Supplementary Information

Facile Synthesis and Characterization of Symmetric *N*-[(Phenylcarbonyl) carbamothioyl]benzamide Thiourea: Experimental and Theoretical Investigations

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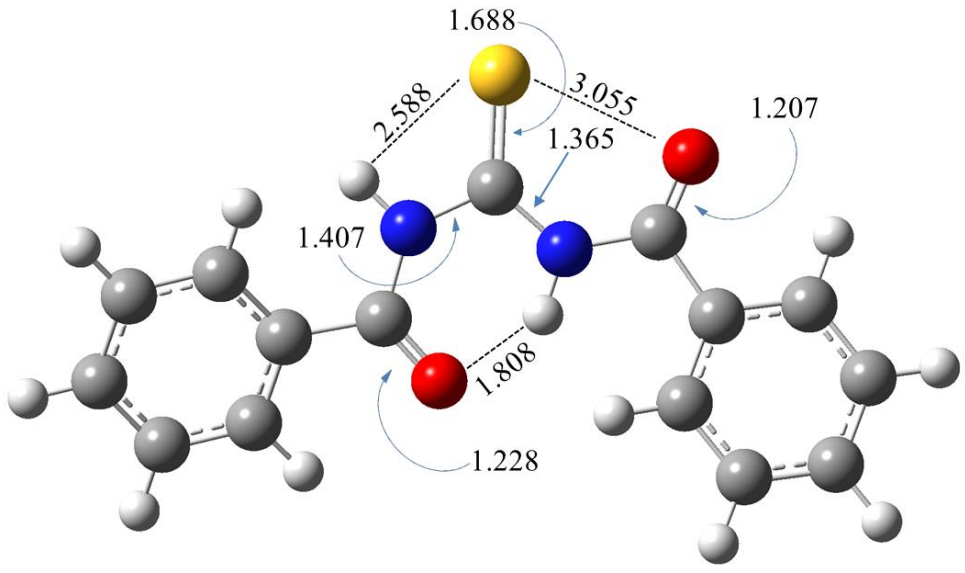

Figure S1. Optimized BT structure and bond length (in Å), obtained at B3LYP/6-311++G(2d,2p) level.

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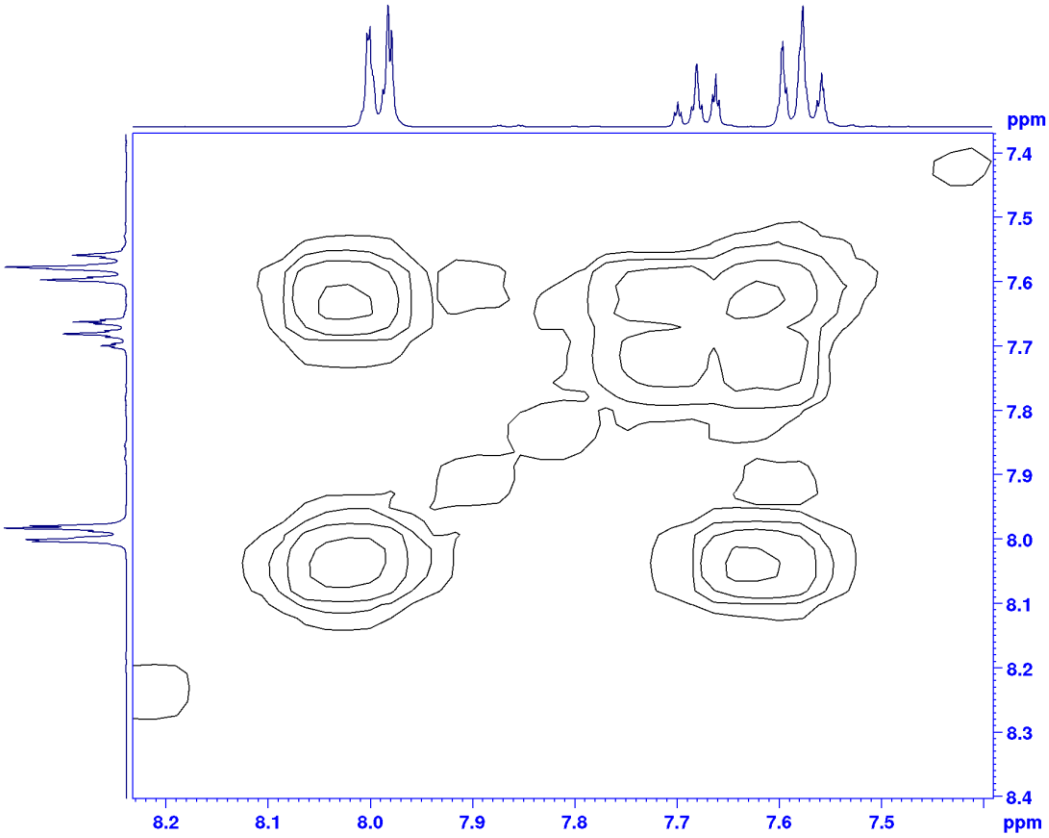


Figure S2. ^{1}H-^{1}H COSY experiments (400.21 MHz, CD_2Cl_2) of BT.

