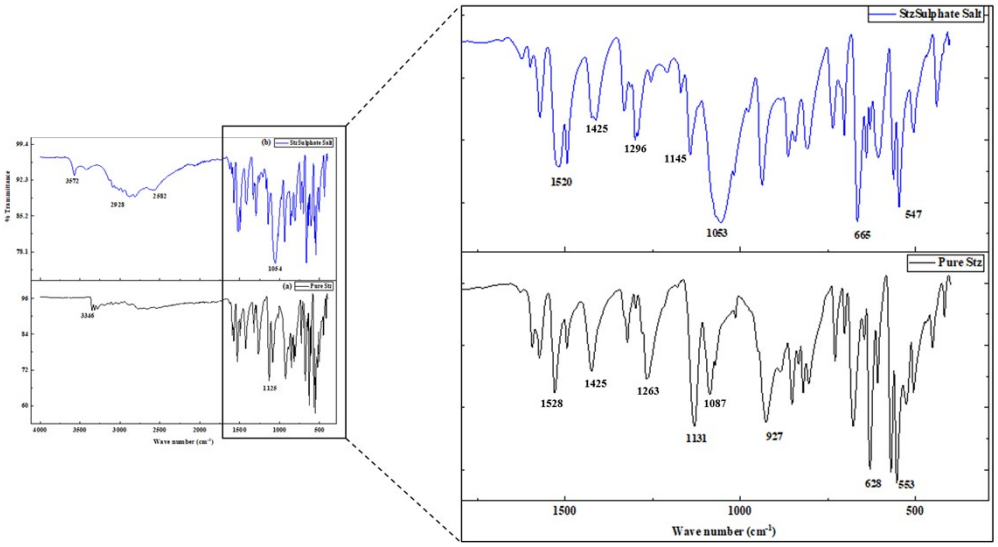


Figure S4: FTIR spectra of (a) sulphathiazole, and (b) $(HSTZ)_2(SO_4)$ (Left-side), and on the right side are the expanded regions 1800 cm^{-1} to 450 cm^{-1}.

