

Complete Publication List of Pavel Soldán

Research papers in impacted journals

1. K. Huml, **P. Soldán**, and K. Zimmermann:
"Structure analysis of catechol-like molecular fragments",
Collect. Czech. Chem. Commun. **58**, 1242-1254 (1993).
2. **P. Soldán***:
"Symmetry in H_5^+ and D_5^+ complexes",
J. Mol. Spectrosc. **168**, 258-270 (1994).
3. **P. Soldán***:
"Symmetry analysis of molecules consisting of two coaxial rotors using the extended permutation-inversion groups",
J. Mol. Spectrosc. **180**, 249-265 (1996).
4. **P. Soldán** and B. I. Zhilinskii:
"Density of vibrational states of a given symmetry type for octahedral AB_6 molecules",
Chem. Phys. Lett. **258**, 25-29 (1996).
5. **P. Soldán***:
"Extended molecular symmetry groups",
J. Math. Chem. **20**, 331-349 (1996).
6. **P. Soldán**, V. Špirko, and W. P. Kraemer:
"Symmetry analysis of the vibrational dynamics of $H_3D_2^+$ and $H_2D_3^+$ complexes",
J. Mol. Spectrosc. **183**, 212-217 (1997).
7. V. Špirko, W. P. Kraemer, and **P. Soldán**:
"Vibrational dynamics of H_5^+ and its deuterated isotopomers",
J. Mol. Spectrosc. **183**, 218-223 (1997).
8. E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"Geometries and binding energies of $Rg.NO^+$ cationic complexes ($Rg = He, Ne, Ar, Kr,$
and Xe)",
J. Phys. Chem. A **102**, 6858-6864 (1998).
9. **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"Interaction energies of the $Na^+.Rg$ complexes ($Rg = He, Ne, and Ar$): basis set consid-
erations for Na^+ ",
J. Chem. Soc., Faraday Trans. **94**, 3307-3312 (1998).
10. **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"Spectroscopy and thermodynamics of $NaO^+(X^3\Sigma^-)$: relevance to atmospheric chem-
istry",
J. Phys. Chem. A **102**, 9040-9046 (1998).
11. E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"The heat of formation of $NaO^+(X^3\Sigma^-)$ and $NaO(X^2\Pi)$ ",
Chem. Phys. Lett. **295**, 354-358 (1998).
12. L. A. Jones, E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"PCCP",
Phys. Chem. Chem. Phys. **1**, 391-395 (1999).
13. V. Špirko, **P. Soldán***, and W. P. Kraemer:
"Adiabatic energies and perturbative non-adiabatic corrections for coulombic three-particle
systems in hyperspherical harmonics formalism",
J. Phys. B **32**, 429-441 (1999).

