Supplementary Table S4 Relative energy for the H-abstraction reactions at different H atoms of H_{NH2}, $H_{cis\text{-}CH3}$ and $H_{trans\text{-}CH3}$ sites of UDMH by H and CH_3 at CCSD(T)/CBS//M062X/def2-TZVP level (unit: kcal/mol).

H atom	Reactions	Relative energy (TS)	Relative energy (Products)
H(inside)	UDMH + H = $HNN(CH_3)_2 + H_2$	1.9	-23.9
H(outside)	UDMH + H = $HNN(CH_3)_2 + H_2$	6.8	-23.9
H(inside)	UDMH + H = cis-$H_2NN(CH_3)CH_2 + H_2$	5.2	-11.8
H(outside)	UDMH + H = cis-$H_2NN(CH_3)CH_2 + H_2$	9.4	-11.8
H(plane)	UDMH + H = cis-$H_2NN(CH_3)CH_2 + H_2$	9.9	-11.8
H(inside)	UDMH + H = trans-$H_2NN(CH_3)CH_2 + H_2$	5.3	-11.4
H(outside)	UDMH + H = trans-$H_2NN(CH_3)CH_2 + H_2$	10.1	-11.4
H(plane)	UDMH + H = trans-$H_2NN(CH_3)CH_2 + H_2$	9.8	-11.4
H(inside)	UDMH + CH_3 = $HNN(CH_3)_2 + CH_4$	6.4	-23.0
H(outside)	UDMH + CH_3 = $HNN(CH_3)_2 + CH_4$	9.9	-23.0
H(inside)	UDMH + CH_3 = cis-$H_2NN(CH_3)CH_2 + CH_4$	11.1	-10.9
H(outside)	UDMH + CH_3 = cis-$H_2NN(CH_3)CH_2 + CH_4$	14.0	-10.9
H(plane)	UDMH + CH_3 = cis-$H_2NN(CH_3)CH_2 + CH_4$	14.2	-10.9
H(inside)	UDMH + CH_3 = trans-$H_2NN(CH_3)CH_2 + CH_4$	11.2	-10.5
H(outside)	UDMH + CH_3 = trans-$H_2NN(CH_3)CH_2 + CH_4$	14.3	-10.5
H(plane)	UDMH + CH_3 = trans-$H_2NN(CH_3)CH_2 + CH_4$	14.5	-10.5