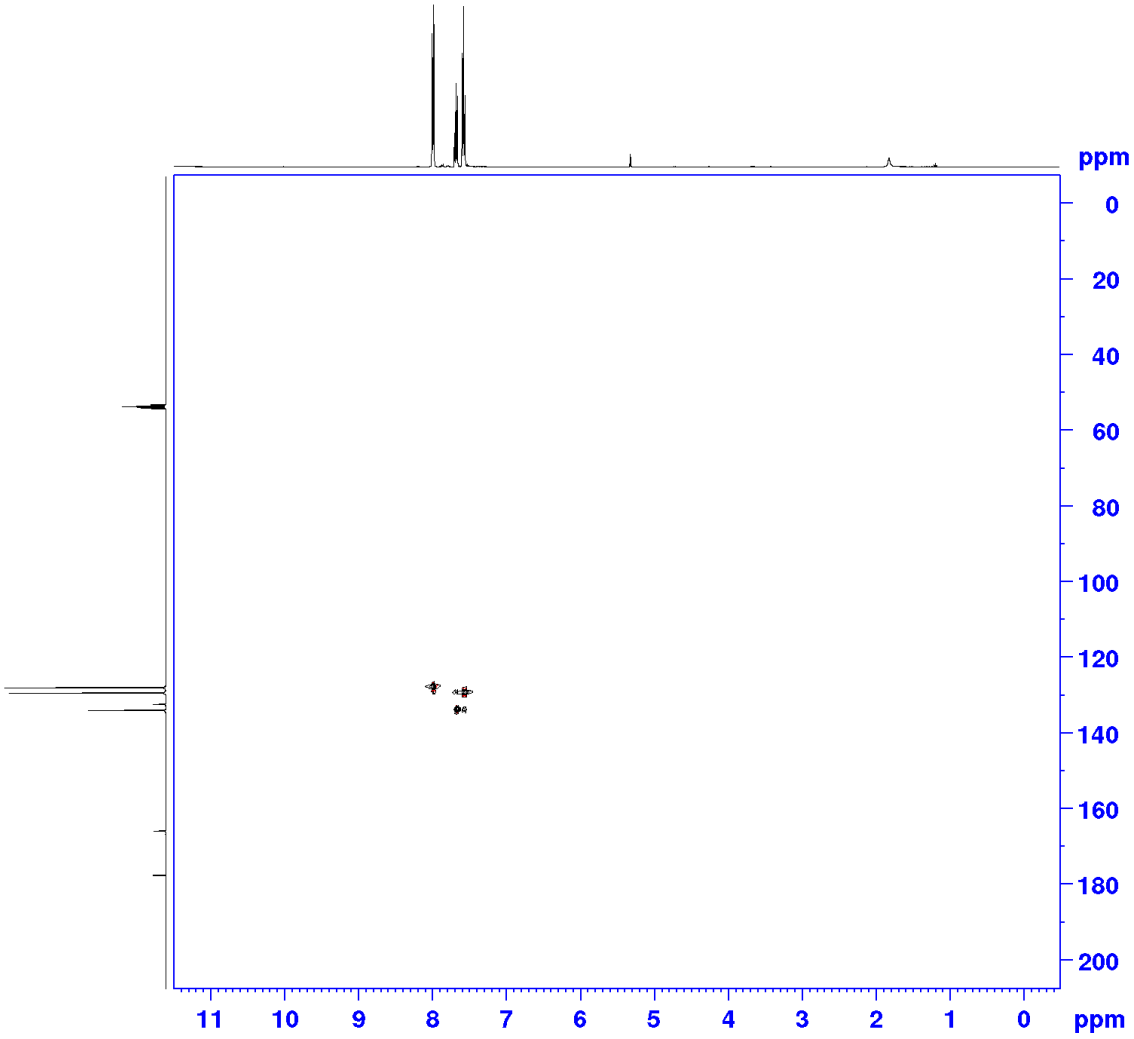


Figure S3. ^{1}H-^{13}C HSQC experiments (400.21 MHz, CD_2Cl_2) of BT.

