[$PhSO_2CHCNLi$.TMEDA] **1**

Table 1. Crystal data and structure refinement for k4.

Identification code	k4
Empirical formula	C14 H22 Li N3 O2 S
Formula weight	303.35
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 8.7582(4) A alpha = 90 deg. b = 9.5126(5) A beta = 91.471(3) deg. c = 20.4591(12) A gamma = 90 deg.
Volume	1703.95(16) A^3
Z, Calculated density	4, 1.182 Mg/m^3
Absorption coefficient	0.196 mm^-1
F(000)	648
Crystal size	0.30 x 0.25 x 0.15 mm
Theta range for data collection	1.99 to 26.00 deg.
Index ranges	0<=h<=10, -11<=k<=11, -25<=l<=25
Reflections collected / unique	5898 / 3260 [R(int) = 0.0700]
Completeness to 2theta = 26.00	91.7%
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3260 / 0 / 197
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0673, wR2 = 0.1626
R indices (all data)	R1 = 0.0977, wR2 = 0.1821
Largest diff. peak and hole	0.431 and -0.347 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for k4.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	1283(1)	9062(1)	967(1)	31(1)
O(1)	1475(2)	8216(2)	1560(1)	36(1)
O(2)	1099(3)	8319(2)	352(1)	37(1)
N(1)	-748(3)	11081(3)	2191(1)	39(1)
N(2)	-1189(3)	5543(3)	1429(1)	46(1)
N(3)	2093(4)	4895(3)	1384(2)	48(1)
C(1)	-171(4)	10171(3)	1057(2)	33(1)
C(2)	-462(3)	10676(3)	1676(2)	32(1)
C(3)	3027(3)	10011(3)	907(1)	31(1)
C(4)	3211(4)	10897(3)	379(2)	37(1)
C(5)	4560(4)	11631(3)	321(2)	44(1)
C(6)	5721(4)	11494(4)	789(2)	51(1)
C(7)	5526(4)	10626(4)	1317(2)	53(1)
C(8)	4184(4)	9871(4)	1382(2)	43(1)
C(9)	-611(7)	4217(7)	1142(3)	47(2)
C(10)	968(7)	4480(7)	842(3)	45(2)
C(11)	-2116(10)	6560(8)	1061(4)	59(2)
C(12)	-2140(9)	4856(9)	1872(4)	55(2)
C(13)	3476(10)	5455(8)	1061(4)	51(2)
C(14)	2485(8)	3737(6)	1797(3)	42(2)
Li(1)	810(6)	6433(5)	1858(2)	36(1)
C(15)	916(16)	4008(17)	1133(9)	77(4)
C(16)	-311(17)	4654(16)	900(8)	72(4)
C(17)	-1833(11)	6371(9)	889(5)	23(2)
C(18)	-2453(13)	5295(13)	1964(5)	41(3)
C(19)	3104(17)	5392(15)	914(7)	53(4)
C(20)	3120(2)	4060(16)	1896(7)	71(4)

Table 3. Bond lengths [A] and angles [deg] for k4.

S(1)-O(2)	1.448(2)
S(1)-O(1)	1.462(2)
S(1)-C(1)	1.668(3)
S(1)-C(3)	1.780(3)
O(1)-Li(1)	1.899(6)
N(1)-C(2)	1.155(4)
N(1)-Li(1)#1	1.976(6)
N(2)-C(12)	1.408(8)
N(2)-C(17)	1.459(9)
N(2)-C(11)	1.459(8)
N(2)-C(9)	1.486(7)
N(2)-C(16)	1.588(14)
N(2)-C(18)	1.595(11)
N(2)-Li(1)	2.115(6)
N(3)-C(19)	1.406(14)
N(3)-C(15)	1.418(14)
N(3)-C(14)	1.425(6)
N(3)-C(13)	1.493(8)
N(3)-C(10)	1.516(7)
N(3)-C(20)	1.576(14)
N(3)-Li(1)	2.098(6)
C(1)-C(2)	1.384(4)
C(1)-H(1)	0.84(4)
C(3)-C(4)	1.384(4)
C(3)-C(8)	1.391(4)
C(4)-C(5)	1.380(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.374(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.388(5)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(10)	1.549(10)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
Li(1)-N(1)#2	1.976(6)

C(15)-C(16)	1.32(2)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
O(2)-S(1)-O(1)	117.43(13)
O(2)-S(1)-C(1)	109.62(14)
O(1)-S(1)-C(1)	109.15(15)
O(2)-S(1)-C(3)	105.36(14)
O(1)-S(1)-C(3)	104.79(13)
C(1)-S(1)-C(3)	110.22(15)
S(1)-O(1)-Li(1)	136.7(2)
C(2)-N(1)-Li(1)#1	165.1(3)
C(12)-N(2)-C(17)	121.0(5)
C(12)-N(2)-C(11)	108.0(5)
C(17)-N(2)-C(11)	18.6(4)
C(12)-N(2)-C(9)	94.1(6)
C(17)-N(2)-C(9)	106.8(5)
C(11)-N(2)-C(9)	123.4(5)
C(12)-N(2)-C(16)	119.7(8)
C(17)-N(2)-C(16)	87.5(8)
C(11)-N(2)-C(16)	106.0(8)
C(9)-N(2)-C(16)	26.2(5)
C(12)-N(2)-C(18)	19.3(5)
C(17)-N(2)-C(18)	109.8(6)
C(11)-N(2)-C(18)	93.7(6)
C(9)-N(2)-C(18)	113.2(6)
C(16)-N(2)-C(18)	138.2(9)
C(12)-N(2)-Li(1)	114.6(4)
C(17)-N(2)-Li(1)	113.5(4)
C(11)-N(2)-Li(1)	113.1(4)
C(9)-N(2)-Li(1)	102.6(3)
C(16)-N(2)-Li(1)	95.0(6)
C(18)-N(2)-Li(1)	110.8(5)
C(19)-N(3)-C(15)	114.7(9)
C(19)-N(3)-C(14)	121.3(7)
C(15)-N(3)-C(14)	85.2(7)
C(19)-N(3)-C(13)	17.2(7)
C(15)-N(3)-C(13)	130.0(8)
C(14)-N(3)-C(13)	110.6(4)
C(19)-N(3)-C(10)	89.8(6)
C(15)-N(3)-C(10)	29.3(7)
C(14)-N(3)-C(10)	112.0(4)

