Polish J. Chem., **78**, 1967–1968 (2004) **DISCUSSION**

The Space Group of Tribenzyl[4-phenyl-1,3,4-thiodiazolyl-2-mercapto-5(*H*)-thione]tin(IV)

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A recent report in this *Journal* presents the refinement of the crystal structure of $C_{29}H_{26}N_2S_3Sn$ in the triclinic *P*-1 space group [1]; the choice of space group is odd since the α and γ angles of the unit cell are 90°. The structure is better described in monoclinic $P2_1/n$ (Table 1, Fig. 1). The revision of the space group from the deposited crystallographic-information-file was effected by using the method detailed in [2,3].

Table 1. Atomic coordinates for $C_{29}H_{26}N_2S_3Sn$ in $P2_1/n$ (a = 9.744, b = 16.338, c = 17.957 Å; β = 100.735°).

Sn1	0.7261	0.7438	0.7131
S1	0.7507	0.7357	0.5797
S2	0.5664	0.6451	0.4536
S3	0.3111	0.5411	0.4058
N1	0.5110	0.6571	0.5869
N2	0.4080	0.6103	0.5435
C1	0.9205	0.8018	0.7574
C2	0.9748	0.8487	0.6972
C3	0.9327	0.9288	0.6795
C4	0.9854	0.9711	0.6238
C5	1.0801	0.9333	0.5859
C6	1.1222	0.8532	0.6036
C7	1.0695	0.8109	0.6593
C8	0.7071	0.6222	0.7575
C9	0.8181	0.6127	0.8283
C10	0.9352	0.5653	0.8247
C11	1.0378	0.5548	0.8890
C12	1.0234	0.5917	0.9569
C13	0.9063	0.6391	0.9605
C14	0.8037	0.6496	0.8962
C15	0.5460	0.8173	0.7209
C16	0.4694	0.7797	0.7787
C17	0.3720	0.7184	0.7553

Table 1 (continuation)

C18	0.3040	0.6807	0.8075
C19	0.3333	0.7043	0.8832
C20	0.4307	0.7656	0.9066
C21	0.4987	0.8033	0.8544
C22	0.6023	0.5785	0.5803
C25	0.1618	0.5955	0.5530
C26	0.0597	0.5622	0.5886
C27	0.0977	0.5119	0.6515
C28	0.2379	0.4950	0.6788
C29	0.3400	0.5283	0.6432

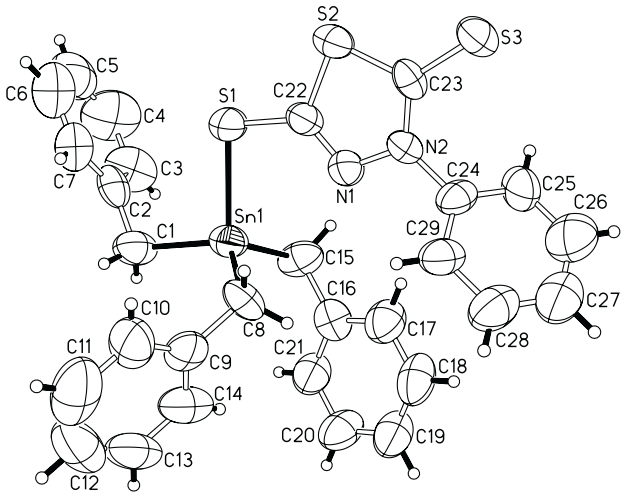

Figure 1. Crystal structure of $C_{29}H_{26}N_2S_3Sn$.

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