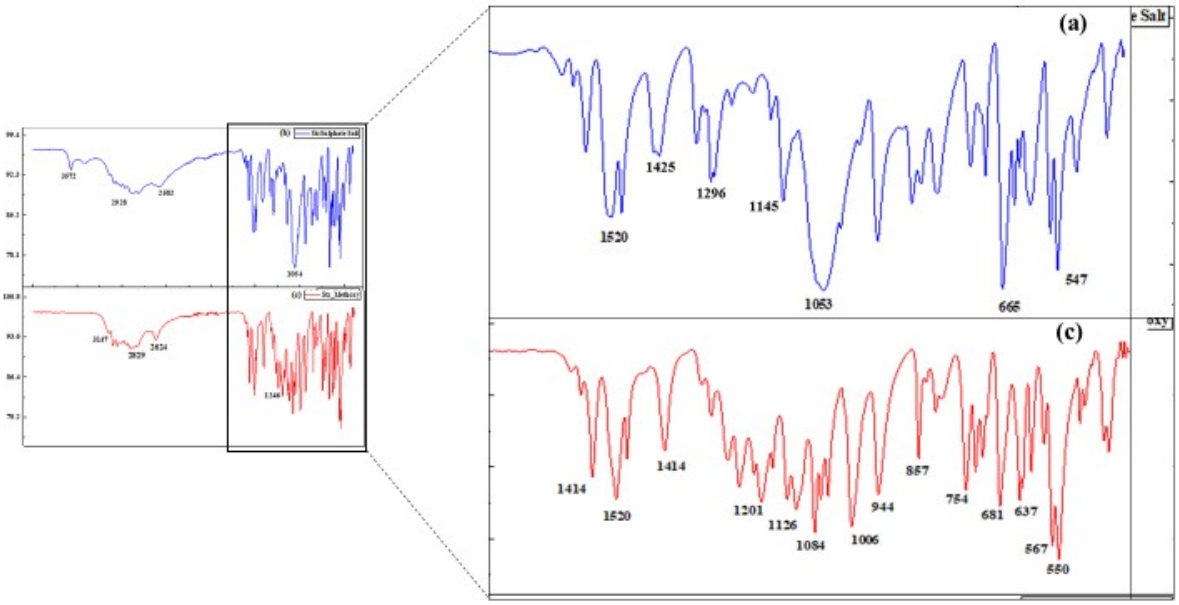
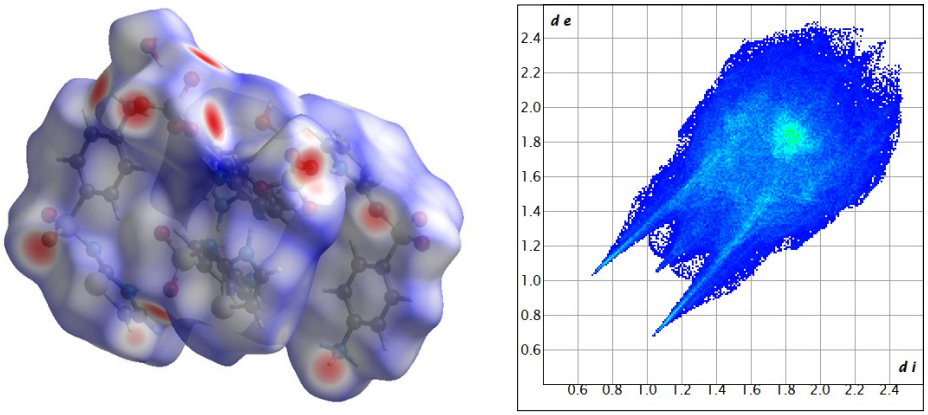
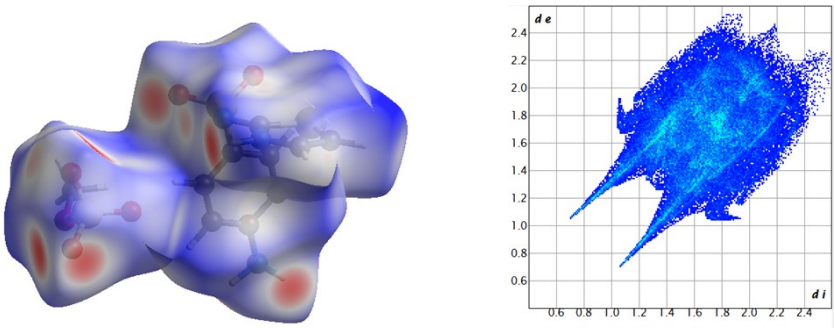


Figure S5: FTIR Spectra of (a) $(HSTZ)(MeOSO_3)$, and (b) $(HSTZ)_2(SO_4)$, (Left-side) and the expanded region 1800 cm^{-1} to 450 cm^{-1} (right side).



(i) **(ii)**

Figure S6 : (i) Hirshfeld surface, (ii) Fingerprint plot of the sulphate salt.



(i) **(ii)**

Figure S7 : (i) Hirshfeld surface and (ii) Fingerprint plot of the methyl sulphate salt

