

Catalytic role of borane and alane in hydrogen release from cyclic amine adducts $C_nH_{2n+1}N \cdot XH_3$ [$X=B, Al$; $n = 2-5$]: a theoretical interpretation

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Supporting Information

Table S1 Calculated wt% values for hydrogen storage of the cyclic amine-borane and amine-alane compounds

	Species	wt%
$C_nH_{2n+1}N \cdot BH_3$ ($n = 2-5$)	$C_2H_5N \cdot BH_3$ (1_{ab})	3.5
	$C_3H_7N \cdot BH_3$ (2_{ab})	2.8
	$C_4H_9N \cdot BH_3$ (3_{ab})	2.4
	$C_5H_{11}N \cdot BH_3$ (4_{ab})	2.0
$C_nH_{2n+1}N \cdot AlH_3$ ($n = 2-5$)	$C_2H_5N \cdot AlH_3$ (1_{aal})	2.8
	$C_3H_7N \cdot AlH_3$ (2_{aal})	2.3
	$C_4H_9N \cdot AlH_3$ (3_{aal})	2.0
	$C_5H_{11}N \cdot AlH_3$ (4_{aal})	1.8