Hyperradial calculations

24th March 2020

1 Neon Potential

n	E_{0n}^{BO}	E_{0n}^{adia}	E_{1n}^{BO}	E_{1n}^{adia}	E_{2n}^{BO}	E_{2n}^{adia}	E_{3n}^{BO}
0	-42.42	-38.47	-26.49	-14.25	-19.48		-14.86
1	-30.77	-23.43	-20.60	-12.79	-13.42		
2	-24.78	-16.01	-14.51				
3	-18.08	-12.96	-13.05				
4	-14.29	-12.44					
5	-13.49						

Table 1: Born–Oppenheimer energies E^{BO} and adiabatic energies E^{adia}. The effective three-body potential was calculated with $N_\theta = N_\phi = 40$ and $N_\rho = 215$. The ground state energy of the Ne dimer is $-11.99\,\mathrm{cm}^{-1}$ and is taken as referense value for a bound three-body state.

$\nu_{\max}$	$E_{00}^{\nu_{\max}}$	$E_{01}^{\nu_{\max}}$	$E_{02}^{\nu_{\max}}$	$E_{03}^{\nu_{\max}}$	$E_{04}^{\nu_{\max}}$	$E_{10}^{\nu_{\max}}$	$E_{11}^{\nu_{\max}}$	$E_{12}^{\nu_{\max}}$	$E_{20}^{\nu_{\max}}$	$E_{21}^{\nu_{\max}}$	$E_{30}^{\nu_{\max}}$
0	-38.47	-23.43	-16.01	-12.96	-12.44	...	...	...	...	...	...
1	-40.86	-24.46	-21.88	-20.56	-15.06	-13.32	-12.87	-12.80	...	...	...
2	-41.08	-25.29	-24.33	-22.92	-19.58	-14.74	-13.87	-13.04	-12.92	-12.32	...
3	-41.29	-26.02	-25.09	-23.72	-20.67	-16.25	-14.48	-14.09	-13.00	-12.85	-12.12

Table 2: Ground and excited state energies $E_{\nu n}^{\nu_{\max}}$ calculated with an increasing number of channels.

The Neon potential used was the one developed by Aziz and Chen 1977. Referera till deras artikel

$$V(r) = \epsilon V^*(x) \tag{1}$$

$$V^*(x) = A * \exp(-\alpha^* x + \beta^* x^2) - F(x)[c_6/x^6 + c_8/x^8 + c_{10}/x^{10}], \qquad (2)$$

where

$$F(x) = \begin{cases} \exp[-(D/x - 1)^2], & x < D \\ 1, & x \geq D \end{cases} \qquad (3)$$