Excited-states and spectroscopic properties of superoxide anion: a theoretical study including spin-orbit coupling

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Figure I. PECs of 9 $\Omega = 3/2$ states of O_2^- anion.

1- $X^2\Pi_{g,3/2}$, 2- $a^4\Sigma_{u,3/2}^-$, 3- $1^4\Sigma_{g,3/2}^+$, 4- $A^2\Pi_{u,3/2}$,

5- $1^4\Pi_{u,3/2}$, 6- $1^4\Sigma_{g,3/2}^-$, 7- $2^4\Sigma_{u,3/2}^-$, 8- $2^4\Pi_{g,3/2}$, 9- $2^4\Sigma_{g,3/2}^-$.

Figure II. PECs of 9 $\Omega = 3/2$ states of O_2^- anion.

1- $1^4\Delta_{g,3/2}$, 2- $1^2\Delta_{u,3/2}$, 3- $1^4\Sigma_{u,3/2}^+$, 4- $1^4\Pi_{g,3/2}$, 5- $1^2\Delta_{g,3/2}$,

6- $2^2\Pi_{g,3/2}$, 7- $2^2\Pi_{u,3/2}$, 8- $2^4\Pi_{u,3/2}$, 9- $1^4\Delta_{u,3/2}$.

Figure III. PECs of 8 $\Omega = 5/2$ states of O_2^- anion.

1- $1^4\Delta_{g,5/2}$, 2- $1^2\Delta_{u,5/2}$, 3- $1^4\Pi_{u,5/2}$, 4- $2^4\Pi_{u,5/2}$,

5- $1^4\Pi_{g,5/2}$, 6- $1^4\Delta_{u,5/2}$, 7- $1^2\Delta_{g,5/2}$, 8- $2^4\Pi_{g,5/2}$.

Figure IV. PECs of 4 $\Omega = -1/2$ and 2 $\Omega = 7/2$ states of O_2^- anion.

1- $1^4\Delta_{g,7/2}$, 2- $1^4\Pi_{u,-1/2}$, 3- $1^4\Pi_{g,-1/2}$,

4- $2^4\Pi_{u,-1/2}$, 5- $2^4\Pi_{g,-1/2}$, 6- $1^4\Delta_{u,7/2}$.

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