Supplementary information.

Table 1S. Total energies (E°_0), Hartree, sum of electronic and thermal enthalpies H°_{298}, Hartree and standard entropies S°_{298}, J mol^{-1}, K^{-1} for the investigated compounds.

B3LYP/LANL2DZ(d,p) level of theory.

Compound	E°_0	H°_{298}	S°_{298}
H_2	-1.1774302	-1.163913	130.3
HBr	-13.7733722	-13.764200	198.5
$AlBr_3$	-41.7196349	-41.709200	349.3
AlH_3	-3.7778843	-3.755332	207.3
$_{ring}$**A**	-218.5238884	-218.408501	419.3
($_{ring}$**A**)$_2$	-437.0696907	-436.836581	676.1
TS1	-436.9713774	-436.746407	642.8
Intermediate	-423.2458412	-423.028831	594.2
TS2	-423.1748923	-422.965455	575.6
$_{chain}$**A**	-218.4833606	-218.368799	447.3
A$_2$	-437.0620358	-436.829490	681.5
I$_a$	-204.5819865	-204.483162	361.2
I$_b$	-204.5479437	-204.449485	398.6
I$_{2a}$	-409.3823024	-409.179877	521.3
I$_{2b}$	-409.3168602	-409.115831	593.6
I$_{2c}$	-409.3168352	-409.115870	606.5
I$_{3a}$	-614.1209861	-613.816227	694.5
I$_{3b}$	-614.0343492	-613.731490	783.7
I$_{3c}$	-614.0342976	-613.731431	776.3
I$_4$	-818.8037934	-818.399331	921.2
I$_6$	-1228.246765	-1227.638396	1208.3
I'$_6$	-1145.328747	-1144.817247	769.8
I'$_8$	-1582.330737	-1581.582958	1312.1
A'	-204.6600463	-204.561487	353.8
A'$_{2a}$	-409.4269528	-409.226070	516.7
A'$_{2b}$	-409.4248457	-409.224013	517.5
A'$_{3a}$	-614.1573514	-613.854895	680.9
A'$_{3b}$	-614.1538736	-613.851221	693.8
A'$_{2a}$($AlBr_3$)$_2$	-492.9858725	-492.758016	888.4
Ladder L	-902.9857657	-902.621907	1162.5
$_{ring}$**A_H**	-193.2131485	-193.089834	331.5
Ladder_H	-776.5089953	-776.103860	727.5