

Complete Publication List of Pavel Soldán

Research papers

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 $Rg\text{NO}^+$ cationic complexes ($Rg = \text{He}, \text{Ne}, \text{Ar}, \text{Kr}$, 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 ($Rg = \text{He}, \text{Ne}$, and Ar): basis set considerations 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 $\text{NaO}^+(X^3\Sigma^-)$: relevance to atmospheric chemistry",
J. Phys. Chem. A **102**, 9040-9046 (1998).
11. E. P. F. Lee, **P. Soldán**, and T. G. Wright:
"The heat of formation of $\text{NaO}^+(X^3\Sigma^-)$ and $\text{NaO}(X^2\Pi)$ ",
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 $\text{NaO}_2^+(X^3\Sigma^-)$ 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 ($\text{Rg} = \text{He}, \text{Ne}$ 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. Dagdigan, and E. P. F. Lee:
"The $\text{NO}(X^2\Pi)\text{-Ne}$ 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+} ",
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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, RaF₂: 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 LiO(X²Π;A²Σ⁺) and LiO⁺(X³Σ⁻;A³Π): 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 (X²Σ⁺; A²Π) and their cations (X³Σ⁻; A³Π)",
Phys. Chem. Chem. Phys. **3**, 4863-4869 (2001).
31. **P. Soldán**, E. P. F. Lee, and T. G. Wright:
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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",
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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 Na⁺·X (X = O, O₂, N₂, CO₂ and H₂O): 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 Li⁺·Rg and Li⁺·Rg transport coefficients (Rg=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 Hg²⁺: energetics of Hg·H₂O, Hg²⁺·H₂O 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 Na + Na₂ 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 Na⁺·Rg and transport coefficients of Na⁺ in Rg (Rg=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 K⁺-Rg and transport coefficients of K⁺ in Rg (Rg=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 M⁺-Rg and transport coefficients of M⁺ in Rg (M=Rb-Fr; Rg=He-Rn)",
Phys. Chem. Chem. Phys. **6**, 4233-4239 (2004).
43. **P. Soldán** and J. M. Hutson:
"On the interaction of NH(X^{3Σ-}) 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 Li + Li₂ collisions: bosonic and fermionic cases",
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45. G. Quéméner, P. Honvault, J.-M. Launay, **P. Soldán**, D. E. Potter, and J. M. Hutson:
"Ultracold quantum dynamics: spin-polarized K + K₂ collisions with three identical bosons or fermions",
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46. M. T. Cvitaš, **P. Soldán**, J. M. Hutson, P. Honvault, and J.-M. Launay:
"Ultracold collisions involving heteronuclear alkali metal dimers",
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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",
Phys. Rev. A **75**, 012704 (2007).
50. M. T. Cvitaš, **P. Soldán**, J. M. Hutson, P. Honvault, and J.-M. Launay:
"Interactions and dynamics in Li + Li₂ ultracold collisions",
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51. **P. Soldán** and V. Špirko:
"Tuning *ab initio* data to scattering length: the a^{3Σ+} state of KRb",
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52. M. Rubeš, **P. Soldán**, P. Nachtigall, and O. Bludský:
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53. O. Bludský, M. Rubeš, and **P. Soldán**:
"*Ab initio* investigation of intermolecular interactions in solid benzene",
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54. 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).
55. **P. Soldán**:
"Lowest quartet states of Li_2A ($\text{A}=\text{Na, K, Rb, Cs}$)",
Phys. Rev. A **77**, 054501 (2008).
56. 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).
57. A. Simoni, J.-M. Launay, and **P. Soldán**:
"Feshbach resonances in ultracold atom-molecule collisions",
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58. **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",
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59. R. Guérout, **P. Soldán**, M. Aymar, J. Deiglmayr, and O. Dulieu:
"Core Repulsion Effects in Alkali Trimers",
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60. **P. Soldán**:
"Potential energy surface for spin-polarized rubidium trimer",
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61. **P. Soldán**:
"Lowest quartet states of heteronuclear alkali-metal trimers ",
Phys. Rev. A **82**, 034701 (2010).
62. 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 $1^2\text{E}'$ and $1^2\text{E}'''$ ",
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63. **P. Soldán**, and W. P. Kraemer:
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64. L. Augustovičová and **P. Soldán**:
"*Ab initio* properties of MgAlk (Alk = Li, Na, K, Rb, Cs)",
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65. L. Augustovičová, V. Špirko, W. P. Kraemer, and **P. Soldán**:
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Review articles

1. K. Huml and **P. Soldán**:
“Symetrie molekul a analýza informací ze strukturních datových bank”,
Chem. Listy **89**, 547-555 (1995). (in Czech)
2. **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.
3. P. Honvaut, J.-M. Launay, **P. Soldán**, M. T. Cvitaš, and J. M. Hutson:
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in *Interactions of Cold Atoms and Molecules*,
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4. J. M. Hutson and **P. Soldán**:
“Molecule formation in ultracold atomic gases”,
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5. J. M. Hutson and **P. Soldán**:
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6. **P. Soldán**:
“Boseho-Einsteinova kondenzace: od atomů k molekulám”,
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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