

For successfully carrying out R-matrix calculations, a good description of the excited states of the neutral molecule around the equilibrium is needed, obtained by an ab-initio method in a relatively small basis. It is also necessary to have potential curves of the neutral molecule and the anion that are consistent with the experimentally obtained values for the molecule and are used to set up the initial parameters of these calculations. In this work we are trying to find a description of the excited states and to obtain reference curves in order to perform R-matrix calculations for two molecules, BeH and OH. For BeH we propose a description of the excited states by the SA-CASSCF method with an active space of 6,2,2,0 and in the aug-cc-pVDZ basis. Similarly for OH a description by the SA-CASSCF method with an active space of 6,2,2,0 or 7,3,3,0 and an in an aug-cc-pVDZ basis should be used, where we have also found a setting of the weights of the states in the SA-CAS-SCF method significantly improving the shape of the curves. We have not yet been able to perform the R-matrix calculations because of insufficient time.