14. E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"The heat of formation of $\text{NaO}_2^+(\tilde{X}^3\Sigma^-)$ and $\text{NaO}_2(\tilde{X}^2A_2)$ ",
Chem. Phys. Lett. **301**, 317-324 (1999).
15. **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"Interatomic potentials for the $\text{Na}^+\cdot\text{Rg}$ complexes (Rg = He, Ne and Ar)",
Mol. Phys. **97**, 139-149 (1999).
16. V. Špirko, O. Engkvist, **P. Soldán**, H. L. Selzle, E. W. Schlag, and P. Hobza:
"Structure and dynamics of the benzene dimer",
J. Chem. Phys. **111**, 572-582 (1999).
17. **P. Soldán**, E. P. F. Lee, L. A. Jones, and T. G. Wright:
"Thermodynamics of $\text{NO}^+\cdot\text{N}_2$: atmospheric relevance",
J. Phys. Chem. A **103**, 5547-5550 (1999).
18. **P. Soldán**, V. Špirko, E. P. F. Lee, and T. G. Wright:
"Structure and potential energy surface for NaN_2^+ ",
J. Chem. Phys. **111**, 3420-3425 (1999).
19. **P. Soldán**, E. P. F. Lee, S. D. Gamblin, and T. G. Wright:
"Structure and stability of the $\text{Na}^+\cdot\text{CO}_2$ and $\text{Na}^+\cdot\text{H}_2\text{O}$ complexes",
Chem. Phys. Lett. **313**, 379-384 (1999).
20. **P. Soldán**, E. P. F. Lee, S. D. Gamblin, and T. G. Wright:
"Photoionization of $\text{NaO}(X^2\Pi;A^2\Sigma^+)$ and the absorption/emission spectra of the lowest cationic states",
Phys. Chem. Chem. Phys. **1**, 4947-4954 (1999).
21. **P. Soldán*** and J. M. Hutson:
"On the long-range and short-range behavior of potentials from reproducing kernel Hilbert space interpolation",
J. Chem. Phys. **112**, 4415-4416 (2000).
22. **P. Soldán**, E. P. F. Lee, S. D. Gamblin, and T. G. Wright:
" Na_2O and Na_2O^+ : Thermodynamics and low-lying electronic states",
J. Phys. Chem. A **104**, 3317-3325 (2000).
23. E. P. F. Lee, J. Lozeille, **P. Soldán**, and T. G. Wright:
"Calculations on the unstable $\text{CO}^-(X^2\Pi)$ anion",
Chem. Phys. Lett. **336**, 479-487 (2001).
24. M. H. Alexander, **P. Soldán**, T. G. Wright, Y. Kim, H. Meyer, P. J. Dagdigian, and E. P. F. Lee:
"The $\text{NO}(X^2\Pi)$ -Ne complex: II. Investigation of the lower bound states based on new potential energy surfaces",
J. Chem. Phys. **114**, 5588-5597 (2001).
25. **P. Soldán**, E. P. F. Lee, J. Lozeille, J. N. Murrell, and T. G. Wright:
"High-quality interatomic potential for $\text{Li}^+\cdot\text{He}$ ",
Chem. Phys. Lett. **343**, 429-436 (2001).
26. E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"Structure and binding energies of monohydrated Cd and Cd^{2+} ",
J. Phys. Chem. A **105**, 8510-8515 (2001).
27. **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"Static dipole polarizabilities (α) and static second hyperpolarizabilities (γ) of the rare gas atoms (He-Rn)",
Phys. Chem. Chem. Phys. **3**, 4661-4666 (2001).
28. E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"The heaviest group 2 difluoride, RaF_2 : Geometry and ionization energy",
Inorg. Chem. **40**, 4597-5984 (2001).

29. E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"High-level *ab initio* study of $\text{LiO}(X^2\Pi; A^2\Sigma^+)$ and $\text{LiO}^+(X^3\Sigma^-; A^3\Pi)$: the ionization energy of LiO ",
Chem. Phys. Lett. **347**, 481-486 (2001).
30. E. P. F. Lee, J. Lozeille, **P. Soldán**, S. E. Daire, J. M. Dyke, and T. G. Wright:
"*Ab initio* study of RbO , CsO and FrO ($X^2\Sigma^+; A^2\Pi$) and their cations ($X^3\Sigma^-; A^3\Pi$)",
Phys. Chem. Chem. Phys. **3**, 4863-4869 (2001).
31. **P. Soldán***, E. P. F. Lee, and T. G. Wright:
"The intermolecular potential energy surface of the $\text{He}\cdot\text{NO}^+$ cationic complex",
J. Chem. Phys. **116**, 2395-2399 (2002).
32. S. C. Collins, J. M. C. Plane, M. C. Kelley, T. G. Wright, **P. Soldán**, R. J. Rollason, T. J. Kane, A. J. Gerrard, B. W. Grime, J. S. Friedman, S. A. González, Q. Zhou, and M. P. Sulzer:
"A study of the role of ion-molecule chemistry in the formation of sporadic sodium layers",
J. Atmos. Solar-Terr. Phys. **64**, 845-860 (2002).
33. S. E. Daire, J. M. C. Plane, S. D. Gamblin, **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"A theoretical study of the thermodynamics and kinetics of ligand-exchange reactions of $\text{Na}^+\cdot\text{X}$ ($\text{X} = \text{O}, \text{O}_2, \text{N}_2, \text{CO}_2$ and H_2O): Implications for the upper atmosphere",
J. Atmos. Solar-Terr. Phys. **64**, 863-870 (2002).
34. J. Lozeille, E. Winata, **P. Soldán**, E. P. F. Lee, L. A. Viehland, and T. G. Wright:
"Spectroscopy of $\text{Li}^+\cdot\text{Rg}$ and Li^+-Rg transport coefficients ($\text{Rg}=\text{He-Rn}$)",
Phys. Chem. Chem. Phys. **4**, 3601-3610 (2002).
35. **P. Soldán** and J. M. Hutson:
"Near-dissociation states and coupled potential curves for the HeN^+ complex",
J. Chem. Phys. **117**, 3109-3119 (2002).
36. E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"What is the ground electronic state of KO^+ ",
J. Chem. Phys. **117**, 8241-8247 (2002).
37. **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"Microsolvation of Hg and Hg^{2+} : energetics of $\text{Hg}\cdot\text{H}_2\text{O}$, $\text{Hg}^{2+}\cdot\text{H}_2\text{O}$ and HgOH^+ ",
J. Phys. Chem. A **106**, 8619-8626 (2002).
38. **P. Soldán**, M. T. Cvitaš, J. M. Hutson, P. Honvault, and J.-M. Launay:
"Quantum dynamics of ultracold $\text{Na} + \text{Na}_2$ collisions",
Phys. Rev. Lett. **89**, 153201 (2002).
39. **P. Soldán***, M. T. Cvitaš, and J. M. Hutson:
"Three-body non-additive forces between spin-polarized alkali atoms",
Phys. Rev. A **67**, 054702 (2003).
40. L. A. Viehland, J. Lozeille, **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"Spectroscopy of $\text{Na}^+\cdot\text{Rg}$ and transport coefficients of Na^+ in Rg ($\text{Rg}=\text{He-Rn}$)",
J. Chem. Phys. **119**, 3729-3736 (2003).
41. L. A. Viehland, J. Lozeille, **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"Spectroscopy of $\text{K}^+\cdot\text{Rg}$ and transport coefficients of K^+ in Rg ($\text{Rg}=\text{He-Rn}$)",
J. Chem. Phys. **121**, 341-351 (2004).
42. H. L. Hickling, L. A. Viehland, D. T. Shepherd, **P. Soldán**, E. P. F. Lee, and T. G. Wright:
"Spectroscopy of $\text{M}^+\cdot\text{Rg}$ and transport coefficients of M^+ in Rg ($\text{M} = \text{Rb-Fr}$; $\text{Rg} = \text{He-Rn}$)",
Phys. Chem. Chem. Phys. **6**, 4233-4239 (2004).