C(13)-N(3)-C(10)	106.8(4)
C(19)-N(3)-C(20)	105.5(8)
C(15)-N(3)-C(20)	109.6(8)
C(14)-N(3)-C(20)	24.7(6)
C(13)-N(3)-C(20)	91.2(7)
C(10)-N(3)-C(20)	134.6(7)
C(19)-N(3)-Li(1)	115.9(6)
C(15)-N(3)-Li(1)	100.9(6)
C(14)-N(3)-Li(1)	112.8(3)
C(13)-N(3)-Li(1)	114.0(4)
C(10)-N(3)-Li(1)	100.1(3)
C(20)-N(3)-Li(1)	110.2(6)
C(2)-C(1)-S(1)	118.7(2)
C(2)-C(1)-H(1)	122(2)
S(1)-C(1)-H(1)	115(2)
N(1)-C(2)-C(1)	177.9(3)
C(4)-C(3)-C(8)	120.4(3)
C(4)-C(3)-S(1)	118.7(2)
C(8)-C(3)-S(1)	120.9(3)
C(5)-C(4)-C(3)	119.6(3)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(4)-C(5)-C(6)	120.5(3)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(7)-C(6)-C(5)	119.7(3)
C(7)-C(6)-H(6)	120.1
C(5)-C(6)-H(6)	120.1
C(6)-C(7)-C(8)	120.6(3)
C(6)-C(7)-H(7)	119.7
C(8)-C(7)-H(7)	119.7
C(7)-C(8)-C(3)	119.2(3)
C(7)-C(8)-H(8)	120.4
C(3)-C(8)-H(8)	120.4
N(2)-C(9)-C(10)	109.6(5)
N(2)-C(9)-H(9A)	109.7
C(10)-C(9)-H(9A)	109.7
N(2)-C(9)-H(9B)	109.7
C(10)-C(9)-H(9B)	109.7
H(9A)-C(9)-H(9B)	108.2
N(3)-C(10)-C(9)	108.8(5)
N(3)-C(10)-H(10A)	109.9
C(9)-C(10)-H(10A)	109.9
N(3)-C(10)-H(10B)	109.9
C(9)-C(10)-H(10B)	109.9
H(10A)-C(10)-H(10B)	108.3
N(2)-C(11)-H(11A)	109.5
N(2)-C(11)-H(11B)	109.5
N(2)-C(11)-H(11C)	109.5
N(2)-C(12)-H(12A)	109.5
N(2)-C(12)-H(12B)	109.5
N(2)-C(12)-H(12C)	109.5
N(3)-C(13)-H(13A)	109.5
N(3)-C(13)-H(13B)	109.5
N(3)-C(13)-H(13C)	109.5
N(3)-C(14)-H(14A)	109.5

N(3)-C(14)-H(14B)	109.5
N(3)-C(14)-H(14C)	109.5
O(1)-Li(1)-N(1)#2	118.9(3)
O(1)-Li(1)-N(3)	107.6(3)
N(1)#2-Li(1)-N(3)	111.5(3)
O(1)-Li(1)-N(2)	118.8(3)
N(1)#2-Li(1)-N(2)	107.3(3)
N(3)-Li(1)-N(2)	88.6(2)
C(16)-C(15)-N(3)	115.6(14)
C(16)-C(15)-H(15A)	108.4
N(3)-C(15)-H(15A)	108.4
C(16)-C(15)-H(15B)	108.4
N(3)-C(15)-H(15B)	108.4
H(15A)-C(15)-H(15B)	107.4
C(15)-C(16)-N(2)	114.0(13)
C(15)-C(16)-H(16A)	108.8
N(2)-C(16)-H(16A)	108.8
C(15)-C(16)-H(16B)	108.8
N(2)-C(16)-H(16B)	108.8
H(16A)-C(16)-H(16B)	107.7
N(2)-C(17)-H(17A)	109.5
N(2)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
N(2)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(2)-C(18)-H(18A)	109.5
N(2)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
N(2)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(3)-C(19)-H(19A)	109.5
N(3)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
N(3)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(3)-C(20)-H(20A)	109.5
N(3)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
N(3)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x,y+1/2,-z+1/2 #2 -x,y-1/2,-z+1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for k4.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	38(1)	26(1)	28(1)	0(1)	-6(1)	-2(1)
O(1)	47(1)	30(1)	30(1)	5(1)	-8(1)	-1(1)
O(2)	49(1)	32(1)	30(1)	-5(1)	-7(1)	-3(1)
N(1)	44(2)	38(2)	35(2)	-3(1)	-5(1)	6(1)
N(2)	48(2)	45(2)	45(2)	5(1)	-11(1)	-6(1)
N(3)	55(2)	34(2)	55(2)	-4(1)	-2(2)	2(1)
C(1)	35(2)	33(2)	30(2)	2(1)	-8(1)	2(1)
C(2)	29(2)	30(2)	36(2)	3(1)	-6(1)	-1(1)
C(3)	31(2)	28(1)	34(2)	-6(1)	-4(1)	3(1)
C(4)	42(2)	30(2)	38(2)	-1(1)	-2(1)	-1(1)
C(5)	48(2)	31(2)	54(2)	-3(2)	10(2)	-2(2)
C(6)	38(2)	45(2)	71(2)	-14(2)	5(2)	-9(2)
C(7)	35(2)	64(2)	58(2)	-7(2)	-10(2)	-2(2)
C(8)	40(2)	45(2)	43(2)	-1(2)	-7(2)	3(2)
Li(1)	42(3)	33(3)	32(3)	-1(2)	-8(2)	-3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for k4.

