To appear in *Molecular Physics*
Vol. 00, No. 00, 21 August 2014, 1–9

RESEARCH ARTICLE

Stability, metastability and spectroscopic constants of electronic states of NH^- and CH^-

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(*August 2014*)

1. Supplementary materials

Table 1. Definition of spin orbit integrals for CH^- depicted in Figure 1 up to Figure 3.

i $\langle$ A'$^1\Delta$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ C$^3\Pi_x$;m$_s = 1\rangle$	=A'$^1\Delta$—C$^3\Pi$
i $\langle$ E'$^1\Sigma^-$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ C$^3\Pi_x$;m$_s = 1\rangle$	=E'$^1\Sigma^-$—C$^3\Pi$
i $\langle$ A'$^1\Delta$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ A$^3\Pi_x$;m$_s = 1\rangle$	=A'$^1\Delta$—A$^3\Pi$
i $\langle$ E'$^1\Sigma^-$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ A$^3\Pi_x$;m$_s = 1\rangle$	=E'$^1\Sigma^-$—A$^3\Pi$
i $\langle$ C'$^1\Pi_y$;m$_s = 0$ $\mid$ L$_z$S$_z$ $\mid$ C$^3\Pi_x$;m$_s = 1\rangle$	=C'$^1\Pi$—C$^3\Pi$
i $\langle$ C'$^1\Pi_y$;m$_s = 0$ $\mid$ L$_z$S$_z$ $\mid$ A$^3\Pi_x$;m$_s = 1\rangle$	=C'$^1\Pi$—A$^3\Pi$
i $\langle$ C'$^1\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ X$^3\Sigma^-$;m$_s = 1\rangle$	=C'$^1\Pi$—X$^3\Sigma^-$
i $\langle$ C'$^1\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ B$^3\Sigma^-$;m$_s = 1\rangle$	=C'$^1\Pi$—B$^3\Sigma^-$
i $\langle$ C'$^1\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ E$^3\Delta$;m$_s = 1\rangle$	=C'$^1\Pi$—E$^3\Delta$
i $\langle$ A$^3\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ X$^3\Sigma^-$;m$_s = 1\rangle$	=A$^3\Pi$—X$^3\Sigma^-$
i $\langle$ A$^3\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ B$^3\Sigma^-$;m$_s = 1\rangle$	=A$^3\Pi$—B$^3\Sigma^-$
i $\langle$ A$^3\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ E$^3\Delta$;m$_s = 1\rangle$	=A$^3\Pi$—E$^3\Delta$
i $\langle$ C$^3\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ X$^3\Sigma^-$;m$_s = 1\rangle$	=C$^3\Pi$—X$^3\Sigma^-$
i $\langle$ C$^3\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ B$^3\Sigma^-$;m$_s = 1\rangle$	=C$^3\Pi$—B$^3\Sigma^-$
i $\langle$ C$^3\Pi_x$;m$_s = 0$ $\mid$ L$_x$S$_x$ $\mid$ E$^3\Delta$;m$_s = 1\rangle$	=C$^3\Pi$—E$^3\Delta$
i $\langle$ A$^3\Pi_x$;m$_s = 1$ $\mid$ L$_x$S$_x$ $\mid$ $^5\Sigma^-$;m$_s = 2\rangle$	=A$^3\Pi$—$^5\Sigma^-$
i $\langle$ C$^3\Pi_x$;m$_s = 1$ $\mid$ L$_x$S$_x$ $\mid$ $^5\Sigma^-$;m$_s = 2\rangle$	=C$^3\Pi$—$^5\Sigma^-$
i $\langle$ C$^3\Pi_x$;m$_s = 1$ $\mid$ L$_z$S$_z$ $\mid$ C$^3\Pi_y$;m$_s = 1\rangle$	=C$^3\Pi$—C$^3\Pi$
i $\langle$ A$^3\Pi_x$;m$_s = 1$ $\mid$ L$_z$S$_z$ $\mid$ C$^3\Pi_y$;m$_s = 1\rangle$	=A$^3\Pi$—C$^3\Pi$
i $\langle$ A$^3\Pi_x$;m$_s = 1$ $\mid$ L$_z$S$_z$ $\mid$ A$^3\Pi_y$;m$_s = 1\rangle$	=A$^3\Pi$—A$^3\Pi$

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ISSN: 00268976 print/ISSN 13623028 online
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DOI: 10.1080/0026897YYxxxxxxxx
http://www.informaworld.com

Table 2. Definition of spin orbit integrals for NH^- depicted in Figure 4 up to Figure 7.

