Supplementary Materials

Two Tautomers of Thiobarbituric Acid in One Crystal: The Experimental Charge Density Perspective

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Table of contents:

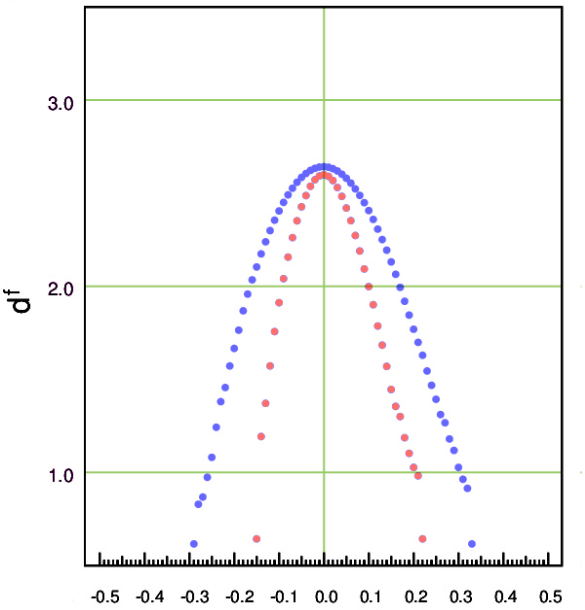

Figure S1. Residual density analysis for the TBA crystal blue whole range. red 0.8 A.

Table S1. Rigid bond test result.

Atom 1	Atom 2	ΔZ_{AB}^2
N1	C2	-0.00036(30)
N1	C6	-0.00027(41)
S2	C2	-0.00019(29)
C2	N3	0.00012(42)
N3	C4	-0.00027(45)
O4	C4	0.00019(45)
C4	C5	0.00039(31)
C5	C6	-0.00040(41)
O6	C6	-0.00002(36)
S12	C12	-0.00004(29)
N11	C12	-0.00011(30)
N11	C16	-0.00030(39)
C12	N13	0.00028(40)
N13	C14	-0.00048(43)
O14	C14	0.00002(49)
C14	C15	-0.00020(33)
C15	C16	0.00045(39)
O16	C16	0.00015(31)
N1	H1	-0.00599(30)
N3	H3	-0.00553(24)
C5	H5	-0.00421(31)
O6	H6	-0.00497(35)
N11	H11	-0.00525(28)
N13	H13	-0.00596(21)
C15	H15A	-0.00390(30)
C15	H15B	-0.00930(30)

Figure S2. Residual electron denisty maps after IAM refinement.