	x	y	z	U(eq)
H(1)	-470(4)	10590(4)	718(18)	43(10)
H(4)	2414	11001	59	44
H(5)	4692	12235	-43	53
H(6)	6649	11998	744	61
H(7)	6318	10543	1640	63
H(8)	4056	9265	1746	51
H(9A)	-1340	3876	800	56
H(9B)	-519	3487	1486	56
H(10A)	1325	3617	623	53
H(10B)	889	5240	512	53
H(11A)	-2967	6074	838	88
H(11B)	-1486	7027	737	88
H(11C)	-2518	7264	1362	88
H(12A)	-2611	5552	2156	83
H(12B)	-1532	4196	2138	83
H(12C)	-2940	4340	1629	83
H(13A)	4194	5824	1394	76
H(13B)	3176	6211	758	76
H(13C)	3967	4698	818	76
H(14A)	1565	3389	2007	63
H(14B)	3232	4042	2133	63
H(14C)	2926	2984	1535	63
H(15A)	1339	3424	781	93
H(15B)	605	3365	1486	93
H(16A)	-1020	3943	710	86
H(16B)	-10	5289	542	86
H(17A)	-2600	5810	648	34
H(17B)	-1019	6639	594	34
H(17C)	-2314	7219	1061	34
H(18A)	-3280	4715	1777	61
H(18B)	-2866	6203	2101	61
H(18C)	-1991	4813	2344	61
H(19A)	3641	4596	721	80
H(19B)	3848	6029	1123	80
H(19C)	2529	5897	570	80
H(20A)	3673	3317	1672	106
H(20B)	2464	3639	2226	106
H(20C)	3844	4705	2110	106

Table 6. Torsion angles [deg] for k4.

O(2)-S(1)-O(1)-Li(1)	-31.1(4)
C(1)-S(1)-O(1)-Li(1)	94.4(3)
C(3)-S(1)-O(1)-Li(1)	-147.6(3)
O(2)-S(1)-C(1)-C(2)	161.5(2)
O(1)-S(1)-C(1)-C(2)	31.6(3)
C(3)-S(1)-C(1)-C(2)	-83.0(3)
Li(1)#1-N(1)-C(2)-C(1)	117(8)
S(1)-C(1)-C(2)-N(1)	-122(9)
O(2)-S(1)-C(3)-C(4)	54.2(3)
O(1)-S(1)-C(3)-C(4)	178.7(2)
C(1)-S(1)-C(3)-C(4)	-64.0(3)
O(2)-S(1)-C(3)-C(8)	-126.0(3)
O(1)-S(1)-C(3)-C(8)	-1.5(3)
C(1)-S(1)-C(3)-C(8)	115.8(3)
C(8)-C(3)-C(4)-C(5)	0.8(5)
S(1)-C(3)-C(4)-C(5)	-179.3(2)
C(3)-C(4)-C(5)-C(6)	-0.5(5)
C(4)-C(5)-C(6)-C(7)	-0.3(5)
C(5)-C(6)-C(7)-C(8)	0.8(6)
C(6)-C(7)-C(8)-C(3)	-0.5(5)
C(4)-C(3)-C(8)-C(7)	-0.3(5)
S(1)-C(3)-C(8)-C(7)	179.9(3)
C(12)-N(2)-C(9)-C(10)	-155.6(6)
C(17)-N(2)-C(9)-C(10)	80.3(6)
C(11)-N(2)-C(9)-C(10)	89.6(6)
C(16)-N(2)-C(9)-C(10)	36.1(13)
C(18)-N(2)-C(9)-C(10)	-158.8(6)
Li(1)-N(2)-C(9)-C(10)	-39.3(6)
C(19)-N(3)-C(10)-C(9)	-164.5(8)
C(15)-N(3)-C(10)-C(9)	46.2(13)
C(14)-N(3)-C(10)-C(9)	71.6(6)
C(13)-N(3)-C(10)-C(9)	-167.2(6)
C(20)-N(3)-C(10)-C(9)	83.7(10)
Li(1)-N(3)-C(10)-C(9)	-48.2(6)
N(2)-C(9)-C(10)-N(3)	63.6(7)
S(1)-O(1)-Li(1)-N(1)#2	-157.1(2)
S(1)-O(1)-Li(1)-N(3)	75.0(4)
S(1)-O(1)-Li(1)-N(2)	-23.4(5)
C(19)-N(3)-Li(1)-O(1)	-4.1(8)
C(15)-N(3)-Li(1)-O(1)	-128.6(8)
C(14)-N(3)-Li(1)-O(1)	142.0(4)
C(13)-N(3)-Li(1)-O(1)	14.7(5)
C(10)-N(3)-Li(1)-O(1)	-98.8(4)
C(20)-N(3)-Li(1)-O(1)	115.5(7)
C(19)-N(3)-Li(1)-N(1)#2	-136.2(7)
C(15)-N(3)-Li(1)-N(1)#2	99.3(9)
C(14)-N(3)-Li(1)-N(1)#2	9.9(5)
C(13)-N(3)-Li(1)-N(1)#2	-117.3(5)
C(10)-N(3)-Li(1)-N(1)#2	129.1(4)
C(20)-N(3)-Li(1)-N(1)#2	-16.5(8)
C(19)-N(3)-Li(1)-N(2)	115.7(7)
C(15)-N(3)-Li(1)-N(2)	-8.8(8)

