

Table S1 Selected interatomic distances (r_a /pm) and mean amplitudes of vibration (u /pm)
for S(NBu¹)₂ from the GED study.^{a,b}

No.	Atom pair	r_a /pm	u /pm ^c
u_1	C(6) - C(4)	152.6(2)	5.7(2)
u_2	C(6) - H(12)	111.8(1)	7.6(2)
u_3	N(2) - S(1)	153.8(3)	4.2 (tied to u_1)
u_4	N(3) - S(1)	156.5(4)	4.3 (tied to u_1)
u_5	C(10) - C(9)	250.1(5)	6.5(6)
u_6	C(7) - C(6)	250.4(5)	6.5 (tied to u_5)
u_7	C(5) ... S(1)	258.4(9)	5.1 (tied to u_{11})
u_8	C(9) ... S(1)	283.4(11)	10.6(5)
u_9	C(4) ... S(1)	267.3(7)	5.2(tied to u_5)
u_{10}	C(6) ... S(1)	322.2(6)	11.4(tied to u_8)
u_{12}	C(4) - N(2)	146.2(4)	5.6(tied to u_1)
u_{13}	C(5) - N(3)	147.0(4)	5.6(tied to u_1)
u_{14}	C(10) ... S(1)	359.7(8)	30.0 (20)
u_{16}	C(7) ... S(1)	385.9(8)	9.7(tied to u_{14})
u_{17}	N(3) ... N(2)	265.7(8)	6.1(6)
u_{18}	C(6)-N(2)	246.4(8)	7.7(tied to u_{17})
u_{19}	C(7) ... N(2)	235.2(9)	7.1(tied to u_{17})
u_{20}	C(9) ... N(3)	253.7(9)	7.1(tied to u_{17})
u_{21}	C(10) ... N(3)	238.4(7)	7.6(tied to u_{17})
u_{22}	C(8) ...N(2)	246.4(8)	7.7(tied to u_{17})

Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2002

u_{23}	C(11) ... N(3)	238.4(7)	7.6(tied to u_{17})
u_{24}	C(4) ... N(3)	313.3(9)	12(1)
u_{25}	C(8) ... N(3)	322.3(9)	24.2(tied to u_{24})
u_{27}	C(5) ... N(2)	397.6(6)	5.7(5)
u_{28}	C(9) ... N(2)	437.3(11)	9.3(tied to u_{27})
u_{29}	C(7) ... N(3)	460.6 (8)	8.6(tied to u_{27})
u_{30}	C(10) ... N(2)	483.4(9)	15.6(tied to u_{27})
u_{32}	C(8) ... C(5)	459.4(11)	20.6(tied to u_{27})
u_{34}	C(5) ... C(4)	460.0(8)	9.9(tied to u_{27})
u_{35}	C(10) ... C(8)	479.1(19)	29.4((tied to u_{27})
u_{37}	C(9) ... C(4)	537.1(12)	15.0(10)
u_{38}	C(10) ... C(4)	525.5(12)	25.9(tied to u_{37})
u_{40}	C(9) ... C(8)	555.4(12)	33.7(tied to u_{37})
u_{42}	C(11) ... C(8)	540.5(16)	45.1(tied to u_{37})
u_{44}^d	C(7) ... C(5)	605.6(77)	10.5(9)
u_{45}^d	C(9) ... C(7)	667.6(13)	12.4(9)
u_{46}	C(10) ... C(7)	672.4(12)	21.9(tied to u_{45})

^a See Figure 1 for atom numbering; all other distances were included in the refinement, but are not listed here.

^b Estimated standard deviations, obtained in the least-squares refinement, are given in parentheses.

^c Amplitudes not refined were fixed at the values obtained using the HF/6-31G* force field.

^d Restraints applied to u_{44} [10.2(10)] and u_{45} [11.5(11)].

Table S2 Least-squares correlation matrix ($\times 100$) for $S(NBu^t)_2$.^a

	p_7	p_9	p_{11}	p_{12}	u_1	u_{17}	k_1
p_9	64						
p_{11}		-71					
u_5	-64	-68					
u_8		52	-52				
u_{14}						-64	
u_{17}	-76						
k_1				-54	58		
k_2							50

^a Only elements with absolute values $\geq 50\%$ are shown; k_1 and k_2 are scale factors.

