

Supplement-Table 1: calculated total energy (in hartree, where -169.0 hartree should be added to the values given) for the lowest ten  $^2\Sigma^+$  states of  $\text{NaLi}^+$  at different values of the internuclear distance R (bohr).

Supplement-Table 2: calculated total energy (in hartree, where -169.0 hartree should be added to the values given) for the lowest six  $^2\Pi$  and two  $^2\Delta$  states of  $\text{NaLi}^+$  at different values of the internuclear distance R (bohr).

Supplement-Table 3: calculated total energy (in hartree, where -169.0 hartree should be added to the values given) for the lowest nine  $^1\Sigma^+$  states of  $\text{NaLi}$  at different values of the internuclear distance R (bohr).

Supplement-Table 4: calculated total energy (in hartree, where -169.0 hartree should be added to the values given) for the lowest eight  $^3\Sigma^+$  states of  $\text{NaLi}$  at different values of the internuclear distance R (bohr).

Supplement-Table 5: calculated total energy (in hartree, where -169.0 hartree should be added to the values given) for the lowest seven  $^1\Pi$  states of  $\text{NaLi}$  at different values of the internuclear distance R (bohr).

Supplement-Table 6: calculated total energy (in hartree, where -169.0 hartree should be added to the values given) for the lowest seven  $^3\Pi$  states of  $\text{NaLi}$  at different values of the internuclear distance R (bohr).

Supplement-Table 7: calculated total energy (in hartree, where -169.0 hartree should be added to the values given) for the lowest four  $^1\Delta$  and lowest four  $^3\Delta$  states of  $\text{NaLi}$  at different values of the internuclear distance R (bohr).

Supplementary Table 8. Comparison of the vibrational levels  $E_v$  ( $\text{cm}^{-1}$ ) for  $\text{B}^1\Pi$  ( $J=1$ ),  $\text{C}^1\Sigma^+$  ( $J=0$ ) and  $\text{D}^1\Pi$  ( $J=1$ ) of  $\text{Na}^7\text{Li}$ , with respect to the electronic minimum energy in each case calculated in the present work with previous theoretical and experimental data.