i $\langle$ $B^2\Delta$;$m_s = -0.5$ | L_xS_x | $X^2\Pi_y$;$m_s = 0.5\rangle$ =$B^2\Delta$—$X^2\Pi$
i $\langle$ $D^2\Sigma^+$;$m_s = -0.5$ | L_xS_x | $X^2\Pi_y$;$m_s = 0.5\rangle$ =$D^2\Sigma^+$—$X^2\Pi$
i $\langle$ $C^2\Sigma^+$;$m_s = -0.5$ | L_xS_x | $X^2\Pi_y$;$m_s = 0.5\rangle$ =$C^2\Sigma^+$—$X^2\Pi$
i $\langle$ $B^2\Delta$;$m_s = -0.5$ | L_xS_x | $E^2\Pi_y$;$m_s = 0.5\rangle$ =$B^2\Delta$—$E^2\Pi$
i $\langle$ $D^2\Sigma^+$;$m_s = -0.5$ | L_xS_x | $E^2\Pi_y$;$m_s = 0.5\rangle$ =$D^2\Sigma^+$—$E^2\Pi$
i $\langle$ $C^2\Sigma^+$;$m_s = -0.5$ | L_xS_x | $E^2\Pi_y$;$m_s = 0.5\rangle$ =$C^2\Sigma^+$—$E^2\Pi$
i $\langle$ $X^2\Pi_x$;$m_s = -0.5$ | L_xS_x | $A^2\Sigma^-$;$m_s = 0.5\rangle$ =$X^2\Pi$—$A^2\Sigma^-$
i $\langle$ $E^2\Pi_x$;$m_s = -0.5$ | L_xS_x | $A^2\Sigma^-$;$m_s = 0.5\rangle$ =$E^2\Pi$—$A^2\Sigma^-$
i $\langle$ $X^2\Pi_x$;$m_s = -0.5$ | L_xS_x | $B^2\Delta$;$m_s = 0.5\rangle$ =$X^2\Pi$—$B^2\Delta$
i $\langle$ $E^2\Pi_x$;$m_s = -0.5$ | L_xS_x | $B^2\Delta$;$m_s = 0.5\rangle$ =$E^2\Pi$—$B^2\Delta$
i $\langle$ $X^2\Pi_x$;$m_s = 0.5$ | L_zS_z | $X^2\Pi_y$;$m_s = 0.5\rangle$ =$X^2\Pi$—$X^2\Pi$
i $\langle$ $X^2\Pi_x$;$m_s = 0.5$ | L_zS_z | $E^2\Pi_y$;$m_s = 0.5\rangle$ =$X^2\Pi$—$E^2\Pi$
i $\langle$ $E^2\Pi_x$;$m_s = 0.5$ | L_zS_z | $E^2\Pi_y$;$m_s = 0.5\rangle$ =$E^2\Pi$—$E^2\Pi$
i $\langle$ $B^2\Delta$;$m_s = 0.5$ | L_zS_z | $A^2\Sigma^-$;$m_s = 0.5\rangle$ =$B^2\Delta$—$A^2\Sigma^-$
i $\langle$ $D^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $A^2\Sigma^-$;$m_s = 0.5\rangle$ =$D^2\Sigma^+$—$A^2\Sigma^-$
i $\langle$ $C^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $A^2\Sigma^-$;$m_s = 0.5\rangle$ =$C^2\Sigma^+$—$A^2\Sigma^-$
i $\langle$ $B^2\Delta$;$m_s = 0.5$ | L_zS_z | $B^2\Delta$;$m_s = 0.5\rangle$ =$B^2\Delta$—$B^2\Delta$
i $\langle$ $D^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $B^2\Delta$;$m_s = 0.5\rangle$ =$D^2\Sigma^+$—$B^2\Delta$
i $\langle$ $C^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $B^2\Delta$;$m_s = 0.5\rangle$ =$C^2\Sigma^+$—$B^2\Delta$
i $\langle$ $A^2\Sigma^-$;$m_s = 0.5$ | L_xS_x | $B'^4\Pi_x$;$m_s = 1.5\rangle$ =$A^2\Sigma^-$—$B'^4\Pi$
