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## CV Appendix

Exhaustive list of publications in reverse chronological order

154. **J. Kłos**, M. H. Alexander, Q. Ma and P. Dagdigian
"The interaction of NO($X^2\Pi$) with $H_2$: Ab initio potential energy surfaces and bound states"
J. Chem. Phys. **146**, 114301 (2017)

153. B. Jiang, P. Kumar, **J. Kłos**, M. H. Alexander, B. Poirier and H. Guo
"First-principles C band absorption spectra of $SO_2$ and its isotopologues"
J. Chem. Phys. **146**, 154305 (2017)

152. P. Kumar, B. Jiang, H. Guo, **J. Kłos**, M. H. Alexander, and B. Poirier
"Photoabsorption Assignments for the $\tilde{C}^1B_2 \leftarrow \tilde{X}^1A_1$ Vibronic Transitions of $SO_2$, Using New Ab Initio Potential Energy and Transition Dipole Surfaces"
J. Phys. Chem. A **121** , 1012 (2017)

151. **J. Kłos**, M. Kim, YH. Wang and M. H. Alexander
"Chemical Control and Spectral Fingerprints of Electronic Coupling in Carbon Nanostructures"
J. Phys. Chem. C **120**, 29476 (2016)

150. **J. Kłos**, M. Hapka, G. Chałasiński, P. Halvick and T. Stoecklin
"Theoretical study of the buffer-gas cooling and trapping of CrH($X^6\Sigma^+$) by $^3$He atoms"
J. Chem. Phys. **145**, 214305 (2016)

149. P. Dagdigian, **J. Kłos**, M. Warehime and M. H. Alexander
"Accurate transport properties for O($^3$P)–H and O($^3$P)–$H_2$"
J. Chem. Phys. **145**, 164309 (2016)

148. V. Beutner, S. G. Zhang, H. Meyer and **J. Kłos**
"The near-IR spectrum of NO($\tilde{X}^2\Pi$)-He detected through excitation into the $\tilde{A}$-state continuum: A joint experimental and theoretical study"
J. Chem. Phys. **145**, 124318 (2016)

147. B. Joalland, N. Jamal-Eddine, **J. Kłos**, F. Lique, Y. Trolez, J.-C. Guillemin, S. Carles and L. Biennier
"Low-Temperature Reactivity of $C_{2n+1}N^-$ anions with Polar Molecules"
J. Phys. Chem. Lett. **7**, 2957 (2016)

146. C. Orek, **J. Kłos**, F. Lique, and N. Bulut
"*Ab initio* studies of the Rg-$NO^+$($X^1\Sigma^+$) van der Waals complexes (Rg = He, Ne, Ar, Kr, and Xe)"
J. Chem. Phys. **144**, 204303 (2016)

145. **J. Kłos**, M. H. Alexander, P. Kumar, B. Poirier, B. Jiang and H. Guo
"New ab initio adiabatic potential energy surfaces and bound state calculations for the singlet ground X and excited C states of $SO_2$"
J. Chem. Phys. **144**, 174301 (2016)

144. K. M. Hickson, J.-C. Loison, F. Lique, and **J. Kłos**
"An Experimental and Theoretical Investigation of the C($^1$D) + $N_2$ $\rightarrow$ C($^3$P) + $N_2$ Quenching Reaction at Low Temperature"
J. Phys. Chem. A **120**, 2504 (2016)

143. **J. Kłos**, S. G. Zhang and H. Meyer
"The near-IR spectrum of NO($\tilde{X}^2\Pi$)-Ne detected through excitation into the $\tilde{A}$-state continuum: A joint experimental and theoretical study"
J. Chem. Phys. **144**, 114307 (2016)

142. M. Warehime and **J. Kłos**
"Nonadiabatic collisions of CaH with Li: Importance of spin-orbit-induced spin relaxation in spin-polarized sympathetic cooling of CaH"
Phys. Rev. A **92**, 032703 (2015)

141. L. A. Garofalo, M. C. Smith, P. J. Dagdigian, **J. Kłos**, M. H. Alexander, K. A. Boering, and J. Jr-Min Lin
"Electronic quenching of O($^1D$) by Xe: Oscillations in the product angular distribution and their dependence on collision energy"
J. Chem. Phys. **143**, 054307 (2015)

140. P. J. Dagdigian, M. H. Alexander, and **J. Kłos**
"Theoretical investigation of the dynamics of O($^1D \rightarrow ^3P$) electronic quenching by collision with Xe"
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139. J. B. Kim, M. L. Weichman, T. F. Sjolander, D. M. Neumark, **J. Kłos**, M. H. Alexander, and D. E. Manolopoulos
"Spectroscopic observation of resonances in the F+$H_2$ reaction"
Science **349**, 510-513 (2015)