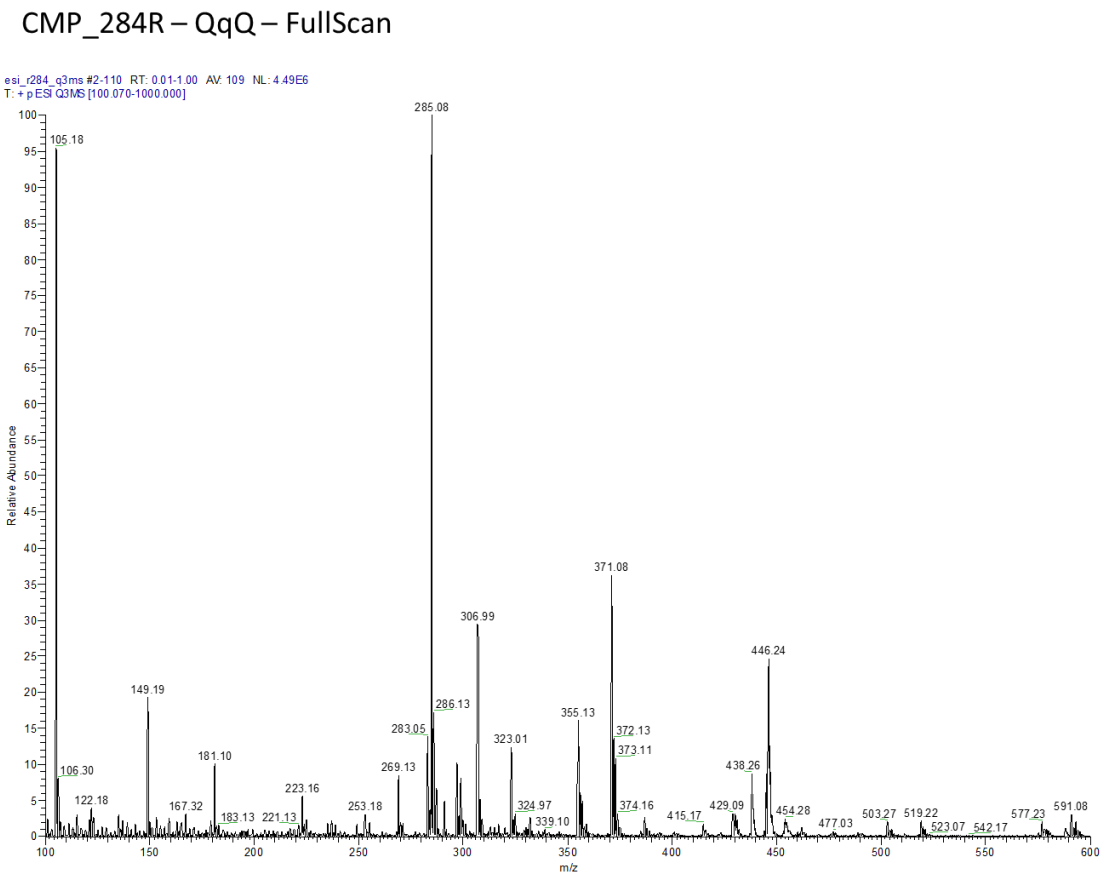


Figure S4. Spectrum of mass (full scan MS) of BT.

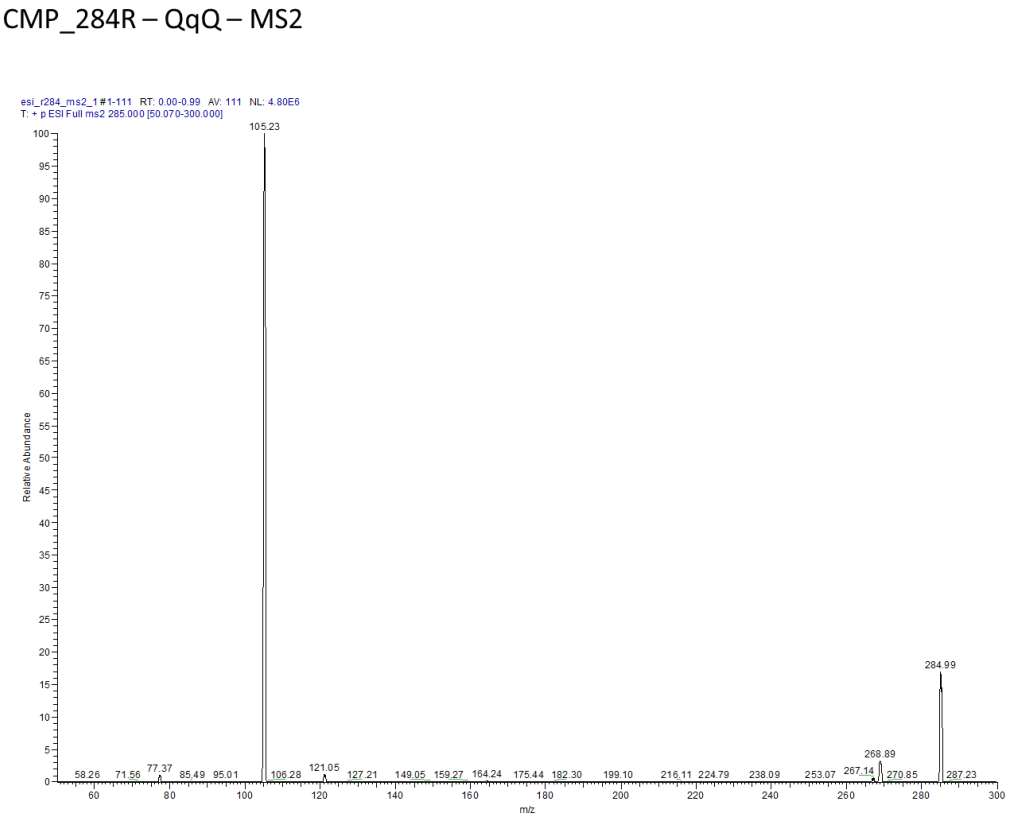


Figure S5. Spectrum of mass (MS/MS) of BT.