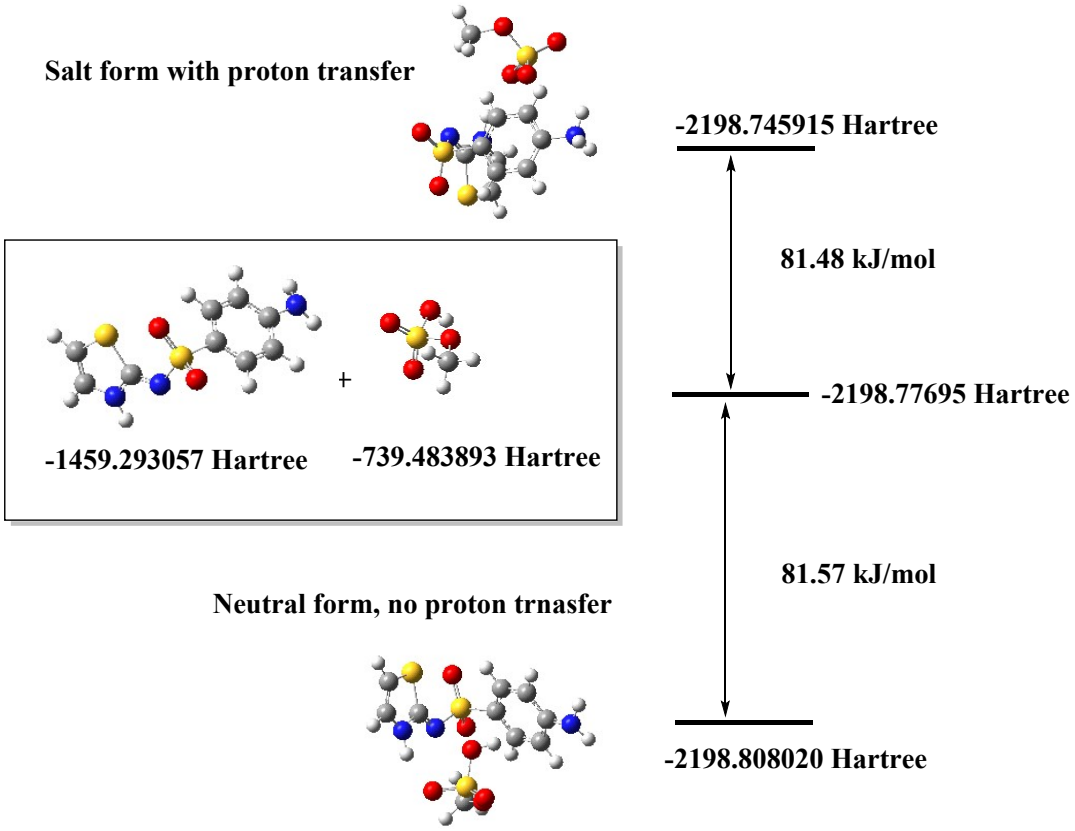


Figure S8: The difference in energy between the sum of energy of neutral components as compared to the energy of methyl-sulphate salt of sulphathiazole and cocrystal of sulphathiazole with methylsulphonica acid.

Table S1: Hydrogen-bond parameters of the sulphate salt

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠D–H···A (°)
N1–H1···O5	0.87	1.87	2.7212(1)	165
N3–H3A···O8	0.89	1.90	2.7862(1)	179
N3–H3B···N11	0.89	2.18	2.9971(1)	153
N3–H3C···O12	0.89	1.87	2.7363(1)	163
N4–H4···O14	0.86	1.94	2.8918(1)	175
N6–H6A···O11	0.89	1.93	2.8183(1)	178
N6–H6A···O12	0.89	2.52	3.0508(1)	119
N6–H6B···O7	0.89	1.96	2.7613(1)	149
N6–H6C···N8	0.89	2.13	2.9141(1)	147
N7–H7···O7	0.78	2.02	2.7974(1)	178
N9–H9A···O6	0.89	2.48	3.0582(1)	123
N9–H9A···O8	0.89	1.96	2.8483(1)	173
N9–H9B···N5	0.89	2.16	2.9256(1)	144
N9–H9C···O14	0.89	1.96	2.7833(1)	153
N10–H10···O13	0.87	1.85	2.7092(1)	169
N12–H12A···O11	0.89	1.91	2.8023(1)	177
N12–H12B···O6	0.89	1.87	2.7237(1)	161
N12–H12C···N2	0.89	2.18	2.9953(1)	151
O17–H17A···O16	0.85	2.02	2.8649(1)	173
O17–H17B···O5	0.85	2.24	2.9551(1)	141
O18–H18A···O9	0.85	1.96	2.8058(1)	173
O18–H18B···O13	0.85	2.17	2.8711(1)	139

Table S2: Hydrogen-bond parameters of the methyl sulphate salt

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠D–H···A (°)
N1–H1A···O1	0.89	2.13	2.9448(3)	152
N1–H1A···O1	0.89	2.31	2.9284(3)	126
N1–H1B···O4	0.89	1.88	2.7546(3)	169
N1–H1C···N2	0.89	2.45	3.0564(3)	121
N1–H1C···O5	0.89	2.14	2.9991(3)	144
N3–H3···O5	0.84	1.99	2.8185(3)	168
C5–H5···O2	0.93	2.55	3.4776(3)	176