Electronic Supplementary Information for:

A theoretical study on laser cooling feasibility of XH (X = As, Sb and Bi): Effects of intersystem crossings and spin-orbit couplings

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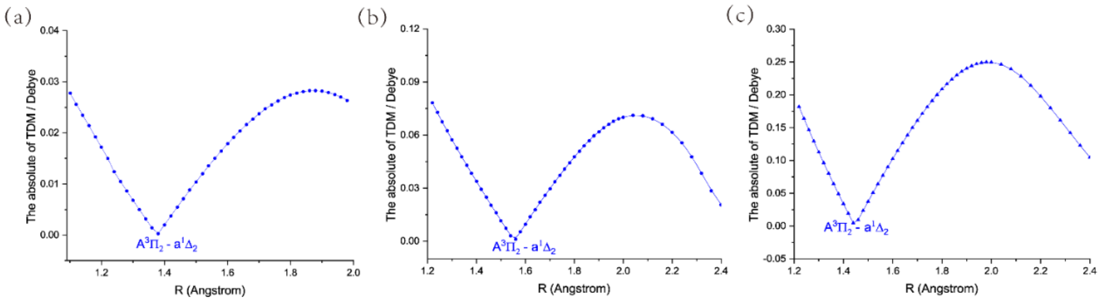

Fig. S1. Transition dipole moments (TDMs) as a function of the interatomic distance (R) for the $A^3\Pi_2$ $\rightarrow$ $a^1\Delta_2$ transition of AsH (a), SbH (b) and BiH (c) at the icMRCI+Q level.

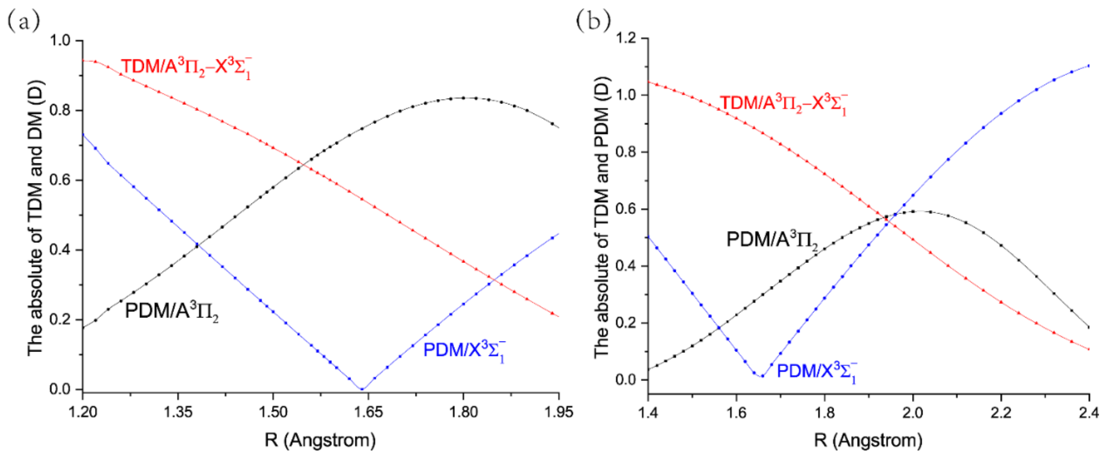

Fig. S2. Permanent dipole moments (PDMs) and transition dipole moments (TDMs) as a function of the interatomic distance (R) for the $X^3\Sigma_1^-$ and $A^3\Pi_2$ states of AsH (a) and SbH (b) at the icMRCI+Q level.

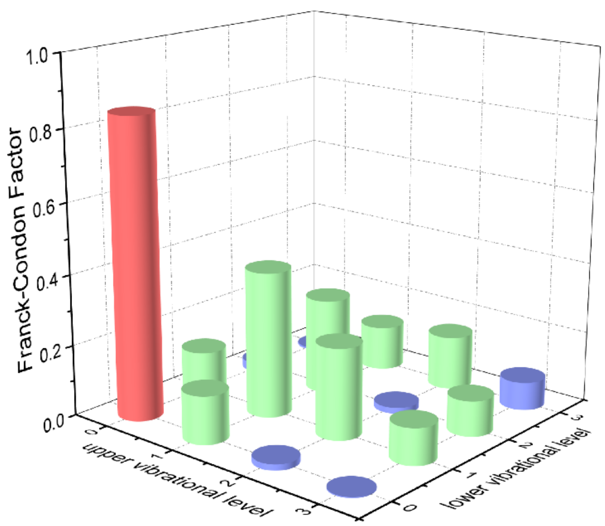

Fig. S3. Franck-Condon factors of the $A^3\Pi_2$ ($v' \leq 3$) $\rightarrow$ $X^3\Sigma_1^-$ ($v \leq 3$) transitions for AsH, calculated at the icMRCI+Q level.

Table S1 The calculated population loss due to the decay channel of intersystem crossings.

	State	Population loss
AsH	$A^3\Pi$ (v′ = 2)	0.0125
SbH	$A^3\Pi$ (v′ = 1)	0.1073
BiH	$A^3\Pi$ (v′ = 1)	0.6247

The population loss due to intersystem crossings has been estimated using the Landau–Zener theory.[1, 2] As shown in Table S1, the obtained decay probability for AsH (v′ = 2) of the $A^3\Pi$ state is 1.3%, and those for SbH (v′ = 1) and BiH (v′ = 1) are 10.7% and 62.5%, respectively.

Table S2 Comparison of the relevant properties for laser cooling of several hydrides.

	R_{00} [a]	$\tau_{v'}$ (ns)[a]	$T_{Doppler}$ (μK) [a]	T_{Recoil} (μK)	λ_{00} (nm) [a]
AsH	0.9662	914	4.18	2.20	338.3
SbH	0.9248	883	4.33	1.13	373.4
BaH	0.9639[b]	120.3[c]	31.7[c]	0.168[c]	905[d]
CH	0.983[e]	536[f]	7.13[f]	7.91[f]	430.9[e]
SiH	0.9954[g]	575[g]	6.65[g]	3.89[g]	412.6[g]

[a] These columns correspond to the main cooling transition. [b] Ref. 3. [c] Ref. 4. [d] Ref. 5. [e] Ref. 6. [f] Ref. 7. [g] Ref. 8.

Notes and references

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