MALDI_MS

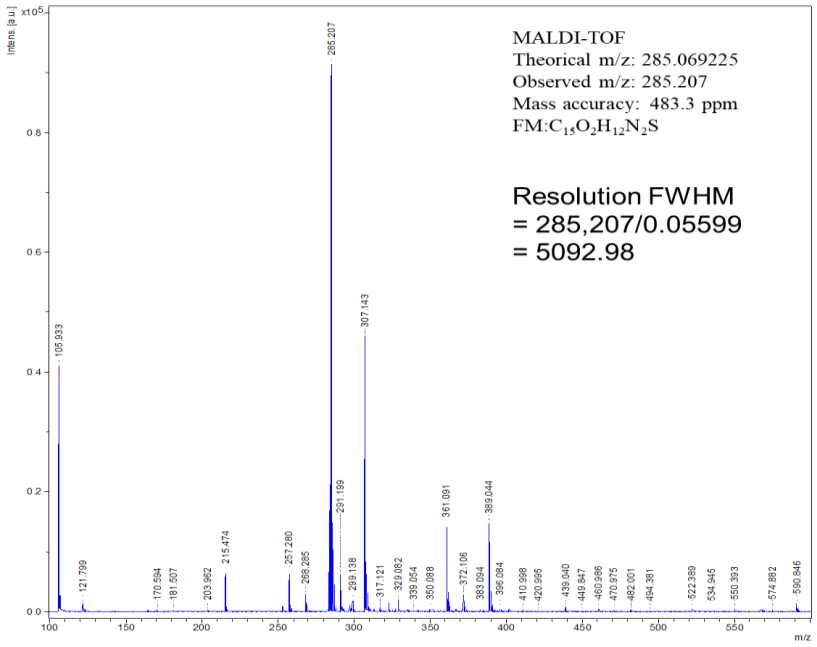
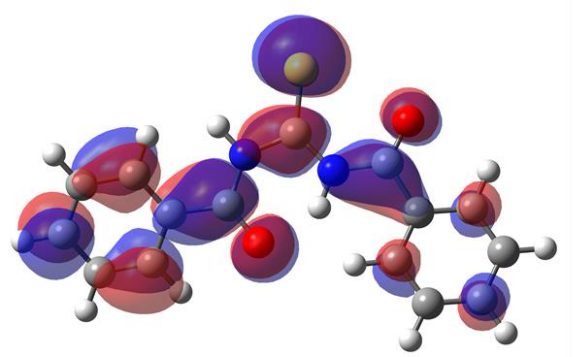
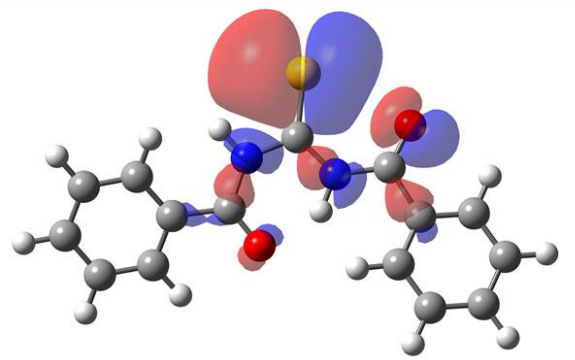


Figure S6. Spectrum of mass (MALDI-MS) of BT.



E_{LUMO} = -2.5551 eV
(First exceted state)

ΔE = 3.6272 eV



E_{HOMO} = -6.1824 eV
(Ground state)

Figure S7. Representation of HOMO and LUMO obtained at B3LYP/6-311++G(2d,2p) level.

NBO analysis

The data of NBO analysis showed that in *cis* conformation there are two equivalent resonant systems, while in *trans*, there is only one and the electronic density more localized resulting in a more negative charge. Furthermore, the charge on oxygen atom that forms the intramolecular hydrogen bond is more negative in *trans* structure when compared to the *cis* form. However, an opposite relation is found for hydrogen atom of the intramolecular hydrogen bond, i.e., it is more positive in *trans* configuration, which means that the hydrogen becomes more acid, as expected by the weakening of NH bond due to the formation of NH---O bond.

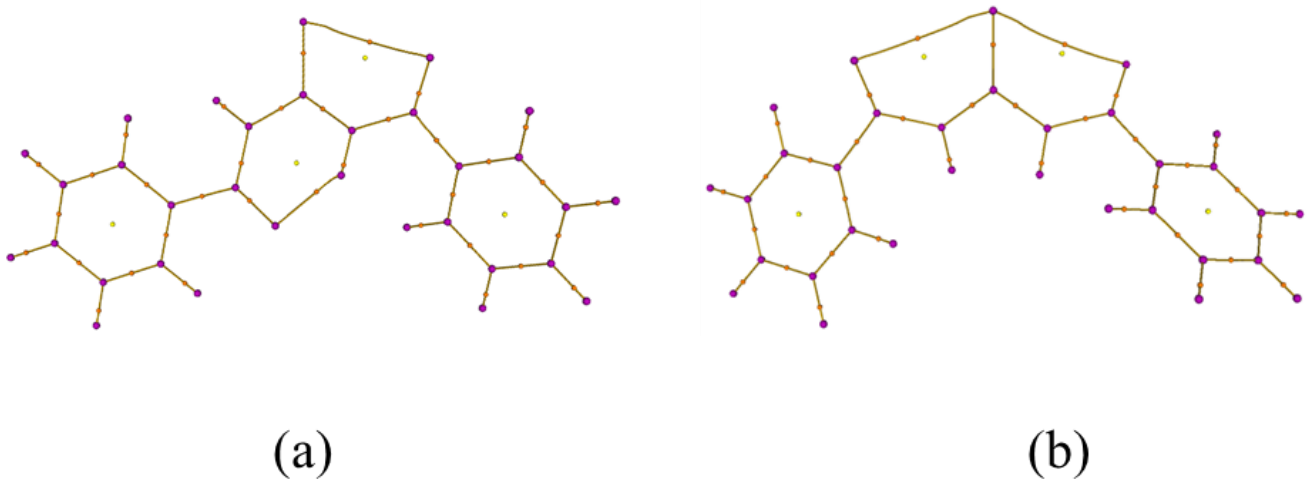


Figure S8. Graphs of (a) *trans*-BT and (b) *cis*-BT with critical points represented by purple (nucleic critical point, NCP), by orange (bond critical point, BCP) and yellow (ring critical point, RCP). Paths are represented by solid lines.

