

List of publications H el ene Bolvin

1. "Hysteresis for noninteracting molecules?"
H. Bolvin, O. Kahn, B. Vekhter *New. J. Chem.* **15**, 889 (1991).
2. "Two-step spin crossover in the new dinuclear compound [Fe(bt)(NCS)₂]₂bpym, with bt=2,2'-bi-2-thiazoline and bpym= 2,2'-bipyridine: experimental investigation and theoretical approach."
J. A. Real, H. Bolvin, A. Bousseksou, A. Dworkin, O. Kahn, F. Varret, J. Zarembowitch *J. Am. Chem. Soc.* **114**, 4650 (1992).
3. "Cooperativity and anticooperativity in spin transition compounds; macroscopic approach and orbital modelization."
H. Bolvin, O. Kahn *Mol. Cryst. Liq. Cryst.* **234**, 275 (1993).
4. "Ising model for low-spin high-spin transitions in molecular compounds; within and beyond the mean-field approximation"
H. Bolvin, O. Kahn *Chem. Phys.* **192**, 295 (1995).
5. "High-spin low-spin transitions in Fe(II) complexes by effective Hamiltonian method"
A. L. Tchougreff, A. V. Soudackov, I. A. Misurkin, H. Bolvin, O. Kahn *Chem. Phys.* **193**, 19 (1995).
6. "Ferromagnetism and spin transition; an attempt of unifying approach"
H. Bolvin, O. Kahn *Chem. Phys. Lett.* **243**, 355 (1995).
7. "The Neel point for spin-transition systems: toward a two-step transition"
H. Bolvin *Chem. Phys.* **211**, 101 (1996).
8. " $d \rightarrow d$ spectrum and high-spin/low-spin competition in d^6 octahedral coordination compounds: *ab-initio* study of potential energy curves."
H. Bolvin *J. Phys. Chem. A* **102**, 7525 (1998).
9. "*Ab initio* calculations of the magnetic coupling between a Ni(II) ion and two nitroxide radicals in *cis* and *trans* positions."
N. Suaud, H. Bolvin, J.-P. Daudey *Inorg. Chem.* **38**, 6089-6095 (1999).
10. "Ab initio study of the two iso-electronic molecules NpO_4^- and UO_4^{2-} " H. Bolvin, U. Wahlgren, O. Gropen, C. Marsden *J. Phys. Chem. A* **105**, 10570-10576 (2001).
11. "On the structure of Np(VII) species in alkaline solution studied by EXAFS and quantum chemical methods"
H. Bolvin, U. Wahlgren, H. Moll, T. Reich, G. Geipel, T. Fangh anel, I. Grenthe *J. Phys. Chem. A* **105**, 11441-11445 (2001)
12. "Amino-methyl-bipyridine bearing two flexible nitronyl nitroxide arms: a new podand for complexation of transition metals in a facial or meridional conformation"
C. Stroh, E. Belorizky, P. Turek, H. Bolvin, R. Ziessel *Inorg. Chem.* **42**, 2938-2949 (2003).
13. "From *ab initio* calculations to model Hamiltonians: the effective Hamiltonian technique as an efficient tool to describe mixed-valence molecules."
H. Bolvin *J. Phys. Chem. A* **107**, 5071-5078 (2003).
14. "Uranyl complexation in fluorinated acids (HF, HBF_4 , HPF_6 and HTf_2N): a combined experimental and theoretical study."
C. Gaillard, A. El Azzi, I. Billard, H. Bolvin, C. Hennig *Inorg. Chem.* **44**, 852 (2005).

15. “(NH₄)₂[Mn(H₂O)₂]₂[Mn(H₂O)][Mo(CN)₇]₂.nH₂O (n=3,4): cations as templates in Mn²⁺/[Mo(CN)₇]⁴⁻ system”
S. Willemin, B. Donnadieu, H. Bolvin, C. Guérin, B. Henner, J. Larionova. *Polyhedron* **24**, 1033-1046 (2005).
16. “An alternative approach to the g-matrix: theory and applications”
H. Bolvin *ChemPhysChem.* **7**, 1575-1589 (2006).
17. “Theoretical determination of the excited states and of g-factors of the Creutz-Taube ion, [(NH₃)₅Ru pyrazine Ru(NH₃)₅]⁵⁺.”
