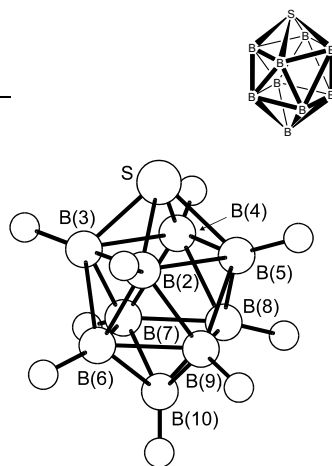


**76      B<sub>9</sub>H<sub>9</sub>S**MW, *ab initio* and DFT  
calculations**1-Thia-*closo*-decaborane(9)****C<sub>4v</sub> assumed**

$r_s$	Å	$\theta_s$	deg
S–B(2)	1.944(2)	B(2)–S–B(3)	59.66(5)
B(2)–B(3)	1.937(1)	B(2)–S–B(4)	89.41(5)
B(2)–B(6)	1.765(3)	B(2)–B(6)–B(3)	66.44(5)
B(6)–B(7)	1.850(2)	B(6)–B(2)–B(9)	63.58(7)
B(6)–B(10)	1.707(1)	B(6)–B(10)–B(7)	65.46(10)
$h^a$	1.435(3)	B(6)–B(10)–B(8)	99.76(2)

Atom	$y_s$ [Å]	$z_s$ [Å]
S	0.0	1.7794
B(10)	0.0	–2.1460
B(2)	1.3678	0.3973
B(6)	1.3151	–1.0378



The axial sulfur atom causes a substantial expansion of the B<sub>4</sub> belt adjacent to sulfur and hence leads to a significant distortion from a regular bicapped square antiprismatic structure.

<sup>a</sup>) Distance between the two BBBB planes.

Møllendal, H., Samdal, S., Holub, J., Hnyk, D.: *Inorg. Chem.* **41** (2002) 4574.