Modelling interactions of cationic dimers in He droplets: microsolvation trends in $He_nK_2^+$ clusters

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Supplementary material

Table S1: Spectroscopic contants, r_e (in Å), ω_e (in cm^{-1}) and D_e (in cm^{-1}) for the K_2^+ at the indicated level of theory or experiment.

Methods/Basis set	r_e	ω_e	$\mathbf{D}_e$
UCCSD(T)/AV6Z	4.80	67.7	6591
MRCI+Q/AV6Z	4.80	66.3	6427
Theory [Ref. [77]]	4.55	72.4	6573
Theory [Ref. [78]]	4.39	73.2	6685
Theory [Ref. [79]]	4.47	73	6688
Expt.[Ref. [80]]	4.40	72.5	6444
Expt.[Ref. [81]]	4.40	73.4	6670
Expt.[Ref. [82]]	-	-	6669.9±0.5

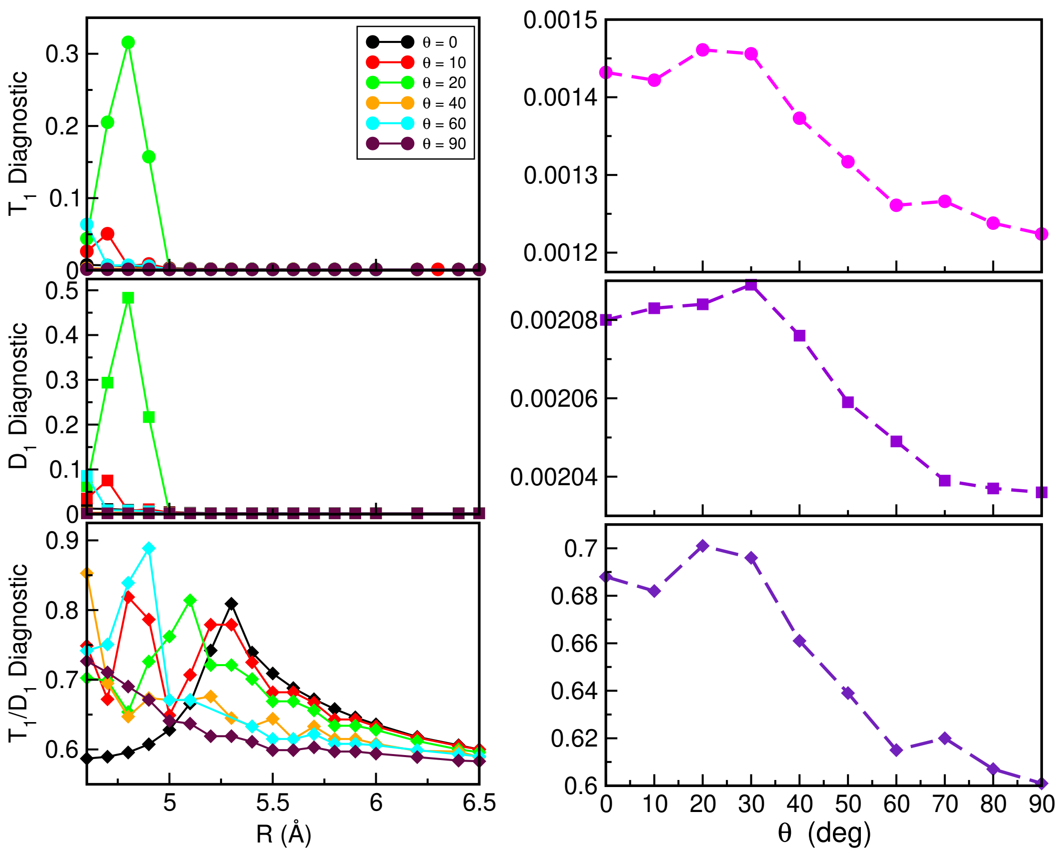

Fig. S1: CC diagnostics as a function of R at the indicated θ values (left panels), and as a function of θ at each $R_e(\theta)$ value (right panels) for the HeK_2^+.