138. S. Marinakis, I. L. Dean, **J. Kłos** and F. Lique
"Collisional excitation of CH($X^2\Pi$) by He: new *ab initio* potential energy surfaces and scattering calculations"
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137. M. Hernández Vera, F. Lique, **J. Kłos**, F. Dumouchel, and J. Rubayo Soneira
"Cyanides/isocyanides abundances in the interstellar medium - IV. Temperature dependence of SiCN/SiNC rate coefficients and astrophysical applications."
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"Quantum mechanical calculations of state-to-state cross sections and rate constants for the F+DCl$\rightarrow$Cl+DF reaction"
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134. H. C. Schewe, Q. Ma, N. Vanhaecke, X. Wang, **J. Kłos**, M. H. Alexander, S. Y. T. van de Meerakker, G. Meijer, A. van der Avoird, and P. J. Dagdigian
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133. T. Perkins, D. Herráez-Aguilar, G. McCrudden, **J. Kłos**, F. J. Aoiz and M. Brouard
"Surface-hopping trajectories for OH($A^2\Sigma^+$) + Kr: Extension to the 1A" state"
J. Chem. Phys. **142**, 144307 (2015)

132. Olga V. Ershova, **J. Kłos**, Nicholas A. Besley, and Timothy G. Wright
"Interaction of the NO 3p$\pi$ (C $^2\Pi$) Rydberg state with RG (RG = Ne, Kr, and Xe): Potential energy surfaces and spec-

troscopy"
J. Chem. Phys. **142**, 034311 (2015)

131. Mick Warehime, **J. Kłos**, and Millard H. Alexander
"A finite-element visualization of quantum reactive scattering. II. Nonadiabaticity on coupled potential energy surfaces"
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130. M. Warehime, E. Johnson and **J. Kłos**
"New XDM-corrected potential energy surfaces for Ar-NO($X^2\Pi$): A comparison with CCSD(T) calculations and experiments"
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The Astrophysical Journal **794**, 33 (2014)

126. E. Karabulut, E. Aslan, **J. Kłos** and N. Bulut
"The effect of initial rotation in the N($^2$D) + $H_2 \rightarrow$ NH($^3\Sigma^-$) + H reaction"
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122. M. Hernández Vera, F. Lique, F. Dumouchel, **J. Kłos**, J. Rubayo Soneira, and M.-L. Senent
"Cyanide/isocyanide abundances in the interstellar medium - II. Inelastic rate coefficients of Al and Mg compounds"
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"Rotational Alignment of NO ($A^2\Sigma^+$) from Collisions with Ne"
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"Near-IR Spectrumn of NO($X^2\Pi$)-Xe: A Joint Experimental-Theoretical Investigation"
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"Collisional excitation of CN($X^2\Sigma^+$) by para- and ortho-$H_2$: Fine-structure resolved transitions"
J. Chem. Phys. **139**, 074301 (2013)

116. M. Hapka, G. Chałasiński, **J. Kłos** and Piotr S. Żuchowski
"First-principle interaction potentials for metastable He($^3S$) and Ne($^3P$) with closed-shell molecules: Application to Penning-ionizing systems"
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"A new potential energy surface for OH($A^2\Sigma^+$)-Kr: The van der Waals complex and inelastic scattering"
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"Properties of the $B^+$-$H_2$ and $B^+$-$D_2$ complexes: A theoretical and spectroscopic study"
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109. Y. Kalugina, F. Lique and **Jacek Kłos**
"Hyperfine collisional rate coefficients of CN with $H_2(j = 0)$"
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"New findings regarding the NO angular momentum orientation in Ar-NO($^2\Pi_{\frac{1}{2}}$) collisions"
Phys. Chem. Chem. Phys. **14**, 9826-9837 (2012)

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"Fine and hyperfine excitation of NH and ND by He: On the importance of calculating rate coefficients of isotopologues"
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"Cold collisions of polyatomic molecular radicals with S-state atoms in a magnetic field: An *ab initio* study of He + $CH_2$(X) collisions"
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"*Ab Initio* studies of the interaction potential for the Xe-NO($X^2\Pi$) van der Waals complex: Bound states and fully quantum and quasi-classical scattering"
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"Nonreactive scattering of the $O^+$+$H_2$: A time-dependent wave packet approach
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95. Svetlana Kotochigova, Alexander Petrov, Maria Linnik, **Jacek Kłos** and Paul Julienne
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93. F. Lique, **J. Kłos**,
"Hyperfine excitation of CN(X) by He"
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"Collisional angular momentum depolarization of OH(A) and NO(A) by Ar: A comparison of mechanisms"
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"Formation and dynamics of van der Waals molecules in buffer-gas traps"
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