



Spectroscopic, single crystal XRD structure, DFT and molecular dynamics investigation of 1-(3-Chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea

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Table S1. Geometrical parameters (DFT/XRD/MacroModel (OPLS 2005 force field)) of ANF-2

Bond lengths (Å)			
C1 -C2	1.4007/1.4015/1.4139	C1-C6	1.3933/1.3945/1.4078
C1-H23	1.0808/0.9500/1.0811	C2-C3	1.4008/1.3795/1.4102
C2-N7	1.4126/1.4224/1.4214	C3-C4	1.3924/1.3895/1.4114
C3-H24	1.0858/0.9500/1.0802	C4-C5	1.3958/1.3875/1.4116
C4-C19	1.5052/1.4925/1.5215	C5-C6	1.3927/1.3715/1.4083
C5-H25	1.0843/0.9500/1.0805	C6-H26	1.0855/0.9500/1.0806
N7-C8	1.3667/1.3454/1.3605	N7-H27	1.0129/0.8800/1.0081
C8-S9	1.6770/1.6853/1.6608	C8-N10	1.3786/1.3554/1.3563
N10-C11	1.4174/1.4254/1.4217	N10-H28	1.0111/0.8800/1.0114
C11-C12	1.4035/1.3895/1.4147	C11-C16	1.4021/1.3865/1.4107
C12-C13	1.3926/1.3815/1.4086	C12-H29	1.0841/0.9500/1.0815
C13-C14	1.3887/1.3815/1.4078	C13-H30	1.0844/0.9500/1.0801
C14-C15	1.3963/1.3765/1.4102	C14-F18	1.3392/1.3474/1.3537
C15-C16	1.3916/1.3975/1.4093	C15-C17	1.7432/1.7253/1.7261
C16-H31	1.0844/0.9500/1.0805	C19-F20	1.3502/1.3054/1.3334
C19-F21	1.3545/1.3245/1.3322	C19-F22	1.3524/1.2855/1.3333

Bond angles (°)			
C6-C1-C2	119.5/119.2/120.2340	H23-C1-C2	119.8/120.4/120.6137
H23-C1-C6	120.7/120.4/119.1521	C3-C2-C1	119.6/121.0/119.3366
N7-C2-C1	123.8/122.0/122.2689	N7-C2-C3	116.5/117.0/118.2607
C4-C3-C2	120.2/118.7/120.7084	H24-C3-C2	120.2/120.7/120.4668
H24-C3-C4	119.6/120.7/118.8207	C5-C4-C3	120.5/120.8/119.4060
C19-C4-C3	119.6/119.0/119.7311	C19-C4-C5	119.9/120.2/120.8537
C6-C5-C4	119.0/120.3/120.2422	H25-C5-C4	120.2/119.8/119.9687
H25-C5-C6	120.9/119.8/119.7881	C5-C6-C1	121.3/119.9/120.0410
H26-C6-C1	119.0/120.0/119.8736	H26-C6-C5	119.8/120.0/120.0853
C8-N7-C2	131.1/127.3/129.1563	H27-N7-C2	113.4/116.3/115.5294
H27-N7-C8	115.0/116.3/114.9662	S9-C8-N7	127.2/123.2/127.7285
N10-C8-N7	113.9/113.1/112.8811	N10-C8-S9	118.9/123.6/119.2920

C11-N10-C8	129.9/128.2/129.7783	H28-N10-C8	112.3/115.9/113.8344
H28-N10-C11	117.8/115.9/116.3639	C12-C11-N10	122.0/122.4/121.8653
C16-C11-N10	118.4/117.0/118.5514	C16-C11-C12	119.6/120.5/119.4906
C13-C12-C11	120.0/119.7/120.0542	H29-C12-C11	120.0/120.2/120.8212
H29-C12-C13	119.9/120.2/119.1168	C14-C13-C12	119.9/119.8/120.2346
H30-C13-C12	121.3/120.1/120.2838	H30-C13-C14	118.8/120.1/119.4786
C15-C14-C13	120.6/121.2/119.9007	F18-C14-C13	119.5/119.6/119.5603
F18-C14-C15	119.9/119.2/120.5382	C16-C15-C14	119.6/119.3/119.9184
Cl17-C15-C14	119.7/120.7/120.5110	Cl17-C15-C16	120.7/120.0/119.5707
C15-C16-C11	120.2/119.6/120.3753	H31-C16-C11	120.2/120.2/120.5540
H31-C16-C15	119.6/120.2/119.0684	F20-C19-C4	111.8/113.3/111.4456
F21-C19-C4	111.5/112.1/109.0203	F21-C19-F20	106.8/108.0/108.8374
F22-C19-C4	112.0/113.6/110.2578	F22-C19-F20	107.6/106.5/108.4973
F22-C19-F21	106.8/102.5/108.7302		

Dihedral angles (°)			
C1-C2-C3-C4	-0.3/2.1/-2.2	C1-C2-N7-C8	28.3/130.2/49.4
C1-C6-C5-C4	-0.0/1.1/-0.2	C2-C1-C6-C5	-0.7/-0.3/-0.8
C2-C3-C4-C5	-0.5/-1.3/1.2	C2-C3-C4-C19	177.1/178.9/-179.8
C2-N7-C8-S9	5.3/-1.2/5.2	C2-N7-C8-N10	-176.7/-175.8/-178.5
C3-C2-C1-C6	0.8/-1.4/1.9	C3-C2-N7-C8	-154.8/-52.7/-134.9
C3-C4-C5-C6	0.6/-0.4/-0.1	C3-C4-C19-F20	148.3/162.4/160.3
C3-C4-C19-F21	-92.2/-77.1/-79.6	C3-C4-C19-F22	27.4/38.3/39.7
C4-C3-C2-N7	-177.3/-179.1/-178.0	C5-C4-C19-F20	-34.1/-17.7/-20.8
C5-C4-C19-F21	85.4/103.0/99.3	C5-C4-C19-F22	-154.9/-141.3/-141.4
C6-C1-C2-N7	177.6/178.5/177.6	C6-C5-C4-C19	-177.0/-179.6/-179.0
N7-C8-N10-C11	7.8/-179.6/8.9	C8-N10-C11-C12	47.9/47.9/47.2
C8-N10-C11-C16	-134.9/-136.3/-136.3	S9-C8-N10-C11	-174.0/-2.9/-174.5
N10-C11-C12-C13	178.3/177.2/178.3	N10-C11-C16-C15	-176.9/-176.3/-178.4
C11-C12-C13-C14	-1.5/1.2/-0.8	C11-C16-C15-C14	-1.4/-1.4/0.7
C11-C16-C15-Cl17	179.6/177.5/-179.3	C12-C11-C16-C15	0.3/0.3/-1.8
C12-C13-C14-C15	0.4/0.6/-0.3	C12-C13-C14-F18	-179.3/0.0/0.0
C13-C12-C11-C16	1.1/-1.5/1.8	C13-C14-C15-C16	1.0/-1.7/0.4
C13-C14-C15-Cl17	-179.9/177.2/-179.6	C16-C15-C14-F18	-179.3/-178.8/0.0
Cl17-C15-C14-F18	-0.2/-2.5/0.1		