Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Quantum Microsolvation and Size-resolved Energetics of He-Solvated H_2^+ and D_2^+ Cations

Antonio Sarsa[1], María Judit Montes de Oca-Estévez[2], Pablo Villarreal[2], Javier Hernández-Rojas[3], and Rita Prosmiti[2*]

[1] *Departamento de Física, Campus de Rabanales Edif. C2, Universidad de Córdoba, Córdoba E-14071, Spain*

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

[3] *Departamento de Física and IUdEA, Universidad de La Laguna, 38200 Tenerife, Spain*

E-mail: rita@iff.csic.es

Supplementary material

Table S1. Kinetic, potential, total, rotational and translational average energies and corresponding errors (in meV) for the $He_N H_2^+$ clusters as obtained from the quantum DMC calculations.

N	E_{kin}	E_{pot}	E_{tot}	E_{rot}	E_{trans}
1	61.05 ± 0.001	-257.21 ± 0.001	-196.16 ± 0.0004	31.89 ± 0.0008	19.40 ± 0.0005
2	113.44 ± 0.001	-526.04 ± 0.001	-412.60 ± 0.0004	48.81 ± 0.0009	38.92 ± 0.0007
3	118.31 ± 0.004	-563.55 ± 0.003	-445.23 ± 0.003	55.35 ± 0.002	37.50 ± 0.002
4	119.02 ± 0.005	-597.37 ± 0.004	-478.35 ± 0.004	51.90 ± 0.002	37.03 ± 0.002
5	126.09 ± 0.005	-637.21 ± 0.004	-511.12 ± 0.005	50.76 ± 0.002	39.70 ± 0.002
6	136.91 ± 0.005	-679.31 ± 0.004	-542.40 ± 0.005	50.06 ± 0.003	43.13 ± 0.002
7	146.78 ± 0.004	-707.98 ± 0.003	-561.20 ± 0.003	48.75 ± 0.001	46.51 ± 0.002
8	146.43 ± 0.006	-716.04 ± 0.006	-569.61 ± 0.005	46.42 ± 0.003	43.34 ± 0.004
9	147.00 ± 0.01	-724.86 ± 0.01	-577.87 ± 0.01	44.71 ± 0.005	41.01 ± 0.008
10	150.83 ± 0.02	-736.17 ± 0.02	-585.34 ± 0.01	44.99 ± 0.005	43.81 ± 0.009
11	153.39 ± 0.02	-745.27 ± 0.02	-591.88 ± 0.01	45.39 ± 0.003	44.55 ± 0.008
12	155.50 ± 0.02	-753.20 ± 0.02	-597.69 ± 0.01	45.48 ± 0.005	44.83 ± 0.012
13	158.60 ± 0.02	-761.85 ± 0.01	-603.25 ± 0.01	45.43 ± 0.007	45.38 ± 0.014
14	161.56 ± 0.02	-770.59 ± 0.02	-609.03 ± 0.01	45.65 ± 0.008	45.85 ± 0.010
15	163.70 ± 0.02	-777.07 ± 0.02	-613.36 ± 0.01	46.05 ± 0.011	46.00 ± 0.010
16	165.42 ± 0.03	-783.43 ± 0.03	-618.02 ± 0.02	45.84 ± 0.023	46.18 ± 0.010
17	167.49 ± 0.05	-790.09 ± 0.04	-622.61 ± 0.04	45.23 ± 0.055	46.26 ± 0.013
18	169.36 ± 0.06	-795.49 ± 0.08	-626.13 ± 0.03	45.81 ± 0.030	45.87 ± 0.017
19	171.79 ± 0.07	-800.85 ± 0.10	-629.06 ± 0.04	46.20 ± 0.026	45.81 ± 0.030
20	172.86 ± 0.06	-804.58 ± 0.09	-631.72 ± 0.03	46.09 ± 0.022	45.38 ± 0.028
21	174.61 ± 0.05	-808.94 ± 0.07	-634.33 ± 0.03	46.14 ± 0.019	45.10 ± 0.025
22	175.99 ± 0.04	-812.96 ± 0.07	-636.97 ± 0.03	46.20 ± 0.016	44.91 ± 0.020
23	178.86 ± 0.05	-818.20 ± 0.07	-639.34 ± 0.03	46.30 ± 0.015	44.90 ± 0.020
24	179.51 ± 0.05	-821.49 ± 0.08	-641.97 ± 0.03	45.81 ± 0.015	44.61 ± 0.023
25	182.76 ± 0.05	-826.80 ± 0.08	-644.04 ± 0.04	45.79 ± 0.013	44.85 ± 0.021
26	184.04 ± 0.05	-830.17 ± 0.08	-646.13 ± 0.04	45.74 ± 0.012	44.52 ± 0.021
27	187.22 ± 0.04	-834.95 ± 0.07	-647.73 ± 0.04	45.83 ± 0.010	45.56 ± 0.020
28	188.06 ± 0.04	-837.71 ± 0.07	-649.65 ± 0.04	45.55 ± 0.009	44.91 ± 0.019
29	190.74 ± 0.04	-841.75 ± 0.07	-651.01 ± 0.03	45.95 ± 0.009	44.52 ± 0.019
30	193.39 ± 0.04	-845.84 ± 0.07	-652.45 ± 0.03	45.82 ± 0.008	45.02 ± 0.021

Table S2. Kinetic, potential, total, rotational and translational average energies and corresponding errors (in meV) for the $He_N D_2^+$ clusters as obtained from the quantum DMC calculations.

