

PUBLICATIONS

of Jean-François Halet

- 315- Monocarboxylate-Protected Two-Electron Superatomic Silver Nanoclusters with High Photothermal Conversion Performance
H.-H. Wang, J. Wei, a, F. Bigdeli, F. Rouhani, H.-F. Su, L.-X. Wang, S. Kahlal, J.-F. Halet, J.-Y. Saillard, A. Morsali, K.-G. Liu
Nanoscale 2023, 15, 8245–8254 (DOI: 10.1039/d3nr00571b).
- 314- Linear and Nonlinear Optical Properties of Quadrupolar Bithiophene and Cyclopentadithiophene Derivatives as Fluorescent Oxygen Photosensitizers
N. Richy, S. Gam, S. Messaoudi, A. Triadon, O. Mongin, M. Blanchard-Desce, C. Latouche, M. Humphrey, A. Boucekkine, J.-F. Halet, F. Paul
Photochem 2023, 3, 127–154 (doi.org/10.3390/photochem3010009).
- 313- From 8- to 18-cluster electrons Superatoms. Evaluation via DFT Calculations of the Ligand-Protected $W@Au_{12}(dppe)_6$ Cluster Displaying Distinctive Electronic and Optical Properties
J. Wei, D. MacLeod Carey, J.-F. Halet, S. Kahlal, J.-Y. Saillard, A. Muñoz-Castro
Inorg. Chem. 2023, 62, 3047–3055 (doi.org/10.1021/acs.inorgchem.2c03771).
- 312- Enhanced NH_3 sensing performance of Mo cluster-MoS₂ nano-composite thin films via the sulfurization of Mo₆ cluster iodide precursors
M. Zhang, F. Grasset, Y. Masubuchi, T. Shimada, T. K. N. Nguyen, N. Dumait, A. Renaud, S. Cordier, D. Berthebaud, J.-F. Halet, T. Uchikoshi
Nanomaterials 2023, 13, 478 (doi.org/10.3390/nano13030478).
- 311- Eu- and Tb-doped Si₃N₄ and Ge₃N₄: Tuning the colors with one luminescent host
C. Braun, L. Mereacre, Z. Chen, A. Slabon, D. Vincent, X. Rocquefelte, J.-F. Halet
ChemRxiv, Cambridge: Cambridge Open Engage; 2021 (DOI:10.26434/chemrxiv-2021-cvfhf)
RSC Advances 2022, 12, 32318–32326 (DOI: 10.1039/d2ra04663f).
- 310- Trimetallic Chalcogenide Species: Synthesis, Structures, and Aromaticity
S. Kar, D. Chatterjee, J.-F. Halet, S. Ghosh
Molecules 2022, 27, 7473 (13 pages) (doi.org/10.3390/molecules27217473).
- 309- Electronic States for 3d Transition Metal Compounds using Local Structure and Neural Networks
W. Zhang, D. Berthebaud, J.-F. Halet, T. Mori
J. Phys. Chem. A 2022, 126, 7373–7381 (doi.org/10.1021/acs.jpca.2c03901).
- 308- Metal-rich clusters: synthesis, structure and bonding of metallaboranes featuring μ_5 -boride and triply bridging borylene units
A. Nanda Pradhan, B. Keshari Rout, J.-F. Halet, S. Ghosh
Inorg. Chim. Acta 2022, 540, 121045 (9 pages) (doi.org/10.1016/j.ica.2022.121045).
- 307- How structural factors determine linear and nonlinear optical properties of bi-phenyl derivatives? A theoretical answer
S. Gam, S. Messaoudi, J.-F. Halet, A. Boucekkine
New J. Chem. 2022, 46, 13431–13441 (DOI: 10.1039/D2NJ01192A).
- 306- Ligand-Induced Cuboctahedral versus Icosahedral Core Isomerism within Eight-Electron Heterocyclic-Carbene-Protected Gold Nanoclusters
J. Wei, S. Kahlal, J.-F. Halet, A. Muñoz-Castro, J.-Y. Saillard
Inorg. Chem. 2022, 61, 8623–8628 (doi.org/10.1021/acs.inorgchem.2c01022).
- 305- Methyl Viologens of Bis-(4'-ethynylpyridyl)arenes - Structures, Photophysical and Electrochemical Studies, and their Potential Application in Biology

- G. K. Kole, M. Koščak, A. Amar, D. Majhen, K. Božinović, Z. Brkljaca, M. Ferger, M. Evripidis, S. Lorenzen, A. Friedrich, I. Krummenacher, M. Moos, H. Braunschweig, A. Boucekkine, C. Lambert, J.-F. Halet, I. Piantanida, K. Müller-Buschbaum, T. B. Marder
Chem. Eur. J. 2022, 28, e202200753 (22 pages, Hot Paper)
(doi.org/10.1002/chem.202200753).