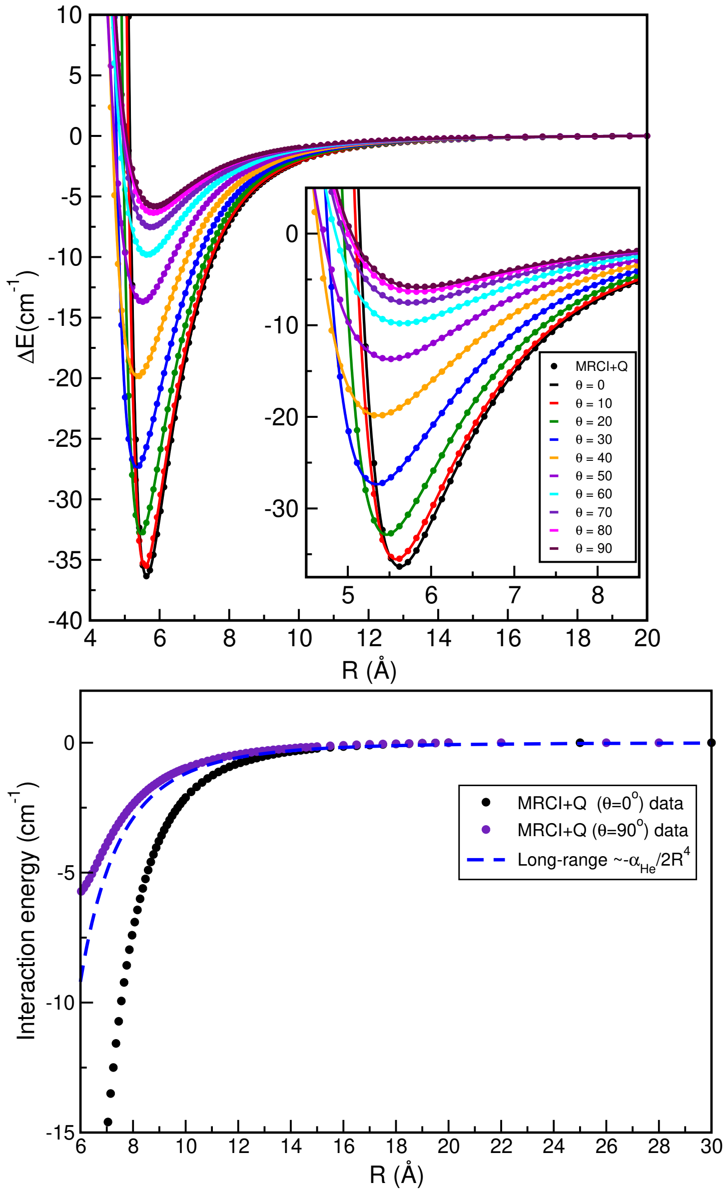

Fig. S2: (Left panel) MRCI+Q interaction energies and RKHS potential curves (left panel) as a function of R and θ coordinates for r_e=4.4 Å for the HeK_2^+. (Right panel) Comparison of the MRCI+Q interactions energies for the indicated θ values with the expected $\sim R^{-4}$ asymptotic behaviour at large values of R (see text).

