Analytical potential energy functions for CO^+ in its ground and excited electronic

Supplementary Material

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TABLE I: The coefficients of PES for CO^+. The parameter c_2 is dimensionless.

Parameters	Calc. [1]	State
c_2	0.706146	$X^2\Sigma^+$
c_2	0.437178	$A^2\Pi$
c_2	0.475807	$B^2\Sigma^+$
$\beta(a_0^{-1})$	0.441367	$X^2\Sigma^+$
$\beta(a_0^{-1})$	0.416943	$A^2\Pi$
$\beta(a_0^{-1})$	0.598974	$B^2\Sigma^+$
$R_e(a_0)$	2.107309	$X^2\Sigma^+$
$R_e(a_0)$	2.350384	$A^2\Pi$
$R_e(a_0)$	2.208653	$B^2\Sigma^+$
$D_e(E_h)$	0.307712	$X^2\Sigma^+$
$D_e(E_h)$	0.214731	$A^2\Pi$
$D_e(E_h)$	0.171737	$B^2\Sigma^+$

[1] G. Herzberg (1950). *Spectra of Diatomic Molecules 2nd ed.* (D. Van Nostrand Company, Princeton, New Jersey)