- 304- Fabrication and characterization of zeolite bulk body containing mesopores and macropores using starch as pore-forming agent
M. Uematsu, K. Ishii, S. Samitsu, E. Bin Ismael, I. Ichinose, N. Ohashi, D. Berthebaud, J.-F. Halet, T. Ishigaki, T. Uchikoshi
Adv. Powder Technol. 2022, 33, 103626 (DOI: 10.1016/j.appt.2022.103626).
- 303- Looking at platinum carbonyl nanoclusters as *superatoms*
J. Wei, R. Marchal, D. Astruc, S. Kahlal, J.-F. Halet, J.-Y. Saillard
Nanoscale 2022, 14, 3946–3957 (DOI: 10.1039/d1nr08216g).
- 302- Insight into The Stability and Electronic and Optical Properties of N-Heterocyclic Carbene Analogues of Halogen/Phosphine Protected Au₁₃ Superatomic Clusters
J. Wei, S. Kahlal, J.-F. Halet, J.-Y. Saillard, A. Muñoz-Castro
J. Chem. Phys. A 2022, 126, 536–545 (doi.org/10.1021/acs.jpca.1c09084).
- 301- Improvement of Thermoelectric Properties via Texturation Using a Magnetic Slip Casting Process – the Illustrative Case of CrSi₂
S. Le Tonquesse, W. Zhang B. Srinivasan, B. Fontaine, T. Hiroto, T. Mori, J.-F. Halet, D. Berthebaud, T. S. Suzuki
Chem. Mater. 2022, 34, 1143–1156 (doi.org/10.1021/acs.chemmater.1c03608).
- 300- Flux synthesis, crystal structure and electronic properties of the layered rare earth metal boride silicide Er₃Si_{5-x}B. An example of a boron/silicon ordered structure derived from the AlB₂ structure type
V. Babizhetskyy, R. Jardin, R. Gautier, B. Fontaine, J.-F. Halet
Z. Naturforsch. B 2021, 76, 869–879 (doi.org/10.1515/znb-2021-0143).
- 299- Two-Photon Absorption Properties of Di- and Multipolar Triarylamino/Tosylamido 1,1,4,4-Tetracyanobutadienes
N. Ripoche, M. Betou, C. Philippe, Y. Trolez, O. Mongin, M. Dudek, Z. Pokladek, K. Matczyszyn, M. Samoc, H. Sahnoune, J.-F. Halet, T. Roisnel, L. Toupet, M. Cordier, G. J. Moxey, M. G. Humphrey, F. Paul
PhysChemChemPhys 2021, 23, 22283–22297 (DOI: 10.1039/D1CP03346H) [2021 HOT PCCP article].
- 298- Two-photon absorption of dipolar and quadrupolar oligothiophene-cored chromophores derivatives containing terminal dimesitylboryl moieties: A theoretical (DFT) structure-property investigation
A. Amar, A. El Kechaj, J.-F. Halet, F. Paul, A. Boucekkine
New J. Chem. 2021, 45, 15074–15081 (doi.org/10.1039/D1NJ01467F).
- 297- Planar triple-decker and capped octahedral clusters of group-6 transition metals
R. Bag, S. Gayen, S. Mohapatra, P. K. S. Antharjanam, J.-F. Halet, S. Ghosh
J. Organomet. Chem. 2021, 952, 122023 (doi.org/10.1016/j.jorganchem.2021.122023).
- 296- On Heteronuclear Isoelectronic Alternatives to Au₁₃(dppe)₅Cl₂: Electronic and Optical Properties of the 18-electron Os@Au₁₂(dppe)₅Cl₂ Cluster from Relativistic DFT Computations
J. Wei, P. L. Rodriguez-Kessler, J.-F. Halet, S. Kahlal, J.-Y. Saillard, A. Muñoz-Castro
Inorg. Chem. 2021, 60, 8173–8180 (doi.org/10.1021/acs.inorgchem.1c00799).