C(14)-N(3)-Li(1)-N(2)	-98.1(4)
C(13)-N(3)-Li(1)-N(2)	134.6(4)
C(10)-N(3)-Li(1)-N(2)	21.0(4)
C(20)-N(3)-Li(1)-N(2)	-124.6(7)
C(12)-N(2)-Li(1)-O(1)	-140.3(5)
C(17)-N(2)-Li(1)-O(1)	4.4(6)
C(11)-N(2)-Li(1)-O(1)	-15.9(6)
C(9)-N(2)-Li(1)-O(1)	119.2(4)
C(16)-N(2)-Li(1)-O(1)	93.8(7)
C(18)-N(2)-Li(1)-O(1)	-119.7(6)
C(12)-N(2)-Li(1)-N(1)#2	-1.7(5)
C(17)-N(2)-Li(1)-N(1)#2	143.0(5)
C(11)-N(2)-Li(1)-N(1)#2	122.6(5)
C(9)-N(2)-Li(1)-N(1)#2	-102.3(4)
C(16)-N(2)-Li(1)-N(1)#2	-127.6(7)
C(18)-N(2)-Li(1)-N(1)#2	18.9(6)
C(12)-N(2)-Li(1)-N(3)	110.4(5)
C(17)-N(2)-Li(1)-N(3)	-105.0(5)
C(11)-N(2)-Li(1)-N(3)	-125.3(5)
C(9)-N(2)-Li(1)-N(3)	9.8(4)
C(16)-N(2)-Li(1)-N(3)	-15.6(7)
C(18)-N(2)-Li(1)-N(3)	130.9(5)
C(19)-N(3)-C(15)-C(16)	-85.6(18)
C(14)-N(3)-C(15)-C(16)	152.1(17)
C(13)-N(3)-C(15)-C(16)	-94.9(17)
C(10)-N(3)-C(15)-C(16)	-51.4(16)
C(20)-N(3)-C(15)-C(16)	156.0(16)
Li(1)-N(3)-C(15)-C(16)	39.7(18)
N(3)-C(15)-C(16)-N(2)	-63(2)
C(12)-N(2)-C(16)-C(15)	-78.3(16)
C(17)-N(2)-C(16)-C(15)	157.1(16)
C(11)-N(2)-C(16)-C(15)	159.4(14)
C(9)-N(2)-C(16)-C(15)	-64.8(18)
C(18)-N(2)-C(16)-C(15)	-85.6(17)
Li(1)-N(2)-C(16)-C(15)	43.7(16)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y+1/2,-z+1/2 #2 -x,y-1/2,-z+1/2

Table 1. Crystal data and structure refinement for k7.

Identification code	k7
Empirical formula	C10 H18 Li N O3 S
Formula weight	239.25
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	P21/a, monoclinic
Unit cell dimensions	a = 10.2227(4) A alpha = 90 deg. b = 6.4498(2) A beta = 94.117(2) deg. c = 19.7438(8) A gamma = 90 deg.
Volume	1298.44(8) A^3
Z, Calculated density	4, 1.224 Mg/m^3
Absorption coefficient	0.240 mm^-1
F(000)	512
Crystal size	0.30 x 0.30 x 0.05 mm
Theta range for data collection	2.07 to 26.00 deg.
Index ranges	0<=h<=12, -7<=k<=7, -24<=l<=24
Reflections collected / unique	4813 / 2545 [R(int) = 0.0551]
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2545 / 0 / 152
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0470, wR2 = 0.0955
R indices (all data)	R1 = 0.0899, wR2 = 0.1093
Largest diff. peak and hole	0.318 and -0.295 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for k7.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	2921(1)	9608(1)	2949(1)	23(1)
O(1)	4039(2)	9028(3)	2573(1)	28(1)
O(2)	1773(2)	8257(3)	2894(1)	30(1)
O(3)	5705(2)	8191(3)	1415(1)	40(1)
N(1)	4152(2)	14420(4)	2258(1)	35(1)
C(1)	2472(3)	12015(4)	2736(1)	29(1)
C(2)	3389(2)	13331(4)	2481(1)	27(1)
C(3)	3527(2)	9419(4)	3837(1)	26(1)
C(4)	4777(2)	10707(5)	3933(1)	37(1)
C(5)	3811(3)	7127(4)	3987(1)	36(1)
C(6)	2481(2)	10245(5)	4278(1)	40(1)
C(7)	6851(3)	7623(6)	1074(2)	59(1)
C(8)	7246(3)	9437(6)	677(2)	63(1)
C(9)	6354(3)	11169(5)	865(2)	55(1)
C(10)	5202(3)	10067(5)	1116(2)	49(1)
Li(1)	5234(4)	7008(7)	2274(2)	28(1)