N	$E_{\rm kin}$	$E_{\rm pot}$	$E_{\rm tot}$	$E_{\rm rot}$	$E_{\rm trans}$
1	49.09 ± 0.001	-274.93 ± 0.001	-225.84 ± 0.0004	23.15 ± 0.0008	12.93 ± 0.0004
2	92.61 ± 0.002	-556.96 ± 0.002	-464.35 ± 0.0006	36.21 ± 0.001	25.62 ± 0.0006
3	98.43 ± 0.004	-595.43 ± 0.003	-497.00 ± 0.002	41.09 ± 0.002	25.59 ± 0.001
4	104.21 ± 0.006	-633.95 ± 0.003	-529.74 ± 0.004	40.15 ± 0.002	26.24 ± 0.001
5	112.811 ± 0.005	-675.17 ± 0.003	-562.36 ± 0.004	40.38 ± 0.003	29.12 ± 0.002
6	121.80 ± 0.005	-715.16 ± 0.004	-593.36 ± 0.003	38.80 ± 0.002	31.21 ± 0.002
7	131.29 ± 0.005	-743.65 ± 0.004	-612.36 ± 0.004	39.20 ± 0.002	32.15 ± 0.002
8	130.73 ± 0.007	-750.98 ± 0.005	-620.25 ± 0.005	36.56 ± 0.002	30.19 ± 0.003
9	131.86 ± 0.01	-759.71 ± 0.01	-627.85 ± 0.007	34.81 ± 0.003	29.39 ± 0.009
10	136.68 ± 0.01	-772.36 ± 0.01	-635.68 ± 0.01	35.49 ± 0.003	30.40 ± 0.007
11	138.44 ± 0.01	-780.90 ± 0.01	-642.46 ± 0.01	35.16 ± 0.003	30.66 ± 0.007
12	139.20 ± 0.01	-787.78 ± 0.01	-648.58 ± 0.01	34.73 ± 0.003	30.41 ± 0.007
13	142.91 ± 0.01	-797.58 ± 0.01	-654.66 ± 0.01	35.32 ± 0.004	31.27 ± 0.010
14	144.60 ± 0.01	-805.07 ± 0.02	-660.48 ± 0.01	35.12 ± 0.005	31.48 ± 0.006
15	146.10 ± 0.02	-811.07 ± 0.02	-664.97 ± 0.01	35.25 ± 0.007	31.60 ± 0.008
16	147.65 ± 0.02	-817.47 ± 0.02	-669.83 ± 0.02	34.50 ± 0.01	31.72 ± 0.007
17	149.07 ± 0.03	-823.40 ± 0.02	-674.33 ± 0.03	34.13 ± 0.03	31.71 ± 0.010
18	150.97 ± 0.04	-828.64 ± 0.06	-677.67 ± 0.03	34.80 ± 0.02	31.37 ± 0.011
19	154.11 ± 0.05	-834.99 ± 0.09	-680.87 ± 0.04	35.04 ± 0.02	31.52 ± 0.022
20	156.41 ± 0.04	-839.66 ± 0.06	-683.24 ± 0.03	35.19 ± 0.01	31.37 ± 0.016
21	158.90 ± 0.04	-844.63 ± 0.06	-685.73 ± 0.03	35.31 ± 0.01	31.40 ± 0.017
22	161.27 ± 0.04	-849.74 ± 0.06	-688.48 ± 0.03	35.26 ± 0.01	31.39 ± 0.018
23	163.57 ± 0.03	-854.50 ± 0.06	-690.93 ± 0.03	35.35 ± 0.008	31.39 ± 0.015
24	166.60 ± 0.05	-860.05 ± 0.08	-693.46 ± 0.04	35.64 ± 0.01	31.49 ± 0.017
25	168.18 ± 0.04	-863.75 ± 0.07	-695.58 ± 0.04	35.71 ± 0.008	31.38 ± 0.014
26	170.09 ± 0.04	-867.72 ± 0.07	-697.63 ± 0.04	35.93 ± 0.009	31.52 ± 0.014
27	173.28 ± 0.04	-872.98 ± 0.07	-699.70 ± 0.04	35.75 ± 0.007	31.49 ± 0.015
28	172.59 ± 0.03	-873.97 ± 0.06	-701.37 ± 0.03	35.73 ± 0.006	31.35 ± 0.014
29	177.54 ± 0.03	-880.29 ± 0.06	-702.75 ± 0.03	35.79 ± 0.005	31.42 ± 0.012
30	177.62 ± 0.03	-882.10 ± 0.06	-704.49 ± 0.03	35.51 ± 0.006	31.37 ± 0.013