i $\langle$ $D^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $C'^4\Sigma^-$;$m_s = 0.5\rangle$ =$D^2\Sigma^+$—$C'^4\Sigma^-$
$\langle$ $D^2\Sigma^+$;$m_s = 0.5$ | L_yS_y | $B'^4\Pi_x$;$m_s = 1.5\rangle$ =$D^2\Sigma^+$—$B'^4\Pi$
$\langle$ $C^2\Sigma^+$;$m_s = 0.5$ | L_yS_y | $B'^4\Pi_x$;$m_s = 1.5\rangle$ =$C^2\Sigma^+$—$B'^4\Pi$
$\langle$ $B^2\Delta$;$m_s = 0.5$ | L_yS_y | $B'^4\Pi_x$;$m_s = 1.5\rangle$ =$B^2\Delta$—$B'^4\Pi$
i $\langle$ $X^2\Pi_y$;$m_s = 0.5$ | L_zS_z | $B'^4\Pi_x$;$m_s = 0.5\rangle$ =$X^2\Pi$—$B'^4\Pi$
i $\langle$ $E^2\Pi_y$;$m_s = 0.5$ | L_zS_z | $B'^4\Pi_x$;$m_s = 0.5\rangle$ =$E^2\Pi$—$B'^4\Pi$
i $\langle$ $X^2\Pi_x$;$m_s = 0.5$ | L_xS_x | $A'^4\Sigma^-$;$m_s = 1.5\rangle$ =$X^2\Pi$— $A'^4\Sigma^-$
i $\langle$ $E^2\Pi_x$;$m_s = 0.5$ | L_xS_x | $A'^4\Sigma^-$;$m_s = 1.5\rangle$ =$E^2\Pi$— $A'^4\Sigma^-$
i $\langle$ $X^2\Pi_x$;$m_s = 0.5$ | L_xS_x | $C'^4\Sigma^-$;$m_s = 1.5\rangle$ =$X^2\Pi$— $C'^4\Sigma^-$
i $\langle$ $E^2\Pi_x$;$m_s = 0.5$ | L_xS_x | $C'^4\Sigma^-$;$m_s = 1.5\rangle$ =$E^2\Pi$— $C'^4\Sigma^-$
i $\langle$ $B^2\Delta$;$m_s = 0.5$ | L_zS_z | $C'^4\Sigma^-$;$m_s = 0.5\rangle$ =$B^2\Delta$—$C'^4\Sigma^-$
i $\langle$ $B^2\Delta$;$m_s = 0.5$ | L_zS_z | $A'^4\Sigma^-$;$m_s = 0.5\rangle$ =$B^2\Delta$— $A'^4\Sigma^-$
i $\langle$ $D^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $A'^4\Sigma^-$;$m_s = 0.5\rangle$ =$D^2\Sigma^+$— $A'^4\Sigma^-$
i $\langle$ $C^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $A'^4\Sigma^-$;$m_s = 0.5\rangle$ =$C^2\Sigma^+$— $A'^4\Sigma^-$
i $\langle$ $B^2\Delta$;$m_s = 0.5$ | L_zS_z | $C'^4\Sigma^-$;$m_s = 0.5\rangle$ =$B^2\Delta$— $C'^4\Sigma^-$
i $\langle$ $D^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $C'^4\Sigma^-$;$m_s = 0.5\rangle$ =$D^2\Sigma^+$— $C'^4\Sigma^-$
i $\langle$ $C^2\Sigma^+$;$m_s = 0.5$ | L_zS_z | $C'^4\Sigma^-$;$m_s = 0.5\rangle$ =$C^2\Sigma^+$— $C'^4\Sigma^-$
i $\langle$ $B'^4\Pi_y$;$m_s = 0.5$ | L_xS_x | $A'^4\Sigma^-$;$m_s = 1.5\rangle$ =$B'^4\Pi$—$A'^4\Sigma^-$
i $\langle$ $B'^4\Pi_x$;$m_s = 0.5$ | L_xS_x | $C'^4\Sigma^-$;$m_s = 1.5\rangle$ =$B'^4\Pi$— $C'^4\Sigma^-$
i $\langle$ $B'^4\Pi_x$;$m_s = 1.5$ | L_zS_z | $B'^4\Pi_x$;$m_s = 1.5\rangle$ =$B'^4\Pi$— $B'^4\Pi$