Table 3. Bond lengths [A] and angles [deg] for k7.

S(1)-O(1)	1.4556(17)
S(1)-O(2)	1.4594(17)
S(1)-C(1)	1.665(3)
S(1)-C(3)	1.821(2)
O(1)-Li(1)	1.908(4)
O(2)-Li(1)#1	1.930(4)
O(3)-C(10)	1.426(3)
O(3)-C(7)	1.440(3)
O(3)-Li(1)	1.952(4)
N(1)-C(2)	1.160(3)
N(1)-Li(1)#2	2.001(5)
C(1)-C(2)	1.385(4)
C(1)-H(1)	0.92(2)
C(3)-C(6)	1.524(3)
C(3)-C(4)	1.525(3)
C(3)-C(5)	1.532(4)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-C(8)	1.481(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.505(5)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.491(4)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
Li(1)-O(2)#3	1.930(4)
Li(1)-N(1)#4	2.001(5)
O(1)-S(1)-O(2)	117.67(11)
O(1)-S(1)-C(1)	108.84(12)
O(2)-S(1)-C(1)	109.40(11)
O(1)-S(1)-C(3)	104.45(10)
O(2)-S(1)-C(3)	104.38(11)
C(1)-S(1)-C(3)	111.98(13)
S(1)-O(1)-Li(1)	151.21(17)
S(1)-O(2)-Li(1)#1	135.66(17)
C(10)-O(3)-C(7)	107.7(2)
C(10)-O(3)-Li(1)	125.9(2)
C(7)-O(3)-Li(1)	124.5(2)
C(2)-N(1)-Li(1)#2	152.2(2)
C(2)-C(1)-S(1)	118.8(2)
C(2)-C(1)-H(1)	122.2(16)
S(1)-C(1)-H(1)	119.0(16)
N(1)-C(2)-C(1)	178.9(3)
C(6)-C(3)-C(4)	110.8(2)
C(6)-C(3)-C(5)	111.0(2)
C(4)-C(3)-C(5)	110.9(2)
C(6)-C(3)-S(1)	108.87(17)
C(4)-C(3)-S(1)	107.90(17)

C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
O(3)-C(7)-C(8)	108.0(3)
O(3)-C(7)-H(7A)	110.1
C(8)-C(7)-H(7A)	110.1
O(3)-C(7)-H(7B)	110.1
C(8)-C(7)-H(7B)	110.1
H(7A)-C(7)-H(7B)	108.4
C(7)-C(8)-C(9)	105.2(2)
C(7)-C(8)-H(8A)	110.7
C(9)-C(8)-H(8A)	110.7
C(7)-C(8)-H(8B)	110.7
C(9)-C(8)-H(8B)	110.7
H(8A)-C(8)-H(8B)	108.8
C(10)-C(9)-C(8)	103.6(3)
C(10)-C(9)-H(9A)	111.0
C(8)-C(9)-H(9A)	111.0
C(10)-C(9)-H(9B)	111.0
C(8)-C(9)-H(9B)	111.0
H(9A)-C(9)-H(9B)	109.0
O(3)-C(10)-C(9)	105.8(2)
O(3)-C(10)-H(10A)	110.6
C(9)-C(10)-H(10A)	110.6
O(3)-C(10)-H(10B)	110.6
C(9)-C(10)-H(10B)	110.6
H(10A)-C(10)-H(10B)	108.7
O(1)-Li(1)-O(2)#3	112.1(2)
O(1)-Li(1)-O(3)	101.8(2)
O(2)#3-Li(1)-O(3)	110.2(2)
O(1)-Li(1)-N(1)#4	102.08(19)
O(2)#3-Li(1)-N(1)#4	111.1(2)
O(3)-Li(1)-N(1)#4	118.8(2)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+3/2,z #2 x,y+1,z #3 x+1/2,-y+3/2,z
#4 x,y-1,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for k7.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	18(1)	25(1)	27(1)	0(1)	2(1)	-1(1)
O(1)	23(1)	28(1)	33(1)	1(1)	9(1)	5(1)
O(2)	23(1)	31(1)	35(1)	2(1)	0(1)	-7(1)
O(3)	41(1)	41(1)	39(1)	13(1)	16(1)	11(1)
N(1)	28(1)	26(1)	51(2)	4(1)	3(1)	1(1)
C(1)	19(1)	30(2)	38(2)	1(1)	3(1)	1(1)
C(2)	26(1)	23(2)	32(2)	-4(1)	-2(1)	1(1)
C(3)	19(1)	33(2)	27(1)	1(1)	4(1)	6(1)
C(4)	29(1)	47(2)	33(2)	5(1)	-4(1)	-10(1)
C(5)	32(2)	41(2)	34(2)	9(1)	4(1)	0(1)
C(6)	31(1)	56(2)	32(2)	-4(2)	5(1)	4(1)
C(7)	69(2)	62(2)	49(2)	7(2)	30(2)	23(2)
C(8)	47(2)	92(3)	52(2)	16(2)	15(2)	2(2)
C(9)	76(2)	47(2)	41(2)	9(2)	0(2)	-14(2)
C(10)	56(2)	48(2)	46(2)	17(2)	19(2)	14(2)
Li(1)	26(2)	29(2)	28(2)	4(2)	3(2)	4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for k7.