The stabilization energy associated with delocalization ("2e-stabilization") is shown in Tables S5 and S6 for the most important NBO donor and acceptor.

Under topological analysis, *trans*-BT and *cis*-BT wave functions reveals the same number and same types of critical points, 32 nucleic critical point (NCP), 35 bond critical point (BCP) and 4 ring critical point (RCP). Nonetheless, *cis*-BT form presents two equivalent BCP between sulfur atom and the two oxygen atoms, while *trans*-BT has only one. This additional BCP, which in *trans* system appears in other spatial region, confers two equivalent RCP that involve S–C–N–C–O fragment, indicating a delocalization of electronic density around this whole region. As in *trans* form there is only one of this S–C–N–C–O fragment, it is expected that charge delocalization would be smaller than in *cis* configuration. Figure S8 shows the graphs of *cis*-BT and *trans*-BR with all critical points and paths connecting them. In *cis*-BT, the path between the critical point in oxygen atom and sulfur atom has length of 3.05 and 3.11 Å, respectively. In *trans*-BT, the path between the CP in oxygen atom and the BCP on the line of hydrogen atom has a length of 1.14 Å and the complement (from BCP until hydrogen NCP) is 0.64 Å, meaning that the distance between the two attractor, bond distance, is 2.04 Å, which is an usual length of a hydrogen bond.

The electronic density (ρ) and the electron localization function (ELF) of those critical points are present in Figures S9 and S10 and Table S7, which show a contour map of the Laplacian of electronic density for both forms, *cis* and *trans*, that indicates the presence of a intramolecular hydrogen bond, in *trans* form, and the presence of a resonance structure formed by the S–C–N–C–O fragment, in *cis*. The higher ρ and ELF values obtained at BCP of O–H–N region display a concentration of charge in the interatomic O–H region and indicates that there is a stronger interaction

between the oxygen atom and the proton. The other bonding regions, which exhibit $\rho(r_c)$ around 0.01 and ELF ranging from 0.02 to 0.04, indicate a moderate interaction and partially covalent nature (van der Waals interaction).

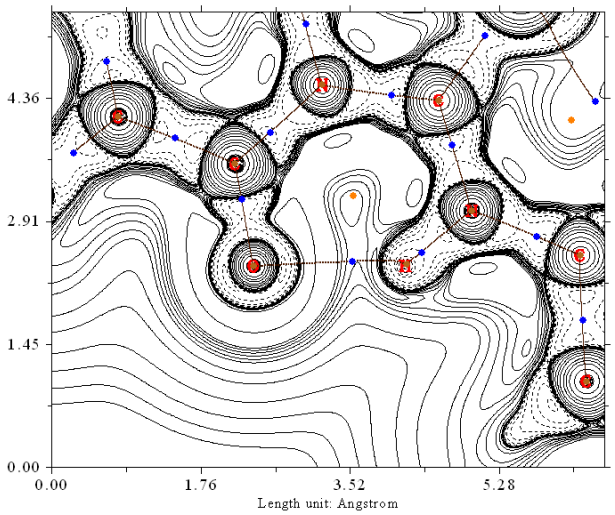


Figure S9. Contour map of the Laplacian of electronic density ($\rho(r)$) for the *trans*-BT with the bond paths linking the N_1, H_1 and O_2 nuclei and the bond critical point superimposed.

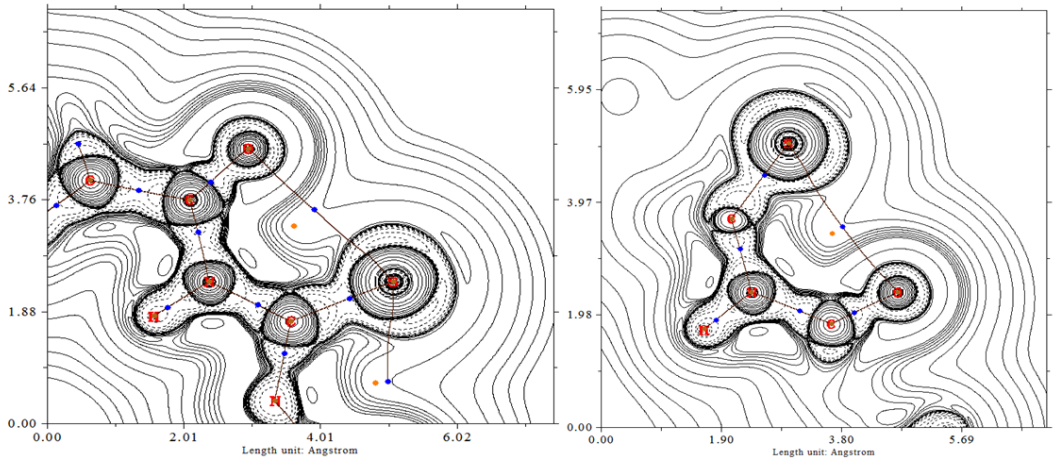


Figure S10. Contour map of the Laplacian of electronic density ($\rho(r)$) for the *cis*-BT with the bond paths closing the two (a, b) S–C–N–C–O systems and forming a RCP.