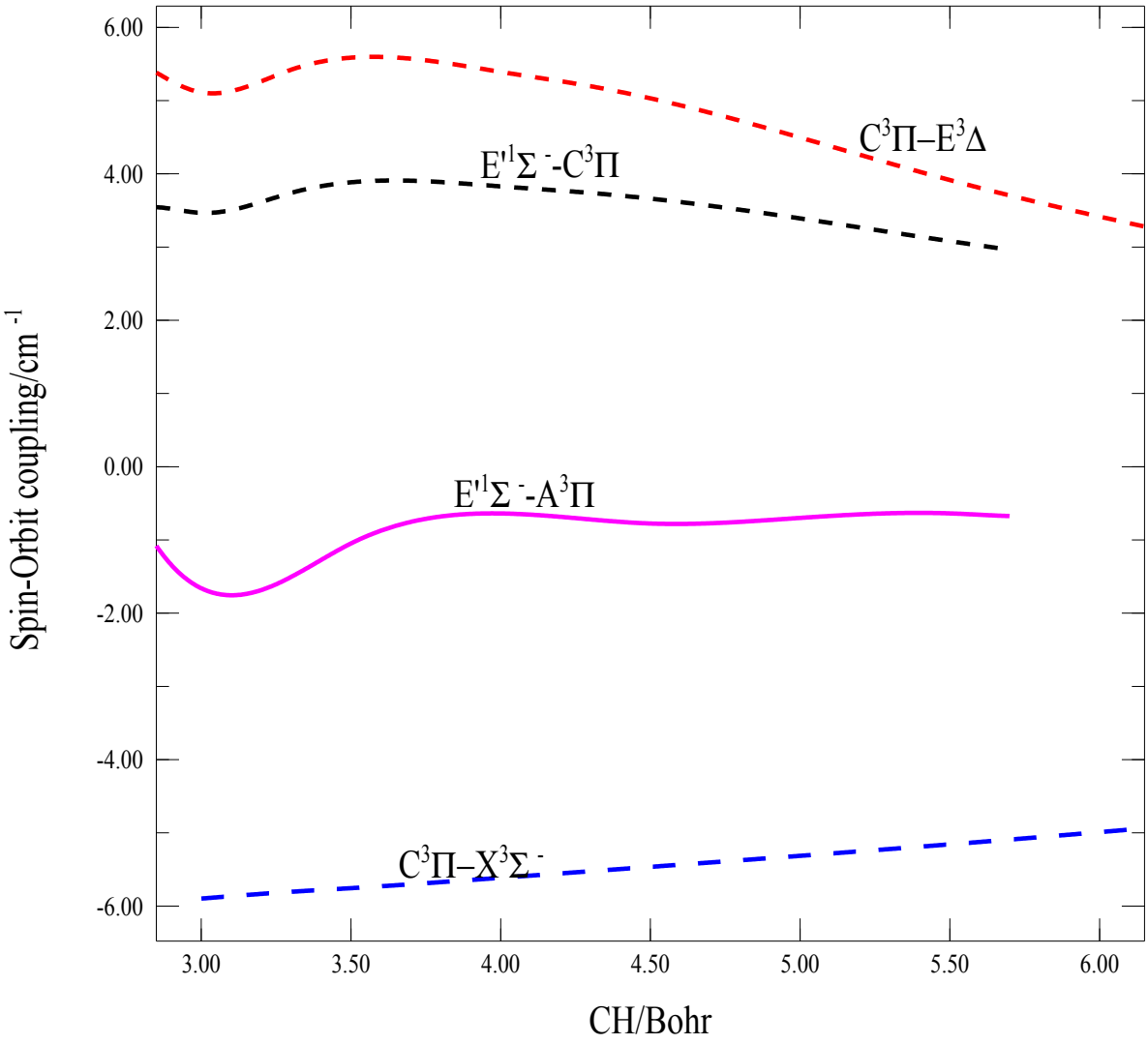

Figure 1. Evolution of the spin-orbit coupling (in cm^{-1}) along the C-H internuclear axis. The definitions are given in Table 1.

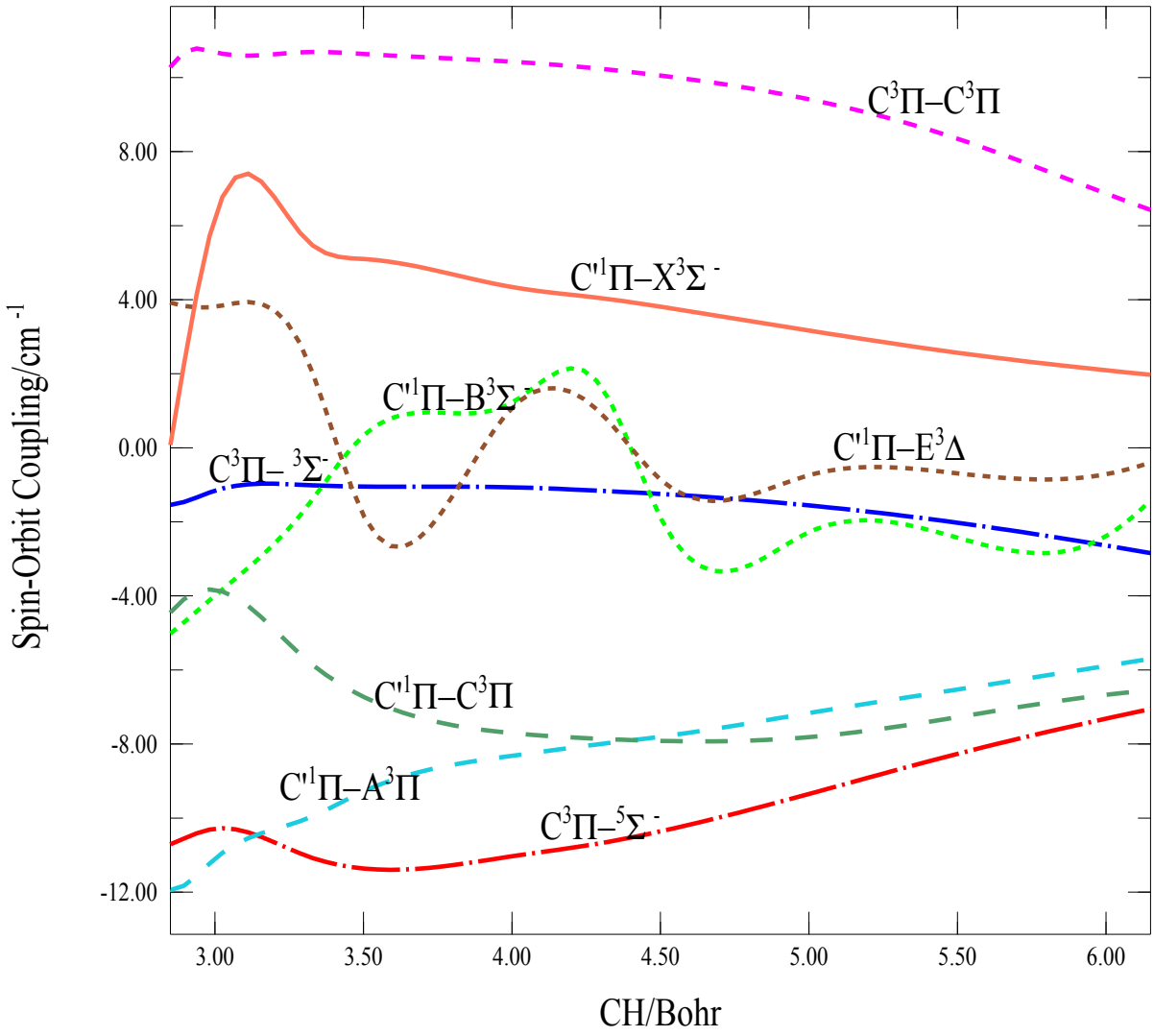

Figure 2. Evolution of the spin-orbit coupling (in cm^{-1}) along the C-H internuclear axis. The definitions are given in Table 1.