Table S3 Interatomic distances (r/pm) and amplitudes of vibration (u/pm) for the restrained GED structure of $S(NBu^t)_3$.^{a,b}

No.	Atom Pair	r_a/pm	u/pm^c
u_1	C(5)-C(8)	150.8(2)	5.0(2)
u_2	S(1)-N(2)	153.5(3)	3.8 (tied to u_1)
u_3	N(2)-C(5)	147.2(4)	5.0 (tied to u_1)
u_4	N(2)...C(8)	250.0(5)	7.4(4)
u_5	C(8)-H(17)	112.9(3)	8.4(3)
u_6	S(1)...C(5)	264.2(4)	8.6(8)
u_7	S(1)...C(8)	331.0(8)	9.6(5)
u_8	S(1)...C(11)	382.3(4)	7.6(6)
u_9	S(1)...C(12)	316.6(7)	9.6 (tied to u_7)
u_{10}	S(1)...H(19)	311.9(24)	20.0 (fixed)
u_{11}	S(1)...H(29)	282.7(27)	20.0 (fixed)
u_{12}	N(2)...N(3)	265.8(5)	4.8(5)
u_{13}	N(2)...H(17)	275.8(22)	16.3 (fixed)
u_{14}	N(2)...H(18)	347.7(7)	9.9 (fixed)
u_{15}	N(2)...H(19)	285.8(21)	16.2 (fixed)
u_{16}	N(3)...C(5)	310.8(7)	8.9 (tied to u_7)

Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2002

u_{17}	N(3)...C(8)	334.2(15)	14.7 (tied to u_7)
u_{18}	N(3)...C(11)	456.4(7)	10.3 (tied to u_{21})
u_{19}	N(3)...C(12)	316.7(12)	14.7 (tied to u_7)
u_{20}	N(4)...C(5)	402.3(4)	6.5 (fixed)
u_{21}	N(4)...C(8)	474.5(8)	13.0(6)
u_{22}^d	N(4)...C(11)	496.0(7)	12.3(8)
u_{23}	N(4)...C(12)	456.6(9)	13.0 (tied to u_{21})
u_{24}	C(5)...C(6)	456.9(7)	12.2 (tied to u_{21})
u_{25}	C(5)...H(17)	219.3(6)	12.7(10)
u_{26}	C(6)...C(8)	474.3(16)	23.3 (tied to u_{21})
u_{27}	C(6)...C(11)	601.7(7)	10.1 (fixed)
u_{28}	C(6)...C(12)	444.5(13)	23.3 (tied to u_{21})
u_{29}	C(7)...C(8)	547.7(8)	9.6 (tied to u_{32})
u_{30}	C(7)...C(11)	510.3(7)	16.4 (fixed)
u_{31}	C(7)...C(12)	526.7(12)	13.4 (fixed)
u_{32}^d	C(8)...C(9)	543.6(16)	24.1(22)
u_{33}	C(8)...C(11)	244.1(7)	11.1(6)
u_{34}^d	C(9)...C(11)	688.2(9)	24.4(17)
u_{35}	C(9)...C(12)	566.4(13)	12.6 (tied to u_{32})
u_{36}	C(10)...C(11)	503.3(22)	40.5 (tied to u_{22})
u_{37}	C(10)...C(12)	579.2(18)	15.8 (tied to u_{32})
u_{38}	C(11)...C(13)	660.0(8)	20.4 (tied to u_{34})
u_{39}	C(11)...C(14)	659.2(12)	24.4 (tied to u_{34})
u_{40}	C(11)...H(17)	272.6(24)	16.4 (fixed)
u_{41}	C(11)...H(18)	270.8(22)	16.5 (fixed)
u_{42}	C(12)...C(13)	468.8(21)	25.7 (fixed)
u_{43}	C(12)...C(14)	493.7(21)	44.5 (tied to u_{22})
u_{44}	C(12)...H(18)	271.5(25)	16.7 (fixed)
u_{45}	C(12)...H(19)	274.5(27)	16.2 (fixed)

^a See Figure 1 for atom numbering; all other distances were included in the refinement, but are not listed here.

^b Estimated standard deviations, obtained in the least-squares refinement, are given in parentheses.

^c Amplitudes not refined were fixed at the values obtained using the HF/6-31G* force field.

^d Restraints were applied to u_{22} [9.3(9)], u_{32} [33.6(34)] and u_{34} [19.6(20)], and also to the ratios of u_4/u_{33} [0.661(33)] and u_6/u_{12} [1.817(91)]. Uncertainties are 5% of the amplitude ratios.

Table S4 Least-squares correlation matrix ($\times 100$) for $S(\text{NBu}^t)_3$.^a

	p_7	p_8	p_{10}	u_6	u_7	u_{12}	u_{25}	k_2
p_4	-50	-70	54					
p_7		63	-54					
p_8			-70					
p_{12}					-79			
u_1								63
u_4				66		62		
u_5				51			56	
u_6						80		

^a Only elements with absolute values $\geq 50\%$ are shown; k_2 is a scale factor.