Table S1. ^{1}H and ^{13}C NMR data summary

Carbon	Chemical shift	Proton	Chemical shift	Multiplicity
2	128.15	4H	8.03	m
3	129.60	4H	7.61	m
4	132.60	2H	7.72	m
1	134.17	–		
5	166.09	–		
6	177.80	–		
Nitrogen		2H	11.75	

Table S2. Vibrational assignments and calculated wave numbers of BT at B3LYP/6-311++G(2d,2p)

Mode No.	Unscaled IR freq. / cm^{-1}	Scaled IR freq. / cm^{-1}	$I^{infrared}$ / (kM mol^{-1})	Scaled Raman freq. / cm^{-1}	Raman intensity	IR and Raman assignments
1	10.13	10.01	0.01	10.33	3.06	τ CCNC
2	25.70	25.38	0.65	26.19	2.77	ω CCNC
3	38.30	37.83	0.24	39.03	1.57	τ CCNC
4	39.26	38.79	0.72	40.02	2.89	τ CCCN
5	51.23	50.60	1.3	52.21	1.07	δ_s CNC + τ CNCN + ω CCCN
6	98.31	97.12	4.53	100.20	1.70	ω CNCN
7	114.25	112.85	0.25	116.44	1.27	τ CNCN
8	119.91	118.45	2.17	122.21	0.64	ω CNCN
9	171.62	169.53	1.11	174.92	3.04	τ CCCC
10	187.05	184.77	6.08	190.65	1.31	τ CCNC + τ CCCC
11	207.62	205.09	0.61	211.61	1.60	δ_s NCS
12	215.47	212.84	1.13	219.61	2.50	ω CCNC + τ CCCC
13	278.56	275.16	11.05	283.91	1.65	ν_s NC + ν_s CC + ν_s NC + δ_s NCO + δ_s CCC
14	328.78	324.77	3.15	335.10	0.58	ρ NCO + δ_s CCC + ρ NCN + ρ CNC
15	384.23	379.54	8.51	391.62	5.16	δ_s NCN + ρ NCO
16	410.82	405.81	0.17	418.72	0.49	τ CCCC
17	411.24	406.22	0.08	419.14	0.93	τ CCCC + τ HCCC
18	423.25	418.09	0.76	431.39	1.60	ω CCCC (ring puckering)
19	440.82	435.44	0.85	449.29	0.18	ω CCCC (ring puckering)
20	456.11	450.54	13.64	464.87	0.61	ω CCCC + CCC + NCO + NCS + CNC +CCN
21	480.40	474.54	1.32	489.63	0.95	ω CCCC + ρ CCC
22	541.04	534.44	31.48	551.44	2.05	δ_s CCN
23	628.48	620.81	19.15	640.56	0.42	ω HNCC + ρ CCC
24	633.82	626.09	1.29	646.00	8.71	δ_s CCC
25	634.73	626.99	2.45	646.93	2.91	τ SNNC + δ_s CCC

Mode No.	Unscaled IR freq. / cm^{-1}	Scaled IR freq. / cm^{-1}	$I^{infrared}$ / (kM mol^{-1})	Scaled Raman freq. / cm^{-1}	Raman intensity	IR and Raman assignments
26	673.41	665.19	13.48	686.35	6.30	ω HNCN +δ_s CCC
27	681.08	672.77	26.91	694.17	7.59	ω HNCN + δ_s CCC
28	698.61	690.09	3.17	712.04	0.12	ω HCCC + ω CCCC
29	703.18	694.61	28.22	716.70	0.20	τ HCCC + ω CCCC
30	705.24	696.63	20.34	718.79	0.85	ρ CCC
31	714.87	706.15	102.27	728.61	0.15	ω HCCC
32	717.47	708.72	17.28	731.26	0.38	ω HCCC
33	797.90	788.17	27.94	813.24	9.11	ω HNCC
34	802.32	792.53	32.1	817.74	15.47	ω HCCC + ν_s SC + ν_{as} CC + ν_s N-C
35	816.05	806.09	18.57	831.73	17.10	ν_s SC + ν_{as} CC + ν_s NC + ω HCCC + ω ONCC
36	823.89	813.83	14.09	839.72	5.00	ω HNCC + ω HCCC
37	858.36	847.89	1.1	874.86	1.62	τ HCCC
38	860.27	849.77	0.87	876.80	0.68	τ HCCC
39	880.86	870.11	1.41	897.79	49.05	ρ CNC + ν_s NC
40	928.26	916.93	60.19	946.10	0.83	δ_s NCO + δ_s NCN + ν_{as} NC + ν_s CC
41	953.09	941.46	1.51	971.41	0.28	τ HCCC
42	954.10	942.46	2.87	972.44	0.91	τ HCCC
43	999.56	987.36	1.69	1018.77	0.18	τ HCCC + ω HCCC
44	1000.90	988.69	0.63	1020.14	0.14	τ HCCC + ω HCCC
45	1018.49	1006.06	0.45	1038.06	0.11	τ HCCC
46	1019.47	1007.04	3.59	1039.07	11.43	δ_s CCC + ν_s CC
47	1019.69	1007.25	1.54	1039.28	80.74	δ_s CCC + ν_s CC
48	1020.42	1007.98	1.9	1040.04	42.70	δ_s CCC + τ HCCC + ν_s CC
49	1047.05	1034.27	20.35	1067.17	5.30	ν_s C-C + ρ CCC
50	1050.35	1037.54	7.14	1070.54	48.14	ν_s C-C + ρ CCC
51	1086.29	1073.04	47.64	1107.17	6.77	ν_{as} NC + ν_s CC + δ_s HCC
52	1094.54	1081.19	58.87	1115.58	19.08	ν_s NC + ν_{as} SC + ν_{as} CC
53	1111.56	1098.00	29.94	1132.92	4.84	ρ HCC
54	1119.17	1105.52	3.55	1140.68	27.20	ρ HCC + ν_{as} CC + ν_s NC
55	1167.54	1153.29	164.91	1189.98	44.85	ν_s NC
56	1186.27	1171.79	9.21	1209.07	6.86	ν_{as} CC
57	1188.13	1173.63	1.13	1210.96	7.34	δ_s HCC
58	1210.75	1195.98	43.96	1234.02	10.72	δ_s HCC + ν_{as} CC
59	1216.44	1201.60	19.5	1239.82	0.67	δ_s HCC
60	1250.18	1234.93	133.22	1274.21	219.07	ν_s CC + ν_{as} NC + ρ HNC
61	1254.31	1239.01	520.22	1278.42	111.81	ν_{as} CC + ν_{as} NC
62	1322.10	1305.97	268.25	1347.51	53.63	ν_{as} NC + ν_s CC