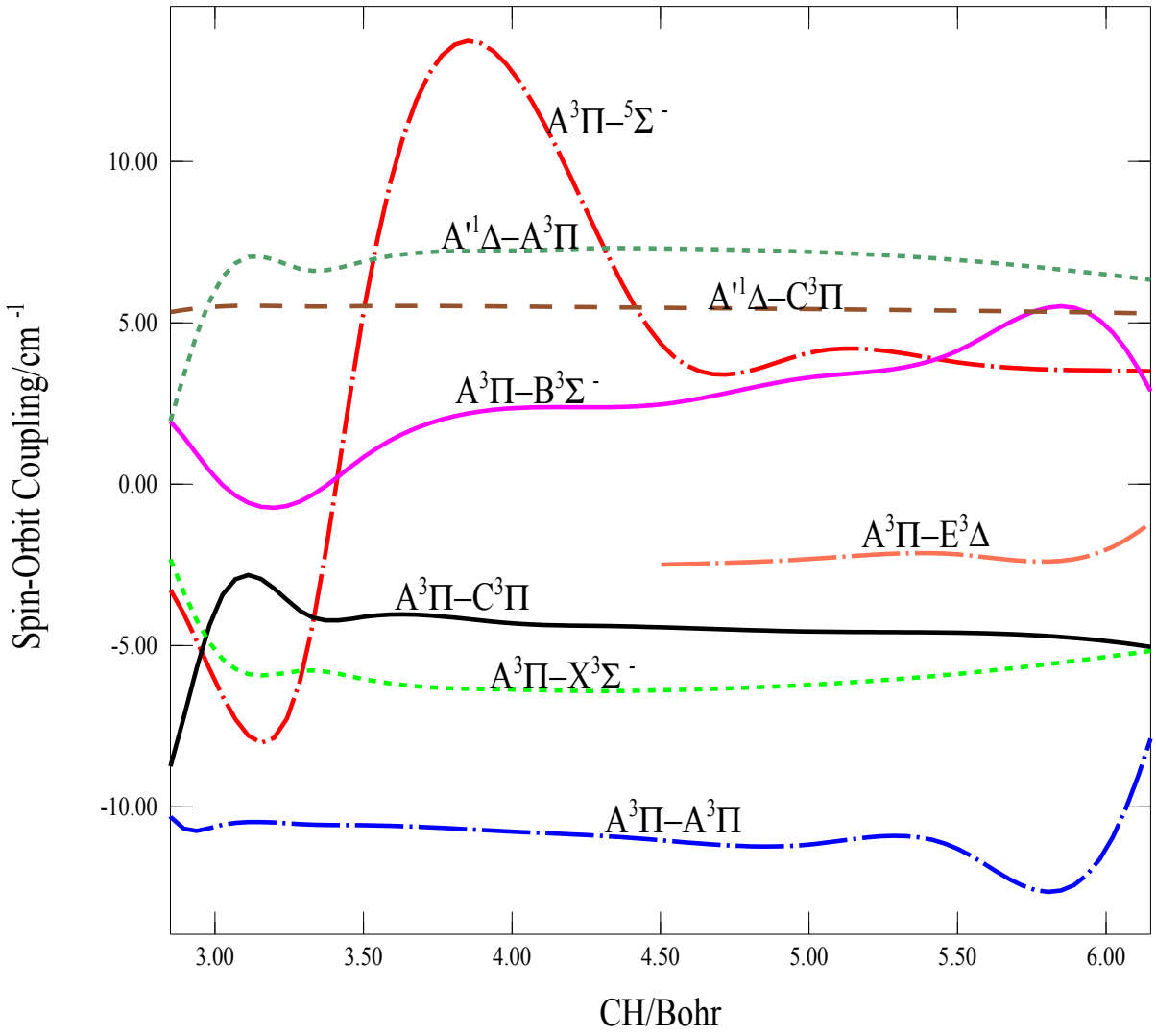

Figure 3. Evolution of the spin-orbit coupling (in cm^{-1}) along the C-H internuclear axis. The definitions are given in Table 1.