- 295- Stereoselective synthesis, structure and DFT studies on fluoro- and nitro-substituted spirooxindole-pyrrolidine heterocyclic hybrids
A. I. Almansour, N. Arumugam, S. M. Soliman, B.S. Krishnamoorthy, J.-F. Halet, R. V. Priya, J. Suresh, D. M. Al-thamili, F. A. Al-aizari, R. S. Kumar
J. Mol. Struct. 2021, 1237, 130396 (doi.org/10.1016/j.molstruc.2021.130396).

- 294- Metal-rich Metallaboranes: Synthesis, Structures and Bonding of Some Bi- and Trimetallic Open Faced Cobaltaboranes
K. Pathak, C. Nandi, J.-F. Halet, S. Ghosh
Inorganics 2021, 9, 28 (doi.org/10.3390/inorganics9040028).
- 293- Electron Counting in High Nuclearity Late Transition Metal Clusters
F. Gam, J. Wei, S. Kahlal, J.-Y. Saillard, J.-F. Halet
In: 50th Anniversary of Electron Counting Paradigms for Polyhedral Molecules (D. M. P. Mingos, ed.), **Struct. Bond.** (Springer) 2021, 188, 69–102
(doi.org/10.1007/430_2021_81).
- 292- Crystal, electronic and magnetic structures of a novel series of intergrowth carbometalates $R_4Co_2C_3$ ($R = Y, Gd, Tb$)
V. Levitskiy, O. Isnard, R. K. Kremer, V. Babizhetskyy, B. Fontaine, X. Rocquefelte, J.-F. Halet, R. Gumeniuk
Dalton Trans. 2021, 50, 4202–4209 (DOI: 10.1039/d1dt00420d).
- 291- Chemistry of group 5 metallaboranes with heterocyclic thiol ligands: a combined experimental and theoretical study
R. Prakash, A. Haridas, K. Bakthavachalam, T. Roisnel, J.-F. Halet, S. Ghosh
Dalton Trans. 2021, 50, 4036–4044 (DOI: 10.1039/d0dt04362a).
- 290- 2- and 2,7-substituted N-methylpyridinium pyrenes and salts – structures, photophysical, electrochemical and spectroelectrochemical studies
G. K. Kole, J. Merz, A. Amar, B. Fontaine, A. Boucekkine, J. Nitsch, S. Lorenzen, A. Friedrich, I. Krummenacher, M. Moos, H. Braunschweig, C. Lambert, J.-F. Halet, K. Müller-Buschbaum, T. B. Marder
Chem. Eur. J. 2021, 27, 2837–2853 (dx.doi.org/10.1002/chem.202004748).
- 289- Tailoring the Thermoelectric and Structural Properties of Cu-Sn based Thiospinel Compounds [$CuM_{1+x}Sn_{1-x}S_4$ ($M = Ti, V, Cr, Co$)]
C. Bourgès, B. Srinivasan, B. Fontaine, P. Sauerschnig, A. Minard, J.-F. Halet, Y. Miyazaki, D. Berthebaud, T. Mori
J. Mater. Chem. C 2020, 8, 16368–16383 (doi.org/10.1039/D0TC04393A).
- 288- $SnCN_2$: A Carbodiimide with an Innovative Approach for Energy Storage Systems and Phosphors in Modern LED Technology
C. Braun, L. Mereacre, W. Hua, T. Stürzer, I. Ponomarev, P. Kroll, A. Slabon, Z. Chen, Y. Damour, X. Rocquefelte, J.-F. Halet, S. Indris
ChemElectroChem 2020, 7, 4550–4561 (DOI: 10.1002/celec.202000765).
- 287- Zwitterionic Mixed-valence Species for the Design of Neutral Clocked Molecular Quantum-dot Cellular Automata
T. Groizard, S. Kahlal, J.-F. Halet
Inorg. Chem. 2020, 59, 15772–15779 (dx.doi.org/10.1021/acs.inorgchem.0c02207).
- 286- A theoretical investigation on conformers of imidazolium salts
A. Ladjarafi, H. Meghezzi, J.-F. Halet
Theor. Chem. Acc. 2020, 139, 135 (doi.org/10.1007/s00214-020-02677-x).
- 285- Towards the Formation of N-Heterocyclic Carbene-Protected Gold Clusters of Various Nuclearities. A Comparison with their Phosphine-Protected Analogs from DFT Calculations
J. Wei, J.-F. Halet, S. Kahlal, J.-Y. Saillard, A. Muñoz-Castro
Inorg. Chem. 2020, 59, 15240–15249 (dx.doi.org/10.1021/acs.inorgchem.0c02219).