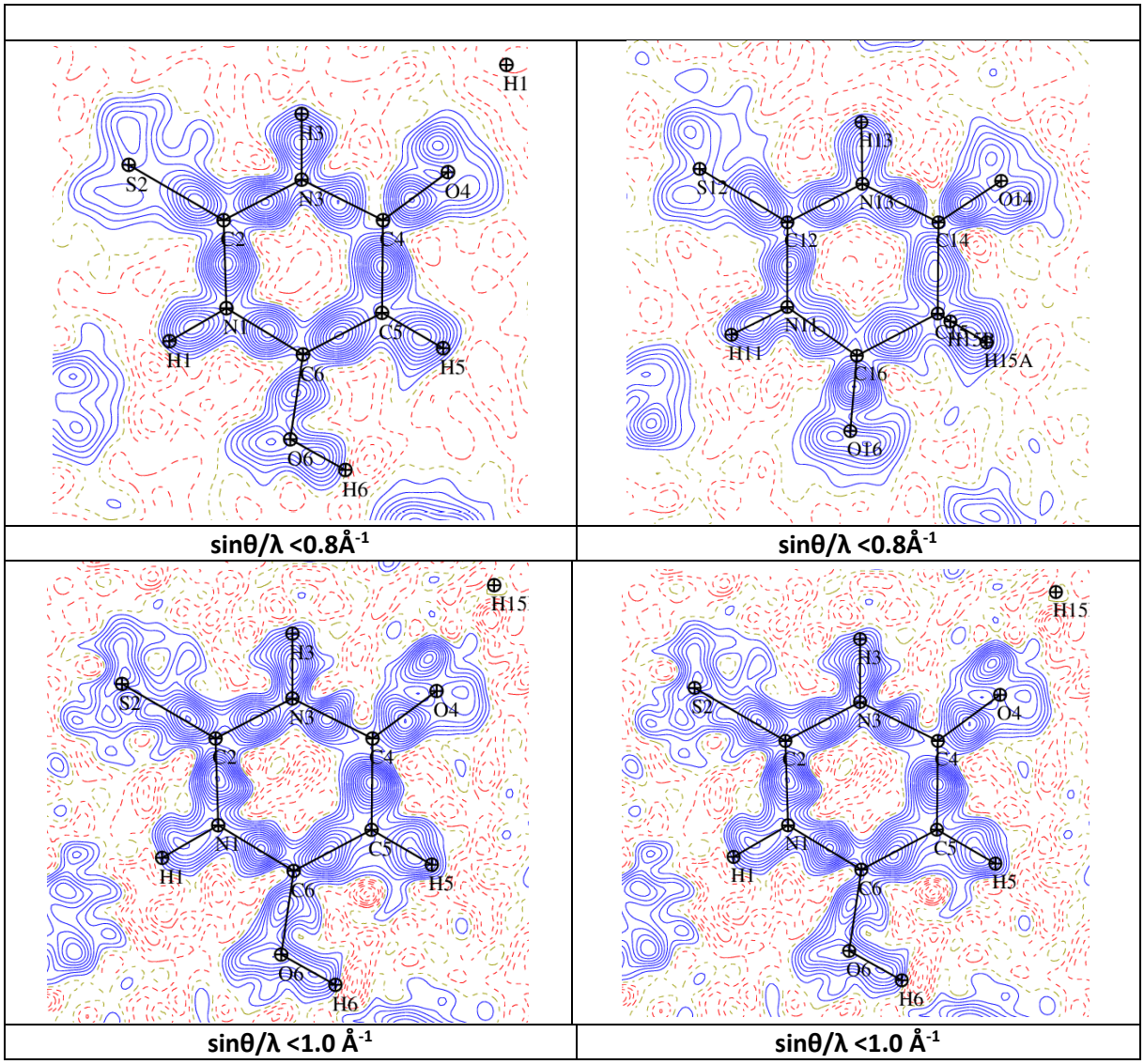

Figure S3. Residual electron denisty maps after multipolar refinement.

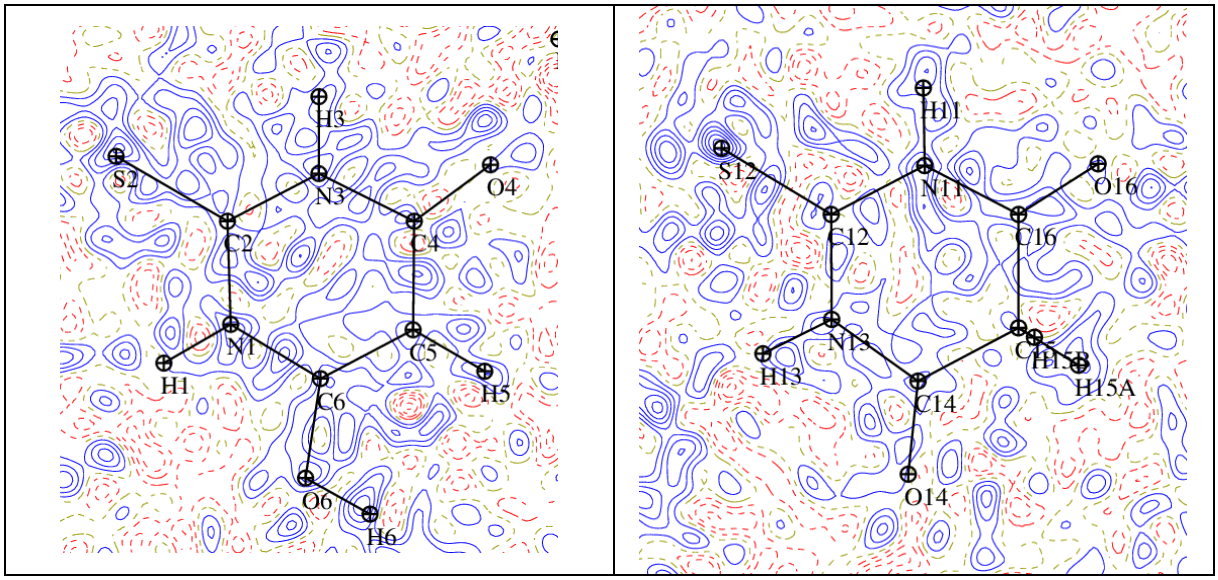

Table S2. Bond critical point characteristics. D12: distance between two atoms; Gcp: kinetic energy density (kJ/mol/Bohr^3); Vcp: potential energy density(kJ/mol/Bohr^3); LAP: laplacian (bcp) (eÅ^{-5})]; RHO: electron density (bcp) (eÅ^{-3})]. ELLIP – ellipticity.