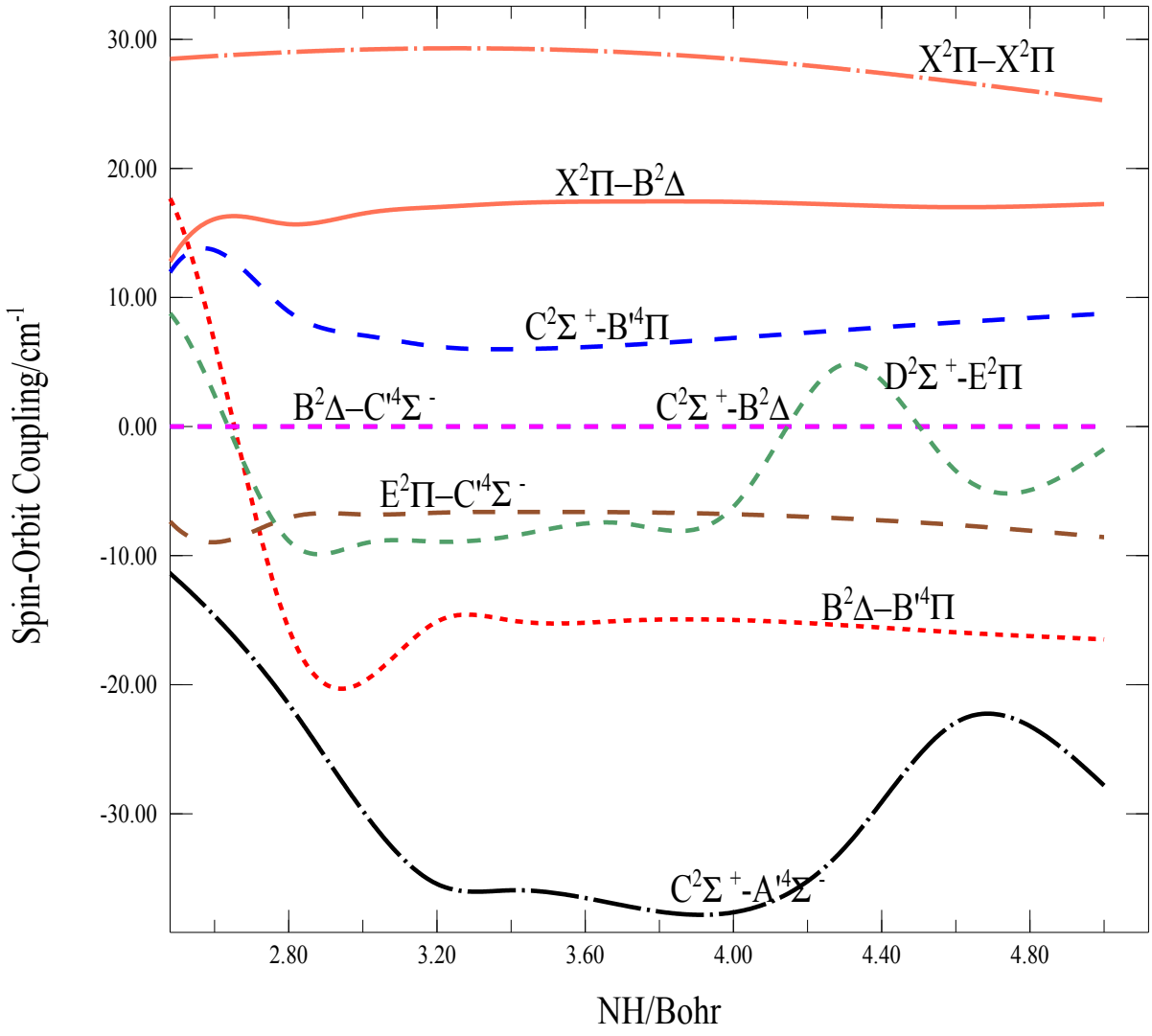

Figure 4. Evolution of the spin-orbit coupling (in cm^{-1}) along the N-H internuclear axis. The definitions are given in Table 2.