	x	y	z	U(eq)
H(4A)	4590	12140	3792	55
H(4B)	5446	10125	3656	55
H(4C)	5101	10685	4412	55
H(5A)	4167	6974	4459	53
H(5B)	4452	6612	3681	53
H(5C)	2998	6328	3918	53
H(6A)	2798	10150	4758	60
H(6B)	1679	9420	4200	60
H(6C)	2292	11696	4162	60
H(7A)	6652	6429	769	70
H(7B)	7571	7223	1411	70
H(8A)	7133	9144	184	75
H(8B)	8175	9800	797	75
H(9A)	6786	12057	1224	66
H(9B)	6090	12038	465	66
H(10A)	4784	10921	1457	59
H(10B)	4543	9766	737	59
H(1)	1620(2)	12420(4)	2786(12)	27(7)

Table 6. Torsion angles [deg] for k7.

O(2)-S(1)-O(1)-Li(1)	-43.7(4)
C(1)-S(1)-O(1)-Li(1)	-168.8(3)
C(3)-S(1)-O(1)-Li(1)	71.5(4)
O(1)-S(1)-O(2)-Li(1)#1	-85.9(2)
C(1)-S(1)-O(2)-Li(1)#1	39.0(3)
C(3)-S(1)-O(2)-Li(1)#1	159.0(2)
O(1)-S(1)-C(1)-C(2)	-23.7(2)
O(2)-S(1)-C(1)-C(2)	-153.5(2)
C(3)-S(1)-C(1)-C(2)	91.3(2)
Li(1)#2-N(1)-C(2)-C(1)	158(14)
S(1)-C(1)-C(2)-N(1)	82(14)
O(1)-S(1)-C(3)-C(6)	173.30(19)
O(2)-S(1)-C(3)-C(6)	-62.6(2)
C(1)-S(1)-C(3)-C(6)	55.7(2)
O(1)-S(1)-C(3)-C(4)	53.0(2)
O(2)-S(1)-C(3)-C(4)	177.13(18)
C(1)-S(1)-C(3)-C(4)	-64.6(2)
O(1)-S(1)-C(3)-C(5)	-66.53(18)
O(2)-S(1)-C(3)-C(5)	57.61(18)
C(1)-S(1)-C(3)-C(5)	175.86(17)
C(10)-O(3)-C(7)-C(8)	13.9(4)
Li(1)-O(3)-C(7)-C(8)	-151.4(3)
O(3)-C(7)-C(8)-C(9)	6.0(4)
C(7)-C(8)-C(9)-C(10)	-22.4(4)
C(7)-O(3)-C(10)-C(9)	-28.4(3)
Li(1)-O(3)-C(10)-C(9)	136.6(3)
C(8)-C(9)-C(10)-O(3)	31.3(3)
S(1)-O(1)-Li(1)-O(2)#3	-90.4(4)
S(1)-O(1)-Li(1)-O(3)	151.9(3)
S(1)-O(1)-Li(1)-N(1)#4	28.6(4)
C(10)-O(3)-Li(1)-O(1)	-1.6(3)
C(7)-O(3)-Li(1)-O(1)	161.0(2)
C(10)-O(3)-Li(1)-O(2)#3	-120.7(3)
C(7)-O(3)-Li(1)-O(2)#3	41.9(4)
C(10)-O(3)-Li(1)-N(1)#4	109.4(3)
C(7)-O(3)-Li(1)-N(1)#4	-87.9(3)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+3/2,z #2 x,y+1,z #3 x+1/2,-y+3/2,z
#4 x,y-1,z

$PhSO_2CH_2CN$ **5**

Table 1. Crystal data and structure refinement for kh5.

Identification code	kh5
Empirical formula	C8 H7 N O2 S
Formula weight	181.21
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pmn21
Unit cell dimensions	a = 8.8415(8) A alpha = 90 deg. b = 10.0748(10) A beta = 90.000(5) deg. c = 4.7850(4) A gamma = 90 deg.
Volume	426.23(7) A^3
Z, Calculated density	2, 1.412 Mg/m^3
Absorption coefficient	0.335 mm^-1
F(000)	188
Crystal size	0.25 x 0.25 x 0.08 mm
Theta range for data collection	2.02 to 26.43 deg.
Index ranges	0<=h<=11, 0<=k<=12, 0<=l<=5
Reflections collected / unique	521 / 521 [R(int) = 0.0000]
Completeness to 2theta = 26.43	99.8%
Absorption correction	None
Max. and min. transmission	0.9737 and 0.9210
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	521 / 1 / 79
Goodness-of-fit on F^2	1.131
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0726
R indices (all data)	R1 = 0.0380, wR2 = 0.0749
Absolute structure parameter	0.06(15)
Largest diff. peak and hole	0.220 and -0.195 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for kh5.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	0	800(1)	870(1)	31(1)
O(1)	-1402(2)	689(2)	-647(4)	37(1)
N(1)	0	-2761(4)	1020(11)	58(1)
C(1)	0	-465(4)	3527(9)	32(1)
C(2)	0	-1769(4)	2161(10)	39(1)
C(3)	0	2261(4)	2867(7)	33(1)
C(4)	1362(3)	2812(3)	3676(7)	41(1)
C(5)	1361(4)	3930(3)	5366(8)	50(1)
C(6)	0	4478(4)	6203(12)	51(1)

Table 3. Bond lengths [A] and angles [deg] for kh5.