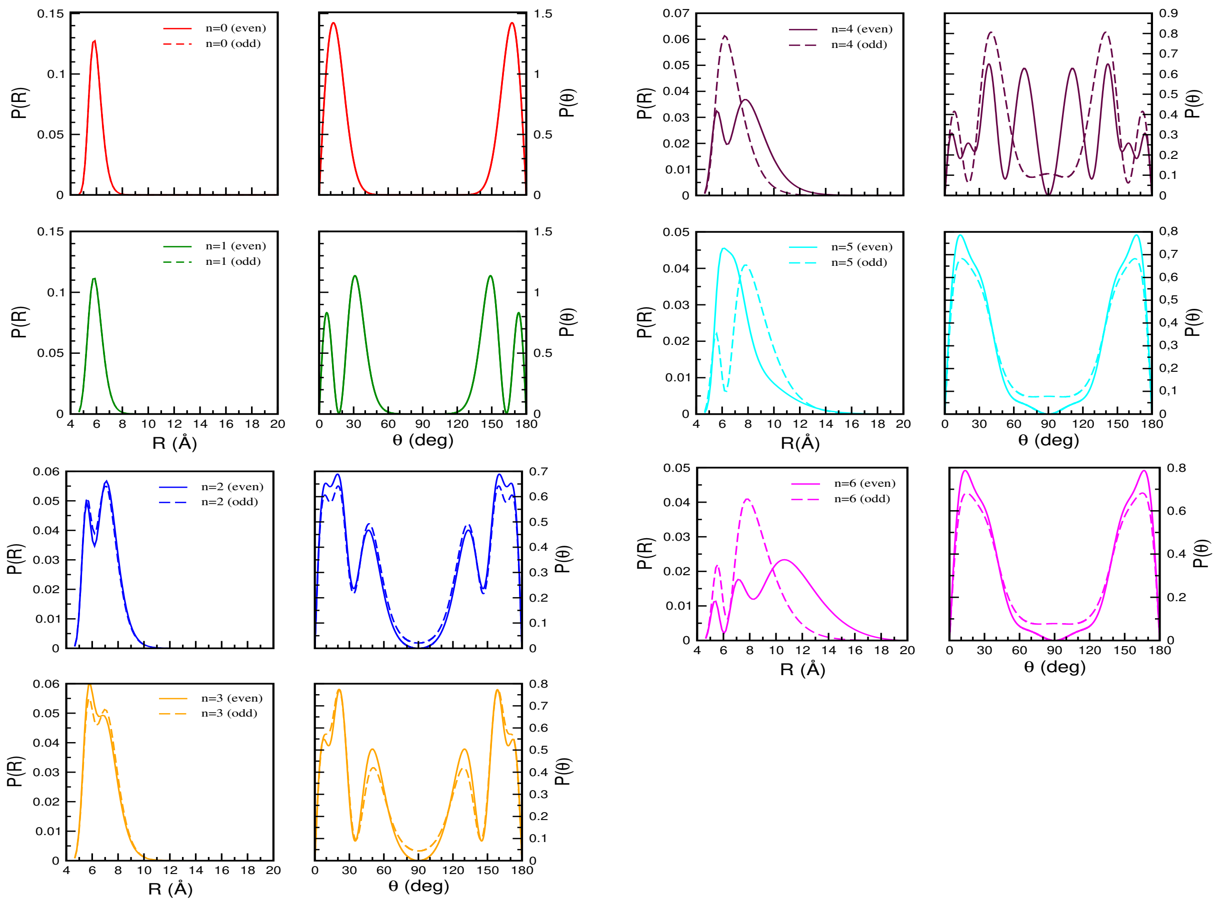

Fig. S3: Radial and angular distributions of all even/odd parity bound states of HeK_2^+ using the MRCI+Q/RKHS surface.

Table S2: Potential energies (in cm^{-1}) of the indicated optimal structures of the $He_nK_2^+$ clusters obtained from the present sum-of-potential approach (see Eq. 4), and comparison with previous theoretical data available[10,46].

N (He atoms)	$(T_1/T_2, L_1/L_2, B_1/B_2)$	**This Work**	**From ref.** [46]	**From ref.** [10]
1	(0/0, 1/0, 0/0)	-36.35	-37.6	-37.41
	(1/0, 0/0, 0/0)	-5.82	-3.8	-
2	(0/0, 0/0, 2/0)	-76.48	-73.9	-
	(0/0, 1/1, 0/0)	-72.69	-74.1	-75.01
	(0/0, 1/0, 1/0)	-71.04	-	-
	(0/0, 2/0, 0/0)	-49.04	-44.8	-
	(1/0, 1/0, 0/0)	-42.18	-41.3	-
	(1/1, 0/0, 0/0)	-11.64	-7.5	-
3	(0/0, 0/0, 3/0)	-123.90	-116.5	-119.40
	(0/0, 1/0, 0/2)	-112.83	-109.4	-
	(0/0, 1/0, 2/0)	-106.13	-82.7	-
	(0/0, 1/2, 0/0)	-85.39	-81.3	-
	(1/0, 1/1, 0/0)	-78.56	-77.8	-
4	(0/0, 0/0, 4/0)	-166.13	-146.4	-156.80
	(0/0, 0/0, 2/2)	-152.97	-143.9	-
	(0/0, 1/1, 2/0)	-142.50	-81.4	-
	(0/0, 2/0, 0/2)	-125.53	-88.5	-
	(0/0, 2/2, 0/0)	-98.08	-116.6	-
	(1/1, 1/1, 0/0)	-84.43	-119.9	-
5	(0/0, 0/0, 5/0)	-204.33	-156.6	-
	(0/0, 0/0, 3/2)	-200.40	-184.9	-
	(0/0, 1/0, 2/2)	-182.42	-154.1	-
	(1/0, 0/0, 2/2)	-158.95	-147.6	-
6	(0/0, 0/0, 0/6)	-251.40	-	-
	(0/0, 0/0, 3/3)	-247.71	-225.0	-
	(0/0, 1/1, 2/2)	-212.32	-164.6	-