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Bulletin of the Korean Chemical Society

Volume 37, Issue 4

Article

# A Study of 15 Singlet Rydberg Series of HeH and Their Correlation with the Rydberg Series of Li

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First published: 14 March 2016

https://doi.org/10.1002/bkcs.10707

Cited by: 2

## Abstract


We theoretically study 37 Rydberg states of HeH derivable from the He(1*s* $^{2}$) + H(*nl*) configuration with *n* Ãƒ Â¢Ã‚Â‰Ã‚Â¤ 5 along with three states with*n* = 6. The multireference configuration interaction method is used to calculate their electronic energy curves (EECs) for the internuclear distance *R* from 0 to 28*a* $_{0}$, which are regarded as the unitedÃƒ Â¢Ã‚Â€Ã‚Â•atom (UA) and separatedÃƒ Â¢Ã‚Â€Ã‚Â•atoms (SA) limits, respectively. The 15 Rydberg series (*nsÃƒ Â•Ã‚Ã‚Â*,

*npÃƒÂ•Ã‚Âƒ*, *ndÃƒÂ•Ã‚Âƒ*, *nfÃƒÂ•Ã‚Âƒ*, *ngÃƒÂ•Ã‚Âƒ*, *ndÃƒÂŽÃ‚Â´*, *nfÃƒÂŽÃ‚Â´*, *ngÃƒÂŽÃ‚Â´*, *ngÃƒÂŽÃ‚Â³*, *npÃƒÂ•Ã‚Â€*, *ndÃƒÂ•Ã‚Â€*, *nfÃƒÂ•Ã‚Â€*, *ngÃƒÂ•Ã‚Â€*, *nfÃƒÂ•Ã‚Â•*, and *ngÃƒÂ•Ã‚Â•*) are identified. Bingel's perturbation theory is used to explain the role of the core part and the Rydberg orbitals in the behavior of EECs at small *R*. Smith's theory of diabatization is directly solved to obtain the diabatic quantum defect curves (QDCs). From the correlations in diabatic QDCs between the UA and SA limits, the following order of orbital energies in the equilibrium region is found: *npÃƒÂ•Ã‚Âƒ* < *nsÃƒÂ•Ã‚Âƒ* < *npÃƒÂ•Ã‚Â€* < *ndÃƒÂ•Ã‚Âƒ* < *ndÃƒÂ•Ã‚Â€* < *nfÃƒÂ•Ã‚Âƒ* < *nfÃƒÂ•Ã‚Â€* < *nfÃƒÂŽÃ‚Â´* < *nfÃƒÂ•Ã‚Â•* < *ndÃƒÂŽÃ‚Â´*, except 5*dÃƒÂŽÃ‚Â´* < 5*fÃƒÂ•Ã‚Â•*. This order is identical to that in oneÃƒÂ¢Ã‚Â€Ã‚Â•electron molecular systems at small *R*, except for the *nsÃƒÂ•Ã‚Âƒ* and *npÃƒÂ•Ã‚Â€* series. The correlation rules are $n_{UA} = n_{SA} + 1$ for the *npÃƒÂ•Ã‚Âƒ* series and $n_{UA} = n_{SA}$ for other series; additionally, $l_{UA} = l_{SA}$ for all cases except for the 2*pÃƒÂ•Ã‚Âƒ* ÃƒÂ¢Ã‚Â€Ã‚Â” *ÃƒÂ•Ã‚Âƒ*1*s* correlation. A reversal of the diabatic dipole moment at avoided crossing points of the *nsÃƒÂ•Ã‚Âƒ* and *npÃƒÂ•Ã‚Âƒ* series is observed, and explained by the behaviors of *ns* and *np* wavefunctions of H at small *R*.



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April 2016

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