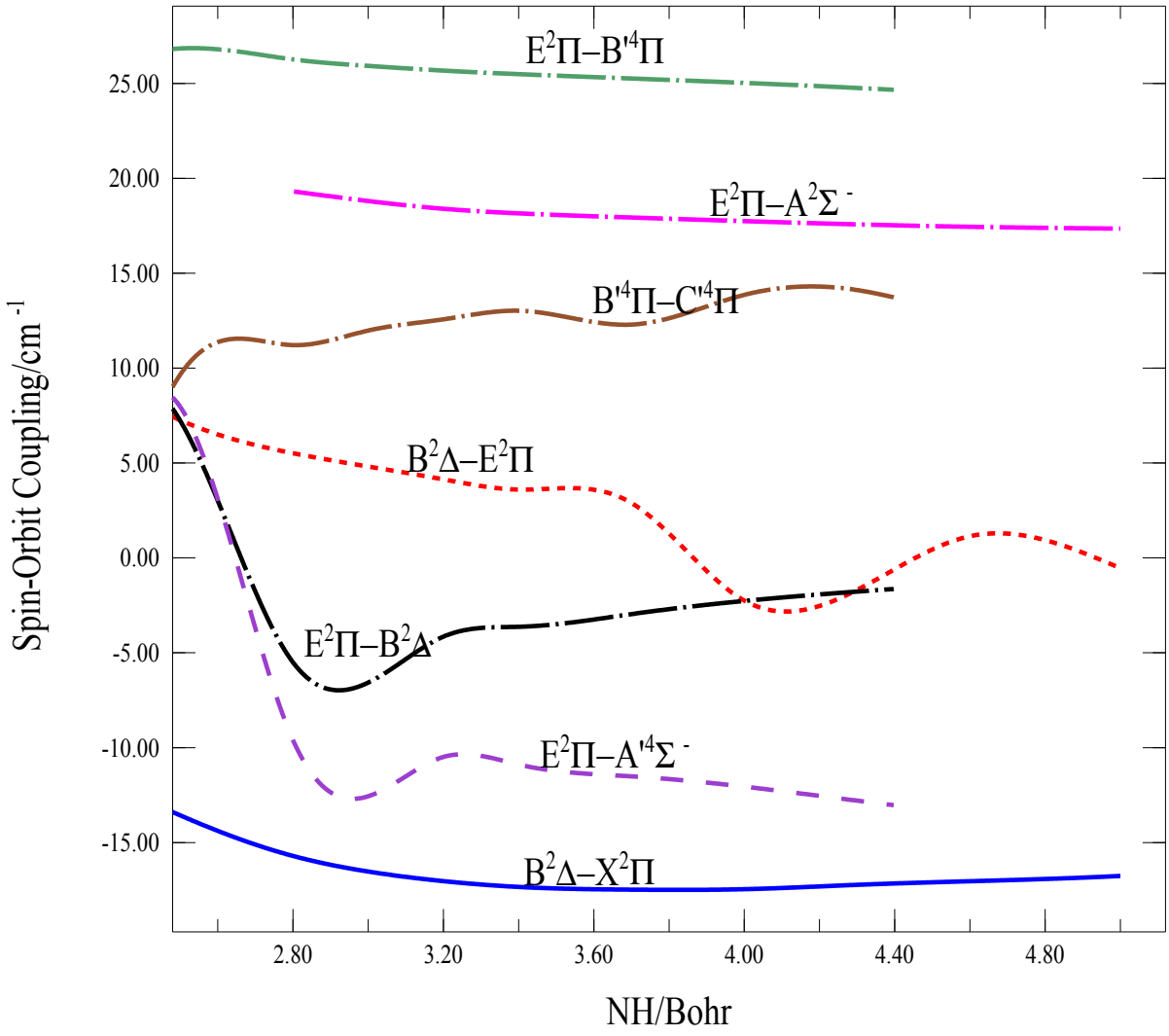

Figure 5. Evolution of the spin-orbit coupling (in cm^{-1}) along the N-H internuclear axis. The definitions are given in Table 2.