S(1)-O(1)	1.4411(17)
S(1)-O(1)#1	1.4412(17)
S(1)-C(3)	1.755(4)
S(1)-C(1)	1.801(4)
N(1)-C(2)	1.139(5)
C(1)-C(2)	1.467(5)
C(1)-H(1)	0.97(3)
C(3)-C(4)#1	1.381(3)
C(3)-C(4)	1.381(3)
C(4)-C(5)	1.386(4)
C(4)-H(2)	0.94(3)
C(5)-C(6)	1.384(4)
C(5)-H(3)	0.97(3)
C(6)-C(5)#1	1.384(4)
C(6)-H(4)	0.92(6)
O(1)-S(1)-O(1)#1	118.72(15)
O(1)-S(1)-C(3)	109.87(9)
O(1)#1-S(1)-C(3)	109.87(9)
O(1)-S(1)-C(1)	107.47(9)
O(1)#1-S(1)-C(1)	107.47(9)
C(3)-S(1)-C(1)	102.08(18)
C(2)-C(1)-S(1)	108.6(3)
C(2)-C(1)-H(1)	115.1(17)
S(1)-C(1)-H(1)	104.6(16)
N(1)-C(2)-C(1)	177.8(5)
C(4)#1-C(3)-C(4)	121.3(4)
C(4)#1-C(3)-S(1)	119.32(18)
C(4)-C(3)-S(1)	119.32(18)
C(3)-C(4)-C(5)	119.3(3)
C(3)-C(4)-H(2)	120.6(19)
C(5)-C(4)-H(2)	120.1(19)
C(6)-C(5)-C(4)	119.6(3)
C(6)-C(5)-H(3)	119(2)
C(4)-C(5)-H(3)	121.1(19)
C(5)-C(6)-C(5)#1	120.9(4)
C(5)-C(6)-H(4)	119.6(2)
C(5)#1-C(6)-H(4)	119.6(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for kh5.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	28(1)	45(1)	20(1)	-3(1)	0	0
O(1)	28(1)	57(1)	27(1)	-3(1)	-3(1)	0(1)
N(1)	51(2)	50(2)	72(3)	-15(3)	0	0
C(1)	29(2)	42(2)	26(2)	-7(2)	0	0
C(2)	32(2)	45(2)	40(2)	-2(2)	0	0
C(3)	35(2)	38(2)	27(2)	0(2)	0	0
C(4)	39(2)	47(2)	38(2)	-3(1)	0(1)	-3(1)
C(5)	51(2)	47(2)	50(2)	-4(2)	-4(2)	-10(1)
C(6)	68(3)	42(2)	44(3)	-4(2)	0	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for kh5.

	x	y	z	U(eq)
H(1)	880(3)	-280(3)	4650(7)	44(8)
H(2)	2280(4)	2440(3)	3070(8)	54(9)
H(3)	2300(3)	4320(2)	6020(10)	56(8)
H(4)	0	5230(5)	7310(13)	66(15)

Table 6. Torsion angles [deg] for kh5.

O(1)-S(1)-C(1)-C(2)	64.42(9)
O(1)#1-S(1)-C(1)-C(2)	-64.42(9)
C(3)-S(1)-C(1)-C(2)	180.0
S(1)-C(1)-C(2)-N(1)	0.000(12)
O(1)-S(1)-C(3)-C(4)#1	24.9(3)
O(1)#1-S(1)-C(3)-C(4)#1	157.2(3)
C(1)-S(1)-C(3)-C(4)#1	-88.9(3)
O(1)-S(1)-C(3)-C(4)	-157.2(3)
O(1)#1-S(1)-C(3)-C(4)	-24.9(3)
C(1)-S(1)-C(3)-C(4)	88.9(3)
C(4)#1-C(3)-C(4)-C(5)	0.9(6)
S(1)-C(3)-C(4)-C(5)	-176.9(3)
C(3)-C(4)-C(5)-C(6)	-0.3(6)
C(4)-C(5)-C(6)-C(5)#1	-0.3(8)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,z

t-$BuSO_2CH_2CN$ **6**

Table 1. Crystal data and structure refinement for kw8.

