

Table S1. Key bond lengths of transition states (TS_{AM} and TS_M).

Structure	Bond length (Å)	
TS _{AM}	C-N	1.17
	B-N	1.68
	C-H	1.18
	B-H	1.45
TS _M	C-N	1.28
	B-N	2.59
	C-H	1.90
	B-H	2.59