H. Bolvin *Inorg Chem* **46**, 417-427 (2007).
18. “A theoretical study of the excited states of AmO₂ⁿ⁺, n=1,2,3.”
F.P. Notter, S. Dubillard, H. Bolvin *J. Chem. Phys.* **128** 164315-164326 (2008).
<http://dx.doi.org/10.1063/1.2889004>
19. “The unique definition of the g tensor of a Kramers doublet”
L.F. Chibotaru, A. Ceulemans, H. Bolvin *Phys. Rev. Lett.* **101** 033003 (2008).
20. “Optical and magnetic properties of the 5f¹AnX₆^{q-} series: a theoretical study.”
F.P. Notter, H. Bolvin *J. Chem. Phys.* **130**, 184310 (2009).
<http://dx.doi.org/10.1063/1.3124193>
21. “Ab initio investigation of spectroscopic parameters for CrX₆³⁻ : the unexpected role of bond length variation - Size really matters “
H. Bolvin *Eur. J. Inorg. Chem.* **2010** 2221 (2010).
22. “The electronic structure of the triiodide ion from relativistic correlated calculations: a comparison of different methodologies”
A.S. Pereira Gomes, L. Visscher, H. Bolvin, T. Saue, S. Knecht, T. Fleig, E. Eliav. *J. Chem. Phys.* **133**, 064305 (2010).
23. “Magnetic memory effect in a transuranic mononuclear complex”
N. Magnani, C. Apostolidis, A. Morgenstern, E. Colineau, J.-C. Griveau, H. Bolvin, O. Walter, R. Caciuffo *Angew. Chem.* **50**, 1696 (2011).
24. “Zero-field splitting of the chalcogen diatomics using relativistic correlated wave-function methods”
J.-B. Rota, S.Knecht, T. Fleig, D. Ganyushin, T. Saue, F. Neese, H. Bolvin. *J. Chem. Phys.* **135**, 114106 (2011).
25. “Ferromagnetic coupling induced by spin-orbit coupling in dipyritylamide linear trinuclear Cu-Pd-Cu and Cu-Pt-Cu complexes”
D. Maynaud, H. Bolvin, W. van den Heuvel, M. Bénard, M.-M. Rohmer, N. Ben Amor *CR Acad. Sci. II B* **15**, 170 (2012).
26. “The case of a strong antiferromagnetic exchange coupling induced by spin polarization of a Mn-Mn partial single bond “
H. Bolvin, F. R. Wagner *Inorg. Chem.* **51**, 7112 (2012).
27. “Single-Ion Magnet behaviour in [U(TpMe₂)₂] “
J. T. Coutinho, M. A. Antunes, L. C. J. Pereira, H. Bolvin, J. Marçaloa, M. Mazzanti, M. Almeida *Dalton Trans.* **41**, 13568 (2012).
28. “Crystal structure diversity in the bis[hydrotris(3,5-dimethylpyrazolyl)borate]iodouranium(III) complex—from neutral to cationic forms”
M. A. Antunes, I. C. Santos, H. Bolvin, L. C. J. Pereira, M. Mazzanti, J. Marçaloa, M. Almeida *Dalton Trans.* **42** 8861 (2013).

29. "A Combined Experimental and Theoretical Study of the Ti₂ + N₂O Reaction"
A. Marzouk, H. Bolvin, P. Reinhardt, L. Manceron, J.P. Perchard, B. Tremblay, M.E. Alikhani *J. Phys. Chem.* **118**, 561 (2014).
