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

A kernel-based machine learning potential and quantum vibrational state analysis of the cationic Argon hydride (Ar_2H^+)

María Judit Montes de Oca-Estévez [1,2,a], Álvaro Valdés[3], and Rita Prosmiti[1*]

[1] *Institute of Fundamental Physics (IFF-CSIC), CSIC, Serrano 123, 28006 Madrid, Spain*

[2] *Atelgraphics S.L., Mota de Cuervo 42, 28043, Madrid, Spain*

[3] *Escuela de Física, Universidad Nacional de Colombia, Sede Medellín, A. A. 3840, Medellín, Colombia*

[a] *Doctoral Programme in Theoretical Chemistry and Computational Modelling, Doctoral School, Universidad Autónoma de Madrid, Spain*

E-mail: rita@iff.csic.es

Supporting Information Available

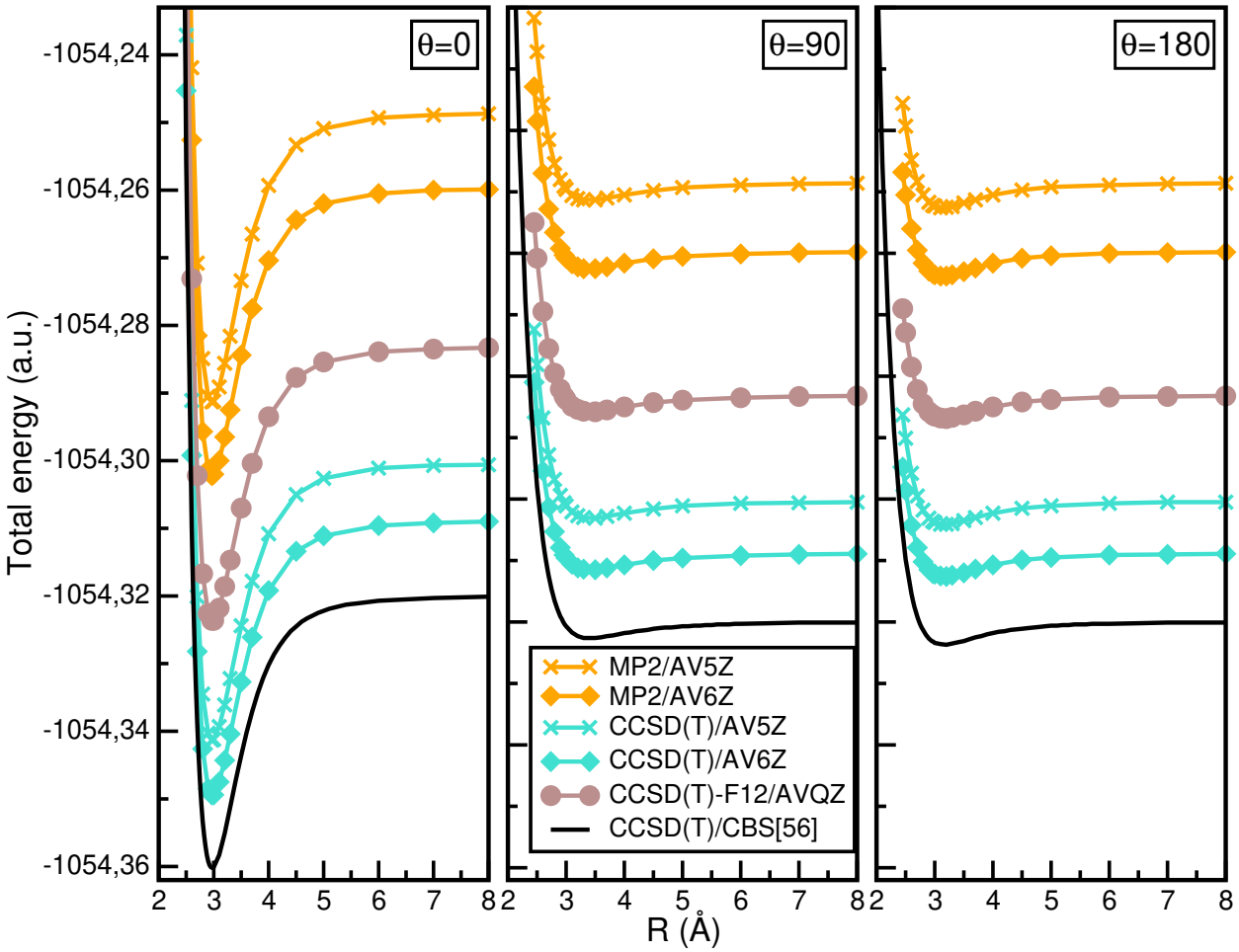

Figure S1: Total electronic energies as a function of R distance at $\theta = 0°$, 90° and 180° from MP2, CCSD(T) and CCSD(T)-F12 calculations using different basis sets for the $[Ar_2H]^+$ cation.

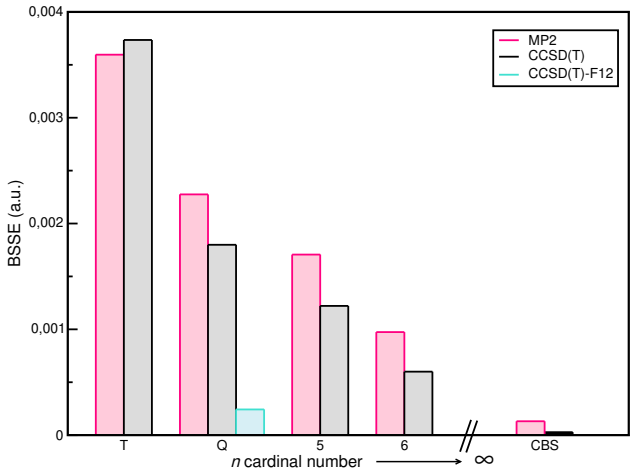

Figure S2: Influence of the BSSE correction in the equilibrium geometry for different level of theory (MP2, CCSD(T) and CCSD(T)-F12) using the correlation consistent basis set family, AVnZ (where n is T, Q, 5 and 6). The CBS[56] extrapolation values are also shown.

Table S1: Vibrational energies (in cm^{-1}) obtained from quantum variational bound states calculations for the indicated $[Ar_2H]^+$ isotopes using the RKHS-ML PES.

No state(v)	$[^{36}Ar_2H]^+$	$[^{40}Ar_2H]^+$
0	1367.00	1356.64
1	1672.85	1647.29
2	1977.67	1937.29
3	2277.06	2222.80
4	2345.57	2333.66
5	2568.05	2501.29
6	2620.43	2595.33
7	2691.07	2678.24
8	2847.75	2770.31
9	2886.17	2848.83
10	2976.01	2948.78
11	3114.23	3028.06
12	3136.68	3088.69
13	3251.07	3211.50
14	3366.04	3273.02
15	3372.78	3315.45
16	3463.53	3438.49
17	3480.38	3451.23
18	3593.15	3503.08
19	3599.43	3532.22