L.p.	atom1	atom2	D12	D1cp	D2cp	RHO	Lapl.	Hessian matrix			Ellip.
cp1	O14	C14	1.2189	0.7882	0.4310	2.9124	-31.52	-29.57	-24.36	22.41	0.21
cp2	O16	C16	1.2296	0.7889	0.4410	2.8708	-36.09	-28.29	-24.04	16.25	0.18
cp3	O4	C4	1.2402	0.7987	0.4422	2.8688	-36.16	-27.96	-24.60	16.41	0.14
cp4	C2	N3	1.3479	0.5586	0.7894	2.3752	-25.39	-20.71	-17.29	12.60	0.20
cp5	N1	C2	1.3522	0.8029	0.5494	2.3538	-25.88	-20.18	-16.97	11.26	0.19
cp6	O6	C6	1.3163	0.8158	0.5008	2.3396	-28.74	-20.45	-18.20	9.91	0.12
cp7	N11	C12	1.3671	0.7704	0.5968	2.3027	-21.41	-19.34	-16.57	14.50	0.17
cp8	C12	N13	1.3614	0.5688	0.7928	2.2743	-22.95	-19.24	-16.03	12.33	0.20
cp9	N1	C6	1.3728	0.8098	0.5638	2.2175	-23.75	-18.60	-15.25	10.10	0.22
cp10	C5	C6	1.3701	0.6174	0.7529	2.1760	-20.22	-17.01	-12.28	9.06	0.39
cp11	N11	C16	1.3715	0.8309	0.5411	2.1417	-24.68	-17.79	-15.03	8.13	0.18
cp12	N13	C14	1.3758	0.8126	0.5635	2.1322	-22.80	-18.55	-14.96	10.71	0.24
cp13	C4	C5	1.4223	0.7203	0.7021	2.0545	-18.81	-16.28	-12.88	10.35	0.26
cp14	N3	H3	1.0090	0.7828	0.2262	2.0324	-28.59	-29.05	-27.78	28.24	0.05
cp15	N13	H13	0.9993	0.7790	0.2204	2.0253	-27.94	-29.86	-28.25	30.18	0.06
cp16	N1	H1	1.0090	0.7901	0.2189	2.0049	-29.82	-29.44	-27.92	27.54	0.05
cp17	N3	C4	1.3944	0.8385	0.5560	1.9936	-19.90	-16.43	-13.59	10.12	0.21
cp18	N11	H11	1.0061	0.7821	0.2241	1.9747	-26.62	-28.18	-26.91	28.47	0.05
cp19	O6	H6	0.9670	0.7830	0.1840	1.9653	-30.93	-34.24	-34.00	37.31	0.01
cp20	C14	C15	1.4969	0.7698	0.7275	1.8321	-13.16	-14.02	-11.76	12.61	0.19
cp21	C5	H5	1.0830	0.7271	0.3560	1.7979	-18.31	-17.41	-16.06	15.16	0.08
cp22	C15	H15A	1.0882	0.7367	0.3521	1.7905	-17.44	-17.17	-16.63	16.37	0.03
cp23	C15	C16	1.4950	0.6947	0.8005	1.7515	-12.02	-12.73	-10.78	11.49	0.18
cp24	C15	H15B	1.0925	0.6944	0.3987	1.7410	-14.34	-15.12	-14.39	15.17	0.05
cp25	S12	C12	1.6582	0.7498	0.9086	1.5831	-6.19	-7.74	-6.15	7.70	0.26
cp26	S2	C2	1.6850	0.7771	0.9082	1.4576	-4.93	-7.03	-5.85	7.96	0.20