30. "Structural and electronic dependence of the single molecule magnet behavior of Dysprosium (III)-complexes"
V. Campbell, H. Bolvin, E. Riviere, R. Guillot, W. Wernsdorfer, T. Mallah *Inorg. Chem.* **53**, 2598 (2014).
31. "Magnetic properties of a fourfold degenerate state: Np⁴⁺ ion diluted in Cs₂ZrCl₆ crystal"
D. Páez Hernández, H. Bolvin *J. Electron. Spectrosc. Relat. Phenom.* **194**, 74 (2014).
<http://dx.doi.org/10.1016/j.elspec.2014.03.002>
32. "Magnetic properties and electronic structure of neptunyl(VI) complexes: Wavefunctions, orbitals, and crystal-field models."
F. Gendron, D. Páez Hernández, F. P. Notter, B. Pritchard, H. Bolvin, J. Autschbach *Chem. Eur. J.* **20**, 7994 (2014).
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33. "Magnetic Resonance Properties of Actinyl Carbonate Complexes and Plutonyl(VI)-trinitrate"
F. Gendron, B. Pritchard, H. Bolvin, J. Autschbach *Inorg. Chem.* **53**, 8577 (2014).
34. "Assessing the exchange coupling in binuclear lanthanide(III) complexes and the slow relaxation of the magnetization in the antiferromagnetically coupled Dy₂ derivative"
C. Y. Chow, H. Bolvin, V. E. Campbell, R. Guillot, J. W. Kampf, W. Wernsdorfer, F. Gendron, J. Autschbach, V. L. Pecoraro, T. Mallah *Chem. Sci.*, **6**, 4148 - 4159, (2015).
DOI: 10.1039/C5SC01029B
35. "Relativistic methods for calculating Electron Paramagnetic Resonance (EPR) parameters"
H. Bolvin, J. Autschbach in Liu, W. (editor), 'Handbook of Relativistic Quantum Chemistry', Springer, Berlin (2016).
36. "Single-ion 4f element magnetism: An ab-initio look at [Ln(COT)]₂⁻"
F. Gendron, B. Pritchard, H. Bolvin, J. Autschbach *Dalton Trans.* **44**, 19886–19900 (2015).
37. "Magnetic Susceptibility of Actinide(III) Cations: Experimental and Theoretical Study."
M. Autillo, L. Guerin, H. Bolvin, P. Moisy, C. Berthon *Phys. Chem. Chem. Phys.* **18**, 6515 (2016).
38. "Predicting Tools for the Nature and Magnitude of Magnetic Anisotropy."
B. Cahier, R. Maurice, T. Mallah, H. Bolvin, N. Guihéry *Magnetochemistry* **2**, 31 (2016).
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39. "Structure, luminescence and magnetic properties of an erbium(III) β-diketonate homodinuclear complex"
P. Martín-Ramos, L.C.J. Pereira, J.T. Coutinho, F. Koprowiak, H. Bolvin, V. Lavín, I.R. Martín, J. Martín-Gilf, M. Ramos-Silva *New. J. Chem.* **40**, 8251-8261 .
DOI: 10.1039/C6NJ01598K
40. "Unraveling σ and π effects on the magnetic anisotropy in cis-NiA₄B₂ complexes: magnetization, HF-HFEPR studies, first principles calculations and orbital model."
G. Charron, E. Malkin, G. Rogez, L. J. Batchelor, S. Mazerat, R. Guillot, N. Guihéry, A. L. Barra, T. Mallah, H. Bolvin *Chem. Eur. J.* **22** 16848-16860 (2016).
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41. "Bi-compartmental Schiff-base with peripheral ester functionalization: Synthesis and magnetic behaviors of bimetallic Zn-Ln complexes (Ln = Dy, Tb, Gd)".
V. Béreau, H. Bolvin, C. Duhayon, J. P. Sutter *Eur. J. Inorg. Chem.* 4988-4995 (2016).
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42. "Paramagnetism of Aqueous Actinide Cations. Part II: Theoretical aspects and new measurements on An(IV)"
M. Autillo, L. Guerin, D. Guillaumont, P. Moisy, H. Bolvin, C. Berthon *Inorg. Chem.* **55**, 12149-12157 (2016).