43. **P. Soldán*** and J. M. Hutson:
"On the interaction of $\text{NH}(X^3\Sigma^-)$ molecules with rubidium atoms: implications for sympathetic cooling and the formation of extremely polar molecules",
Phys. Rev. Lett. **92**, 163202 (2004).
44. M. T. Cvitaš, **P. Soldán**, J. M. Hutson, P. Honvault, and J.-M. Launay:
"Ultracold $\text{Li} + \text{Li}_2$ collisions: bosonic and fermionic cases",
Phys. Rev. Lett. **94**, 033201 (2005).
45. G. Quéméner, P. Honvault, J.-M. Launay, **P. Soldán**, D. E. Potter, and J. M. Hutson:
"Ultracold quantum dynamics: spin-polarized $\text{K} + \text{K}_2$ collisions with three identical bosons or fermions",
Phys. Rev. A **71**, 032722 (2005).
46. M. T. Cvitaš, **P. Soldán**, J. M. Hutson, P. Honvault, and J.-M. Launay:
"Ultracold collisions involving heteronuclear alkali metal dimers",
Phys. Rev. Lett. **94**, 200402 (2005).
47. M. T. Cvitaš, **P. Soldán**, and J. M. Hutson:
"Long range intermolecular forces in triatomic systems:
connecting the atom-diatom and atom-atom-atom representations",
Mol. Phys. **104**, 23-31 (2006).
48. M. Lara, J. L. Bohn, D. E. Potter, **P. Soldán**, and J. M. Hutson:
"Ultracold Rb-OH collisions and prospects for sympathetic cooling",
Phys. Rev. Lett. **97**, 183201 (2006).
49. M. Lara, J. L. Bohn, D. E. Potter, **P. Soldán**, and J. M. Hutson:
"Cold collisions between OH and Rb : The field-free case",
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50. M. T. Cvitaš, **P. Soldán**, J. M. Hutson, P. Honvault, and J.-M. Launay:
"Interactions and dynamics in $\text{Li} + \text{Li}_2$ ultracold collisions",
J. Chem. Phys. **127**, 074302 (2007).
51. **P. Soldán** and V. Špirko:
"Tuning *ab initio* data to scattering length: the $a^3\Sigma^+$ state of KRb ",
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52. O. Bludský, M. Rubeš, and **P. Soldán***:
"*Ab initio* investigation of intermolecular interactions in solid benzene",
Phys. Rev. B **77**, 092103 (2008).
53. P. Nachtigall, M. Rubeš, **P. Soldán**, and O. Bludský:
"Investigation of the benzene-dimer potential energy surface: DFT/CCSD(T) correction scheme",
J. Chem. Phys. **128**, 114102 (2008).
54. **P. Soldán***:
"Lowest quartet states of Li_2A ($\text{A}=\text{Na}, \text{K}, \text{Rb}, \text{Cs}$)",
Phys. Rev. A **77**, 054501 (2008).
55. A. W. Hauser, C. Callegari, **P. Soldán**, and W. E. Ernst:
"On the doublet states of the potassium trimer",
J. Chem. Phys. **129**, 044307 (2008).
56. A. Simoni, J.-M. Launay, and **P. Soldán**:
"Feshbach resonances in ultracold atom-molecule collisions",
Phys. Rev. A **79**, 032701 (2009).
57. **P. Soldán***, P. S. Żuchowski, and J. M. Hutson:
"Prospects for sympathetic cooling of polar molecules: NH with alkali-metal and alkaline-earth atoms – a new hope",
Faraday Discussions **142**, 191-201 (2009).