Table S3. Bond critical points for intermolecular interactions. D12: distance between two atoms; Gcp: kinetic energy density (kJ/mol/Bohr^3); Vcp: potential energy density(kJ/mol/Bohr^3); LAP: Laplacian (bcp) (eÅ^{-5})]; RHO: electron density (bcp) (eÅ^{-3})]. Symmetry codes: [i] 1-x,1-y,-z; [ii] x,1/2-y,1/2+z; [iii] -1+x,1/2-y,1/2+z; [iv]1-x,-y,-z; [v] x,1/2-y,-1/2+z; [vi] 1+x,y,z; [vii] 1-x,-1/2+y,-1/2-z; [viii] 1+x,1/2-y,-1/2+z; [ix] 2-x,1-y,-z; [x] 1-x,-1/2+y,1/2-z; [xi] -x,-y,-z

CP	Atom1	Atom2	Gcp	Vcp	D12	D1cp	D2cp	RHO	LAPL	Hessian matrix		
cp27	O16	H6[i]	111.72	-111.85	1.6832	1.1302	0.5540	0.2793	4.10	-1.67	-1.66	7.44
cp28	O4	H11[ii]	110.88	-100.40	1.7062	1.1325	0.5737	0.2448	4.46	-1.41	-1.37	7.24
cp29	O14	H1[iii]	90.80	-72.82	1.7779	1.1812	0.5982	0.182	3.99	-0.99	-0.96	5.94
cp30	S12	H3[iv]	40.31	-32.25	2.2901	1.5509	0.7470	0.1114	1.78	-0.44	-0.37	2.58
cp31	S2	H13[iv]	37.98	-29.86	2.3052	1.5411	0.7760	0.1045	1.69	-0.45	-0.34	2.48
cp32	O4	H15B	25.12	-19.67	2.3363	1.3797	0.9956	0.0810	1.12	-0.29	-0.25	1.66
cp33	O16	H15B[v]	19.47	-14.50	2.4136	1.4286	1.0177	0.0637	0.90	-0.23	-0.19	1.32
cp34	S12	C12[iv]	11.87	-9.00	3.4031	1.8269	1.5815	0.0488	0.54	-0.08	-0.06	0.68
cp35	S2	C16[vi]	11.76	-8.62	3.3353	1.8221	1.5239	0.0457	0.55	-0.07	-0.03	0.64
cp36	S2	C15[vi]	12.80	-9.10	3.4519	1.7625	1.6925	0.0453	0.61	-0.04	-0.01	0.66
cp37	S12	N1[vii]	13.07	-9.15	3.3687	1.7548	1.6307	0.0445	0.62	-0.10	-0.03	0.75
cp38	S2	H15A[viii]	9.84	-7.41	2.9660	1.8491	1.1481	0.0431	0.45	-0.13	-0.09	0.68
cp39	S12	H5[v]	11.45	-8.10	2.8213	1.7975	1.0656	0.0420	0.54	-0.13	-0.08	0.76
cp40	O6	N1[ix]	12.47	-8.36	3.1644	1.5415	1.6239	0.0392	0.61	-0.10	-0.07	0.79
cp41	S2	C4[v]	9.76	-6.63	3.4504	1.9081	1.5752	0.0349	0.47	-0.05	-0.01	0.53
cp42	C5	C5[i]	7.04	-4.89	3.6531	1.8265	1.8265	0.0301	0.34	-0.08	-0.03	0.44
cp43	O6	O6[ix]	9.13	-5.74	3.3143	1.6572	1.6571	0.0274	0.46	-0.06	-0.01	0.54
cp44	O14	C5[x]	6.13	-3.92	3.5694	1.7158	1.8546	0.0228	0.31	-0.05	-0.02	0.38
cp45	S12	H15B[iv]	5.11	-3.39	3.4197	1.9906	1.5559	0.0224	0.25	-0.03	-0.01	0.30
cp46	O14	N13[xi]	5.89	-3.64	3.5223	1.7267	1.8040	0.0201	0.30	-0.04	-0.01	0.36
cp47	O14	S12[xi]	5.11	-3.20	3.7757	1.6983	2.0994	0.0193	0.26	-0.04	-0.01	0.31
cp48	N13	N13[xi]	4.92	-3.02	3.6910	1.8455	1.8455	0.0176	0.25	-0.03	0.00	0.28