Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

Synthesis and characterization of [{PhC(NBu^t)$_2$}Si(S)SBu^t]: a silicon thioester analogue with the Si(=S)-S-skeleton

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Theoretical calculation data

N	0.41412300	1.09283700	0.10574500
N	0.38950000	-1.05369800	0.33593600
C	1.18230200	-0.00800200	0.05561800
C	0.75177600	2.54052600	0.13209200
C	2.64302300	-0.05370800	-0.24764800
C	1.48635600	2.88979000	1.44159800
C	-0.59006000	3.29415100	0.08507400
C	1.59206900	2.94705600	-1.09227600
C	3.58263400	-0.01522600	0.79210200
C	3.08302100	-0.12476400	-1.57688900
H	0.89460800	2.57423100	2.30710600
H	2.46761600	2.40657400	1.49012400
H	1.64435800	3.97311000	1.50498900
H	-0.40605800	4.37392200	0.10334400
H	-1.14310900	3.05258800	-0.82872900
H	-1.21346100	3.03866100	0.94833200
H	1.70162800	4.03758900	-1.10719500
H	2.59492500	2.51335600	-1.07345800
H	1.09574200	2.64280800	-2.02063900
H	3.24375800	0.03304000	1.82339000
C	4.94777100	-0.04447600	0.50197100
H	2.35652900	-0.14629000	-2.38471500
C	4.44894400	-0.15815100	-1.86047500
H	5.66989900	-0.01253100	1.31385400
C	5.38285600	-0.11666000	-0.82286200

H	4.78186300	-0.21338700	-2.89382000
H	6.44650400	-0.14023800	-1.04621500
Si	-1.07058000	0.08017300	0.61740900
C	-4.08559000	-0.05334900	-0.79882100
C	-4.46947600	-1.23873000	0.09420100
C	-4.46919800	1.28089700	-0.14893800
C	-4.74990900	-0.18571000	-2.17843100
H	-4.20229400	-2.19117100	-0.37700300
H	-3.98252300	-1.17534500	1.07160100
H	-5.55684900	-1.23368600	0.25439400
H	-4.19408300	2.12524900	-0.79032400
H	-5.55741600	1.30943700	0.00312100
H	-3.98710700	1.40219700	0.82516800
H	-5.84073800	-0.17538700	-2.05368900
H	-4.47584600	0.64474200	-2.83829600
H	-4.47301200	-1.12438000	-2.67080400
S	-2.22858500	-0.09080100	-1.20401700
C	0.62601600	-2.51996600	0.31308300
C	1.73296300	-2.91571100	1.30883900
H	1.80698500	-4.00842500	1.35798200
H	2.71172700	-2.52932100	1.01229400
H	1.49691500	-2.54364200	2.31177300
C	-0.69546400	-3.17458500	0.75430000
H	-0.99091600	-2.82916800	1.75035800
H	-1.50251600	-2.93869700	0.05284800
H	-0.57503300	-4.26295200	0.78329200
C	0.97594200	-2.99070000	-1.11175200
H	1.93514500	-2.58597600	-1.44891600
H	1.04899200	-4.08446700	-1.13402000
H	0.19703900	-2.68473000	-1.81857700
S	-1.82681400	0.29328800	2.45353100