58. R. Guérout, **P. Soldán**, M. Aymar, J. Deiglmayr, and O. Dulieu:
“Core Repulsion Effects in Alkali Trimers”,
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59. **P. Soldán***:
“Potential energy surface for spin-polarized rubidium trimer”,
J. Chem. Phys. **132**, 234308 (2010).
60. **P. Soldán***:
“Lowest quartet states of heteronuclear alkali-metal trimers”,
Phys. Rev. A **82**, 034701 (2010).
61. A. W. Hauser, C. Callegari, **P. Soldán**, and W. E. Ernst:
“A Jahn-Teller analysis of K_3 and Rb_3 in the electronic states $1^2E'$ and $1^2E'''$ ”,
Chem. Phys. **375**, 73-84 (2010).
62. **P. Soldán***, and W. P. Kraemer:
“Molecular ion $LiHe^+$: *ab initio* study”,
Chem. Phys. **393**, 135-139 (2012).
63. L. Augustovičová and **P. Soldán***:
“*Ab initio* properties of $MgAlk$ ($Alk = Li, Na, K, Rb, Cs$)”,
J. Chem. Phys. **136**, 084311 (2012).
64. L. Augustovičová, V. Špirko, W. P. Kraemer, and **P. Soldán***:
“Radiative association of $LiHe^+$ ”,
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65. P. S. Żuchowski, M. Kosicki, M. Kodrycka, and **P. Soldán***:
“van der Waals coefficients for systems with ultracold polar alkali-metal molecules”,
Phys. Rev. A **87**, 022706 (2013).
66. L. Augustovičová, V. Špirko, W. P. Kraemer, and **P. Soldán***:
“Radiative association of He_2^+ revisited”,
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67. L. Augustovičová, V. Špirko, W. P. Kraemer, and **P. Soldán***:
“Radiative association of He_2^+ : the role of quartet states”,
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68. L. Augustovičová, W. P. Kraemer, and **P. Soldán***:
“Depopulation of metastable helium by radiative association with hydrogen and lithium ions”,
Astrophys. J. **782**, 46 (2014).
69. L. Augustovičová, **P. Soldán***, W. P. Kraemer, and V. Špirko:
“Potential microwave probes of the proton-to-electron mass ratio at very high redshifts”,
Mon. Not. R. Astron. Soc. **439**, 1136-1139 (2014).
70. A. K. Belyaev, L. Augustovičová, **P. Soldán**, and W. P. Kraemer:
“Non-radiative inelastic processes in lithium-helium ion-atom collisions”,
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71. L. Augustovičová, W. P. Kraemer, and **P. Soldán***:
“Depopulation of metastable helium $He(2^1S)$ by radiative association with hydrogen and lithium ions”,
J. Quant. Spectros. Radiat. Transfer **148**, 27 (2014).
72. M. Urbanek and **P. Soldán***:
“Matter-wave revival of binary mixtures in optical lattices”,
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73. L. Augustovičová, W. P. Kraemer, and **P. Soldán***:
“The role of molecular quadrupole transitions in the depopulation of metastable helium”,
Mon. Not. R. Astron. Soc. **446**, 2738-2743 (2015).
74. A. K. Belyaev, D. S. Rodionov, L. Augustovičová, **P. Soldán**, and W. P. Kraemer:
“Full quantum study of non-radiative inelastic processes in lithium-helium ion-atom collisions”,
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75. L. Augustovičová, M. Zámečnicková, W. P. Kraemer, and **P. Soldán***:
“Radiative association of He(2^3P) with lithium cations”,
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76. M. Urbanek and **P. Soldán***:
“Parallel implementation of the time-evolving block decimation algorithm for the Bose–Hubbard model”,
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77. L. Augustovičová, **P. Soldán**, and V. Špirko:
“Effective hyperfine-structure functions of ammonia”,
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78. M. Zámečnicková, W. P. Kraemer, and **P. Soldán***:
“Radiative association of He(2^3P) with lithium cations: $\Pi \rightarrow \Sigma$ processes”,
J. Quant. Spectros. Radiat. Transfer **191**, 88-95 (2017).
79. M. Zámečnicková and **P. Soldán***:
“Radiative decay of HeLi⁺($b^3\Sigma^+$)”,
Chem. Phys. **500**, 1-6 (2018).
80. M. Urbanek and **P. Soldán***:
“Equilibration in two-dimensional Bose systems with disorders”,
Eur. Phys. J. D **72**, 114 (2018).
81. M. Zámečnicková, W. P. Kraemer, and **P. Soldán***:
“Radiative charge transfer between metastable helium and lithium cations”,
Astrophys. J. **867**, 157 (2018).
82. M. Zámečnicková, **P. Soldán**, M. Gustafsson, and G. Nyman:
“Formation of CO⁺ by radiative association”,
Mon. Not. R. Astron. Soc. **489**, 2954-2960 (2019).
83. M. Zámečnicková, M. Gustafsson, G. Nyman, and **P. Soldán***:
“Formation of CO⁺ by radiative association II”,
Mon. Not. R. Astron. Soc. **492**, 3794–3802 (2020).
84. M. Šimsová-Zámečnicková, **P. Soldán**, and M. Gustafsson:
“Formation of NaCl by radiative association in interstellar environments”,
Astron. and Astrophys. **664**, A5 (2022).
85. M. Šimsová née Zámečnicková, M. Gustafsson, and **P. Soldán***:
“Non-adiabatic dynamics in collisions of sodium and chlorine atoms and their ions”,
Phys. Chem. Chem. Phys. **24**, 25250–25257 (2022).