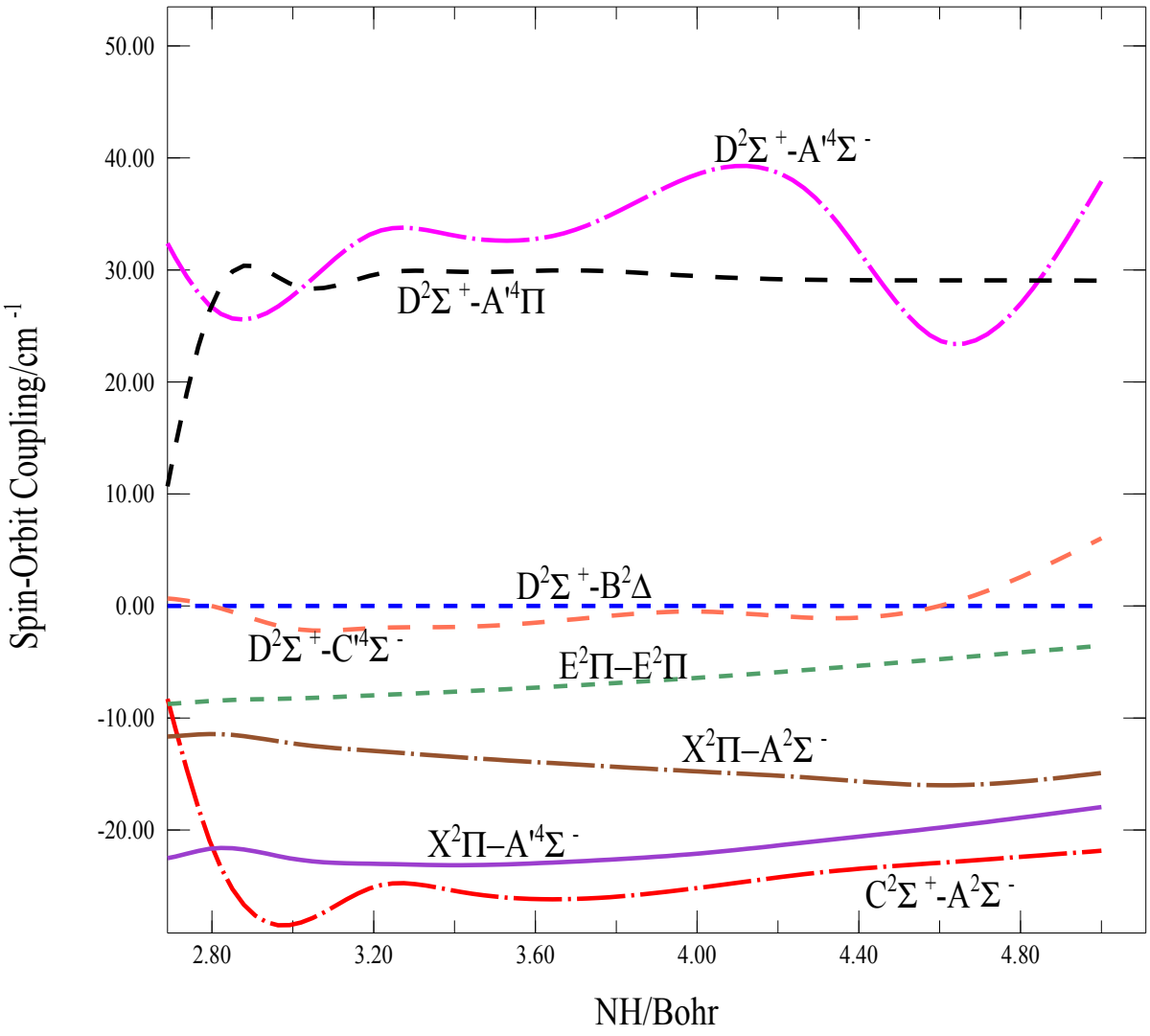

Figure 6. Evolution of the spin-orbit coupling (in cm^{-1}) along the N-H internuclear axis. The definitions are given in Table 2.

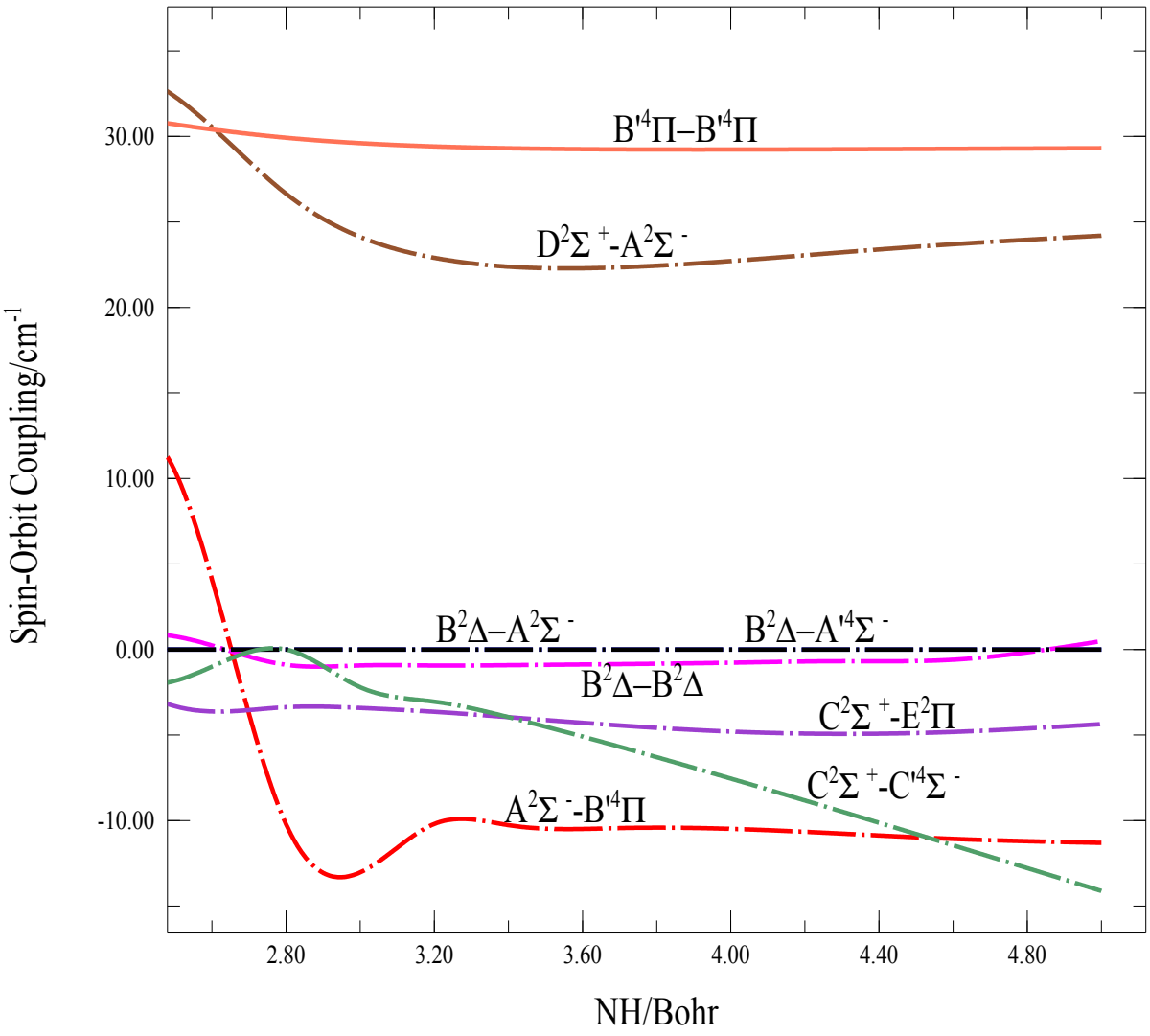

Figure 7. Evolution of the spin-orbit coupling (in cm^{-1}) along the N-H internuclear axis. The definitions are given in Table 2.