Identification code	kw8
Empirical formula	C6 H11 N O2 S
Formula weight	161.22
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pnma
Unit cell dimensions	a = 17.3947(5) A alpha = 90 deg. b = 8.5665(2) A beta = 90 deg. c = 5.47070(10) A gamma = 90 deg.
Volume	815.20(3) A^3
Z, Calculated density	4, 1.314 Mg/m^3
Absorption coefficient	0.340 mm^-1
F(000)	344
Crystal size	0.35 x 0.15 x 0.15 mm
Theta range for data collection	3.34 to 30.00 deg.
Index ranges	0<=h<=24, 0<=k<=11, -7<=l<=7
Reflections collected / unique	1939 / 1121 [R(int) = 0.0221]
Absorption correction	None
Max. and min. transmission	0.9508 and 0.8903
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1121 / 0 / 77
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0300, wR2 = 0.0697
R indices (all data)	R1 = 0.0426, wR2 = 0.0753
Largest diff. peak and hole	0.321 and -0.353 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for kw8.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	2962(1)	2500	5276(1)	17(1)
O(1)	2843(1)	3934(1)	6606(1)	25(1)
N(1)	906(1)	2500	4246(4)	45(1)
C(1)	2317(1)	2500	2686(3)	21(1)
C(2)	1526(1)	2500	3571(3)	28(1)
C(3)	3911(1)	2500	3909(3)	21(1)
C(4)	4002(1)	1010	2388(2)	29(1)
C(5)	4476(1)	2500	6053(3)	35(1)

Table 3. Bond lengths [A] and angles [deg] for kw8.

S(1)-O(1)#1	1.4424(9)
S(1)-O(1)	1.4424(9)
S(1)-C(1)	1.8077(17)
S(1)-C(3)	1.8118(17)
N(1)-C(2)	1.140(3)
C(1)-C(2)	1.459(3)
C(1)-H(1A)	0.944(17)
C(3)-C(5)	1.531(2)
C(3)-C(4)	1.5319(11)
C(3)-C(4)#1	1.5319(11)
C(4)-H(4A)	0.966(18)
C(4)-H(4B)	0.973(18)
C(4)-H(4C)	0.960(19)
C(5)-H(5A)	1.00(3)
C(5)-H(5B)	0.95(2)
O(1)#1-S(1)-O(1)	116.73(7)
O(1)#1-S(1)-C(1)	107.84(5)
O(1)-S(1)-C(1)	107.84(5)
O(1)#1-S(1)-C(3)	109.82(5)
O(1)-S(1)-C(3)	109.82(5)
C(1)-S(1)-C(3)	103.99(8)
C(2)-C(1)-S(1)	108.97(12)
C(2)-C(1)-H(1A)	109.0(11)
S(1)-C(1)-H(1A)	107.5(10)
N(1)-C(2)-C(1)	179.5(2)
C(5)-C(3)-C(4)	110.49(9)
C(5)-C(3)-C(4)#1	110.49(9)
C(4)-C(3)-C(4)#1	112.86(12)
C(5)-C(3)-S(1)	105.58(12)
C(4)-C(3)-S(1)	108.56(9)
C(4)#1-C(3)-S(1)	108.56(9)
C(3)-C(4)-H(4A)	105.8(10)
C(3)-C(4)-H(4B)	113.4(11)
H(4A)-C(4)-H(4B)	110.5(14)
C(3)-C(4)-H(4C)	112.0(10)
H(4A)-C(4)-H(4C)	110.3(14)
H(4B)-C(4)-H(4C)	104.9(15)
C(3)-C(5)-H(5A)	106.9(13)
C(3)-C(5)-H(5B)	111.1(12)
H(5A)-C(5)-H(5B)	107.2(14)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for kw8.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	18(1)	16(1)	18(1)	0	0(1)	0
O(1)	28(1)	23(1)	24(1)	-7(1)	1(1)	2(1)
N(1)	24(1)	60(1)	51(1)	0	-2(1)	0
C(1)	20(1)	19(1)	23(1)	0	-3(1)	0
C(2)	24(1)	27(1)	32(1)	0	-7(1)	0
C(3)	18(1)	26(1)	19(1)	0	1(1)	0
C(4)	29(1)	28(1)	30(1)	-4(1)	5(1)	6(1)
C(5)	21(1)	59(1)	25(1)	0	-4(1)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for kw8.

	x	y	z	U(eq)
H(1A)	2406(10)	1570(2)	1800(2)	29(4)
H(4A)	4525(11)	1020(2)	1800(3)	35(4)
H(4B)	3642(12)	940(2)	1030(3)	43(5)
H(4C)	3909(11)	90(2)	3340(3)	38(4)
H(5A)	5005(16)	2500	5340(4)	35(6)
H(5B)	4428(12)	1570(2)	7000(3)	49(5)

Table 6. Torsion angles [deg] for kw8.

O(1)#1-S(1)-C(1)-C(2)	63.43(4)
O(1)-S(1)-C(1)-C(2)	-63.43(4)
C(3)-S(1)-C(1)-C(2)	180.0
S(1)-C(1)-C(2)-N(1)	180.00(2)
O(1)#1-S(1)-C(3)-C(5)	-64.82(4)
O(1)-S(1)-C(3)-C(5)	64.82(4)
C(1)-S(1)-C(3)-C(5)	180.0
O(1)#1-S(1)-C(3)-C(4)	53.66(11)
O(1)-S(1)-C(3)-C(4)	-176.69(8)
C(1)-S(1)-C(3)-C(4)	-61.51(8)
O(1)#1-S(1)-C(3)-C(4)#1	176.69(8)
O(1)-S(1)-C(3)-C(4)#1	-53.66(11)
C(1)-S(1)-C(3)-C(4)#1	61.52(8)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z