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Review articles in impacted journals

1. K. Huml and **P. Soldán**:
"Symetrie molekul a analýza informací ze strukturních datových bank",
Chem. Listy **89**, 547-555 (1995). (in Czech)
2. J. M. Hutson and **P. Soldán**:
"Molecule formation in ultracold atomic gases",
Int. Rev. Phys. Chem. **25**, 457-526 (2006).
3. J. M. Hutson and **P. Soldán**:
"Molecular collisions in ultracold atomic gases",
Int. Rev. Phys. Chem. **26**, 1-28 (2007).

Other research papers

1. M. Rubeš, **P. Soldán**, P. Nachtigall, and O. Bludský:
“A computationally feasible DFT/CCSD(T) correction scheme for the description of weakly interacting systems”,
Open Chem. Phys. J. **1**, 1-11 (2008).
2. M. Zámečníková, L. Augustovičová, W. P. Kraemer, and **P. Soldán**:
“Formation of molecular ion LiHe⁺ by radiative association of metastable helium He(2³P) with lithium ions”,
J. Phys. Conf. Ser. **635**, 022038 (2015).

Other reviews

1. **P. Soldán**:
“Extended molecular symmetry groups: symmetry analysis of molecules consisting of two coaxial rotors”,
in *Advanced Series in Physical Chemistry IX: Vibration-Rotational Spectroscopy and Molecular Dynamics*,
ed. D. Papoušek, World Scientific Publishing Company, 1997, pp. 461-515.
2. P. Honvault, J.-M. Launay, **P. Soldán**, M. T. Cvitaš, and J. M. Hutson:
“Quantum dynamics of ultracold alkali + alkali dimer collisions”,
in *Interactions of Cold Atoms and Molecules*,
eds. P. Soldán, M. T. Cvitaš, J. M. Hutson, and C. S. Adams, CCP6, 2002, pp. 60-65.
3. **P. Soldán**:
“Boseho-Einsteinova kondenzace: od atomů k molekulám”,
Čs. čas. pro fyz. **58**, 4 (2008). (in Czech)

Books edited

1. S. C. Althorpe, **P. Soldán**, and G. G. Balint-Kurti (editors):
Time-Dependent Quantum Dynamics,
published by CCP6, Daresbury (2001). ISBN 0-9522736-7-5
2. **P. Soldán**, M. T. Cvitaš, J. M. Hutson, and C. S. Adams (editors):
Interactions of Cold Atoms and Molecules,
published by CCP6, Daresbury (2002). ISBN 0-9522736-9-1