Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material:

We present the results of the computations of isolated H_2 and of H_2 embedded into an Ar matrix. We used similar methodology as described in the paper for $CO@Ar_n$.

Table S1: variation of vibrational frequency of H_2 in argon matrix ω_{H2}.

Molecular system	ω_{H2} **(cm^{-1})**	$\Delta\omega_{H2}$ **(cm^{-1})**
H_2	4392.2 4401.2 [a]	
H_2@Ar_{31}	4248.0	144.2
H_2@Ar [b]	4241.6	159.6

a) Ref. [80].

b) Ref. [83].

The spectroscopic properties of dihydrogen embedded in Ar matrix are following the same variations as those noticed for carbon monoxide. See text for more details.