Mode No.	Unscaled IR freq. / cm^{-1}	Scaled IR freq. / cm^{-1}	$I^{infrared}$ / (kM mol^{-1})	Scaled Raman freq. / cm^{-1}	Raman intensity	IR and Raman assignments
63	1331.89	1315.64	10.63	1357.48	3.95	ν asym CC
64	1341.58	1325.21	316.01	1367.36	51.14	ν_{as} NC + ν_{as} CC
65	1362.32	1345.70	7.55	1388.50	2.53	ν_{as} CC
66	1369.77	1353.06	28.42	1396.10	8.65	δ_s HCC
67	1482.07	1463.99	17.2	1510.55	8.84	δ_s CCC + ρ HCC
68	1483.85	1465.74	0.7	1512.37	10.06	ν_{as} CC + ν_s N-C + δ_s CCC + ρ HCC
69	1517.58	1499.07	306.7	1546.75	4.85	δ_s HNC s + δ_s HCC
70	1531.41	1512.73	56.74	1560.85	14.85	δ_s HNC + δ_s HCC
71	1537.37	1518.62	147.41	1566.92	25.48	δ_s HNC + δ_s HCC
72	1588.60	1569.22	1039.43	1619.14	184.87	δ_s HNC
73	1617.82	1598.08	10.38	1648.91	7.03	ν_s CC
74	1620.20	1600.44	11.82	1651.34	12.05	ν_{as} CC
75	1639.13	1619.14	18.63	1670.64	238.46	ν_{as} CC
76	1640.20	1620.19	27.38	1671.72	175.34	ν_{as} CC + δ_s HCC
77	1699.07	1678.34	189.35	1731.72	126.67	ν_s OC
78	1769.28	1747.69	139.67	1803.29	209.58	ν_s OC
79	3172.66	3133.96	2.64	3233.64	39.80	ν_{as} CH
80	3172.73	3134.02	0.02	3233.71	35.62	ν_{as} CH
81	3179.56	3140.77	2.05	3240.67	82.99	ν_{as} CH
82	3182.27	3143.44	5.35	3243.43	139.41	ν_{as} CH
83	3189.97	3151.05	11.64	3251.28	45.05	ν_{as} CH
84	3190.21	3151.29	10.6	3251.52	89.30	ν_{as} CH
85	3198.70	3159.68	10.61	3260.18	244.32	ν_s CH
86	3199.79	3160.75	9.08	3261.29	248.42	ν_s CH
87	3211.08	3171.90	6.09	3272.80	114.06	ν_s CH
88	3211.23	3172.06	4.44	3272.95	149.11	ν_s CH
89	3396.14	3354.71	277.99	3461.41	218.89	ν_s NH
90	3611.76	3567.70	33.1	3681.18	92.14	ν_s NH

Table S3. Natural atomic charges of BT molecule in implicit solvent (acetone)

Atom	*cis*-BT	*trans*-BT	Difference
S1	0.03229	–0.16197	0.19426
O2	–0.55255	–0.64534	0.09279
C1	0.22701	0.29557	–0.06856
H1	0.38711	0.44475	–0.05764
H2	0.38711	0.43123	–0.04412
O1	–0.55254	–0.59597	0.04343
N2	–0.64875	–0.62199	–0.02676
C2	0.68597	0.70678	–0.02081
C9	0.68597	0.70541	–0.01944
N1	–0.64874	–0.64795	–0.00079

