

3-Cyanoazolo[5,1-c][1,2,4]triazines: synthesis and antiviral activity

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SUPPLEMENTARY INFORMATION

X-ray crystal analysis of compound 4b

Crystallographic data for compound 4b

Parameter		Value
Temperature, K		295
Wavelength, Å		1.54184
Formula		C ₆ H ₉ N ₆ O ₄ SNa
Molecular weight		284.24
Crystal system		Orthorhombic
Space group		P 2 ₁ 2 ₁ 2 ₁
Cell lengths, Å	<i>a</i>	5.551 (8)
	<i>b</i>	14.170 (11)
	<i>c</i>	15.284 (9)
Cell angles, deg	α	90.00
	β	90.00
	γ	90.00
Cell volume, Å ³		1202 (2)
Density, g/cm ³		1.570
Number of measured reflections		12823
Number of unique reflections		2045
<i>R</i> -factor		0.0295
Number of refined parameters		188
Residual electron density, e/Å ³ (min/max)		-0.262/0.169

Bond lengths

№	Atom 1	Atom 2	Length, Å	№	Atom 1	Atom 2	Length, Å
1	S1	C1	1.729(2)	17	C2	N3	1.320(3)
2	S1	C6	1.789(2)	18	C2	N4	1.347(2)
3	N1	N2	1.373(2)	19	O2S	H2SA	0.90(3)
4	N1	C2	1.366(2)	20	O2S	H2SB	0.74(3)
5	N1	C5	1.380(2)	21	C4	C3	1.420(3)
6	O1S	Na1	2.328(3)	22	C4	C5	1.436(2)
7	O1S	H1SB	0.72(3)	23	C4	N5	1.333(2)
8	O1S	H1SA	0.87(3)	24	O3S	H3SB	0.86(3)
9	O1	Na1	2.415(2)	25	O3S	H3SA	0.75(3)
10	O1	C5	1.215(2)	26	O3S	Na1	2.391(3)
11	C1	N2	1.322(2)	27	C3	N6	1.142(3)
12	C1	N3	1.356(2)	28	N4	N5	1.309(3)
13	Na1	O2S	2.487(2)	29	N4	Na1	2.624(2)
14	Na1	O3S	2.454(2)	30	C6	H6A	0.960(3)
15	Na1	O3S	2.391(3)	31	C6	H6B	0.961(3)
16	Na1	N4	2.624(2)	32	C6	H6C	0.960(2)

Bond angles

№	Atom 1	Atom 2	Atom 3	Angle, deg	№	Atom 1	Atom 2	Atom 3	Angle, deg
1	C1	S1	C6	101.75(9)	30	N3	C2	N4	126.8(1)
2	N2	N1	C2	110.1(1)	31	Na1	O2S	H2SA	101(2)
3	N2	N1	C5	126.5(1)	32	Na1	O2S	H2SB	103(2)
4	C2	N1	C5	123.3(1)	33	H2SA	O2S	H2SB	108(3)
5	Na1	O1S	H1SB	127(2)	34	C3	C4	C5	118.1(1)
6	Na1	O1S	H1SA	121(2)	35	C3	C4	N5	115.6(1)
7	H1SB	O1S	H1SA	109(3)	36	C5	C4	N5	126.2(1)
8	Na1	O1	C5	161.7(1)	37	Na1	O3S	H3SB	96(2)
9	S1	C1	N2	125.0(1)	38	Na1	O3S	H3SA	101(2)
10	S1	C1	N3	118.8(1)	39	Na1	O3S	Na1	128.01(6)
11	N2	C1	N3	116.1(1)	40	H3SB	O3S	H3SA	110(3)
12	O1S	Na1	O1	88.13(5)	41	H3SB	O3S	Na1	99(2)
13	O1S	Na1	O2S	85.24(5)	42	H3SA	O3S	Na1	120(2)
14	O1S	Na1	O3S	99.95(5)	43	C1	N3	C2	103.4(1)
15	O1S	Na1	O3S	171.22(5)	44	C4	C3	N6	178.2(2)
16	O1S	Na1	N4	87.77(5)	45	C2	N4	N5	115.6(1)
17	O1	Na1	O2S	171.71(5)	46	C2	N4	Na1	121.2(1)
18	O1	Na1	O3S	92.34(5)	47	N5	N4	Na1	121.1(1)
19	O1	Na1	O3S	83.25(5)	48	N1	C5	O1	123.2(1)
20	O1	Na1	N4	99.73(5)	49	N1	C5	C4	108.7(1)
21	O2S	Na1	O3S	83.92(5)	50	O1	C5	C4	128.1(1)
22	O2S	Na1	O3S	103.49(5)	51	C4	N5	N4	122.1(2)
23	O2S	Na1	N4	85.00(5)	52	S1	C6	H6A	109.4(2)
24	O3S	Na1	O3S	82.17(5)	53	S1	C6	H6B	109.5(2)
25	O3S	Na1	N4	165.91(5)	54	S1	C6	H6C	109.5(2)
26	O3S	Na1	N4	91.99(5)	55	H6A	C6	H6B	109.5(2)
27	N1	N2	C1	101.2(1)	56	H6A	C6	H6C	109.5(2)
28	N1	C2	N3	109.2(1)	57	H6B	C6	H6C	109.5(2)
29	N1	C2	N4	124.0(1)					