Table S4. Atomic charges obtained by NBO methodology for BT

Atom	*cis*-BT	*trans*-BT	Difference
S1	0.03229	–0.16197	0.19426
O2	–0.55255	–0.64534	0.09279
O1	–0.55254	–0.59597	0.04343
C3	–0.13864	–0.15410	0.01546
C10	–0.13864	–0.15327	0.01463
C7	–0.19165	–0.20042	0.00877
C5	–0.19165	–0.19823	0.00658
H8	0.23178	0.22654	0.00524
H11	0.23177	0.22802	0.00375
C11	–0.14871	–0.15092	0.00221
C8	–0.14871	–0.15561	0.0069
C12	–0.19691	–0.19891	0.002
C14	–0.19691	–0.19683	–8E-05
N1	–0.64874	–0.64795	–0.00079
C6	–0.17864	–0.17372	–0.00492
H7	0.20967	0.21666	–0.00699
H6	0.20770	0.21573	–0.00803
H12	0.20967	0.21829	–0.00862
H13	0.20769	0.21732	–0.00963
H5	0.20692	0.21734	–0.01042
C13	–0.17864	–0.16813	–0.01051
H14	0.20692	0.21936	–0.01244
C4	–0.19291	–0.17854	–0.01437
C9	0.68597	0.70541	–0.01944
C15	–0.19291	–0.17298	–0.01993
C2	0.68597	0.70678	–0.02081
H15	0.18998	0.21477	–0.02479
N2	–0.64875	–0.62199	–0.02676
H4	0.18998	0.21713	–0.02715
H2	0.38711	0.43123	–0.04412
H1	0.38711	0.44475	–0.05764
C1	0.22701	0.29557	–0.06856

Table S5. NBO analysis of BT in configuration *trans*

Donor NBO	Occupancy	Acceptor NBO	Occupation	Stabilization energy / (kcal mol^{-1})
n_{N2}	1.62255	π*(C12–O30)	0.29969	57.05
n_{N2}		π*(C13–S32)	0.41252	62.62
n_{N1}	1.60188	π*(C13–S32)		79.80
n_{N1}		π*(C14–O31)	0.24623	46.18
n_{O2}	1.86290	π*(C1–C12)	0.05848	17.74
n_{O2}		π*(C12–N26)	0.07853	22.69
n_{O2}		σ*(N28–H29)	0.05473	12.88

Table S6. NBO analysis of BT in configuration *cis*

Donor NBO	Occupation	Acceptor NBO	Occupation	Stabilization energy / (kcal mol^{-1})
n_{N2}	1.66746	π*(C12–O30)	0.24176	47.49
n_{N2}		π*(C13–S32)	0.31106	45.01
n_{N1}	1.66745	π*(C13–S32)		45.02
n_{N2}		π*(C14–O31)	0.24176	47.49
n_{O2}	1.85867	π*(C12–N26)	0.08879	30.24
n_{O1}	1.85867	π*(C14–C15)	0.06713	19.25
n_{O1}		π*(C14–N28)	0.08879	30.24

Table S7. Electronic density and electron localization function at the BCP and RCP (all quantities are in atomic units)

Molecule	CP	Region	$\rho(r_c)$ / a.u.	ELF / a.u.
trans-BT	BCP	O–H–N	0.0401	0.1374
	BCP	S---O	0.0130	0.0432
	RCP	O–C–N–C–N–H	0.0180	0.0215
	RCP	S–C–N–C–O	0.0124	0.0254
cis-BT	BCP	S–O (1)	0.0133	0.0448
	BCP	S–O (2)	0.0122	0.0363
	RCP	S–C–N–C–O (1)	0.0121	0.0274
	RCP	S–C–N–C–O (2)	0.0124	0.0240

CP: critical point; BCP: bond critical point; RCP: ring critical point; ρ(r): electron density distribution function (a.u.: atomic units); ELF: electron localization function.

Table S8. Natural atomic charges of BT molecule in implicit solvent (acetone)

Atom	*cis*-BT	*trans*-BT	Difference
S1	0.03229	–0.16197	0.19426
O2	–0.55255	–0.64534	0.09279
C1	0.22701	0.29557	–0.06856
H1	0.38711	0.44475	–0.05764
H2	0.38711	0.43123	–0.04412
O1	–0.55254	–0.59597	0.04343
N2	–0.64875	–0.62199	–0.02676
C2	0.68597	0.70678	–0.02081
C9	0.68597	0.70541	–0.01944
N1	–0.64874	–0.64795	–0.00079

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelxl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelxl

Bond precision: C-C = 0.0065 A Wavelength=0.71073

Cell: a=5.0620(1) b=11.8620(3) c=21.9680(8)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1319.08(6)	1319.08(6)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C15 H12 N2 O2 S	C15 H12 N2 O2 S
Sum formula	C15 H12 N2 O2 S	C15 H12 N2 O2 S
Mr	284.33	284.33
Dx,g cm-3	1.432	1.432
Z	4	4
Mu (mm-1)	0.248	0.248
F000	592.0	592.0
F000'	592.73	
h,k,lmax	6,14,27	6,14,27
Nref	2655[1578]	1576
Tmin,Tmax	0.939,0.980	
Tmin'	0.820	

Correction method= Not given

Data completeness= 1.00/0.59 Theta(max)= 26.255

R(reflections)= 0.0550(1156) wR2(reflections)= 0.1584(1576)

S = 1.093 Npar= 182

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0065 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H1      ..  H4       ..      1.93 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         1 Note
             C15 H12 N2 O2 S
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     2.078 Check
PLAT914_ALERT_3_C No Bijvoet Pairs in FCF for Non-centro Structure   Please Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.        0 Info
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF   Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        2 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....     0.80 mm
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large     0.10 Report
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        3 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......   Please Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   6 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock shelxl - ellipsoid plot