- 284- Screening of Transition (Y, Zr, Hf, V, Nb, Mo, Ru) and Rare-earth (La, Pr) Elements as Potential Effective Dopants for Thermoelectric GeTe – an Experimental and Theoretical Appraisal
B. Srinivasan, S. Le Tonquesse, A. Gellé, C. Bourgès, L. Monier, I. Ohkubo, J.-F. Halet, D. Berthebaud, T. Mori
J. Mater. Chem. A 2020, 8, 19805–19821 (DOI: 10.1039/D0TA06710E).

- 283- The electron count and electronic structure of bare icosahedral Au₃₂ and Au₃₃ ionic nanoclusters and ligated derivatives
Q. Wang, J.-F. Halet, S. Kahlal, A. Muñoz-Castro, J.-Y. Saillard
Phys. Chem. Chem. Phys. 2020, 22, 20751–20757 (DOI: 10.1039/D0CP03735D).
- 282- Metal Centred *commo*-Bis(metallaselenaborane): Heterotrimetallic Systems Bearing a Zn(II) Center
B. Joseph, R. Prakash, V. Dorcet, T. Roisnel, J.-F. Halet, S. Ghosh
Organometallics 2020, 39, 2942–2946 (doi.org/10.1021/acs.organomet.0c00427).
- 281- Polyhedral M₂B₅ Metallaborane Clusters and Derivatives: An Overview of their Structural Features and Chemical Bonding
R. Prakash, J.-F. Halet, S. Ghosh
Molecules 2020, 25, 3179 (doi.org/10.3390/molecules25143179).
- 280- Rare-earth metal borosilicides R₉Si_{15-x}B₃ (R = Tb, Yb): New ordered structures derived from the AlB₂ structure type
V. Babizhetskyy, V. Levytskyy, R. Jardin, J. Bauer, R. Guérin, R. Gautier, B. Fontaine, J.-F. Halet
Z. Anorg. Allg Chem. 2020, 646, 1168–1175 (doi.org/10.1002/zaac.202000046).
- 279- 1,4-Diethynylbenzene-Bridged [Cp*(dppe)Fe]ⁿ⁺ Units: Effect of 2,5-Ethynyl Groups on the Chemical and Electronic Properties
R. Makhoul, T. Groizard, P. Hamon, T. Roisnel, V. Dorcet, S. Kahlal J.-F. Halet, J.-R. Hamon, C. Lapinte
Eur. J. Inorg. Chem. 2020, 2624–2638 (doi.org/10.1002/ejic.202000345).
- 278- Is the Alumino-boron Carbide Al₃BC a Promising Thermoelectric Material?
A. Huguenot, A. Riot, B. Boucher, B. Fontaine, R. Al Rahal Al Orabi, H. Hillebrecht, T. Mori, J.-F. Halet, R. Gautier
Solid State Sci. 2020, 104, 106205
 (doi.org/10.1016/j.solidstatesciences.2020.106205).
- 277- Theoretical analysis of the Mackay icosahedral cluster Pd₅₅(PⁱPr₃)₁₂(μ₃-CO)₂₀: An open-shell 20-electron superatom
J. Wei, R. Marchal, D. Astruc, J.-Y. Saillard, J.-F. Halet, S. Kahlal
Chem. Eur. J. 2020, 26, 5508–5514 (dx.doi.org/10.1002/chem.202000447).
- 276- Electronic Properties of Poly-yne Carbon Chains and Derivatives with Transition Metal End-Groups
F. Gendron, T. Groizard, B. Le Guennic, J.-F. Halet
Eur. J. Inorg. Chem. 2020, 667–681 (dx.doi.org/10.1002/ejic.201901112) [Hot Topic: Carbon, Graphite, and Graphene].
- 275- Insights into the Optical Properties of Triarylboranes with Strongly Electron-accepting Bis(fluoromesityl)boryl Groups: When Theory Meets Experiment
H. Belaidi, F. Rauch, Z. Zhang, C. Latouche, A. Boucekkine, T. B. Marder, J.-F. Halet
ChemPhotoChem 2020, 4, 173–180 (doi.org/10.1002/cptc.201900256).
- 274- Diborane(6) and its analogues stabilized by the mono-, bi- and trinuclear group 7 templates: Combined experimental and theoretical studies
R. Prakash, A. N. Pradhan, M. Jash, S. Kahlal, M. Cordier, T. Roisnel, J.-F. Halet, S. Ghosh
Inorg. Chem. 2020, 59, 1917–1927 (dx.doi.org/10.1021/acs.inorgchem.9b03217).
- 273- An Experimental and Theoretical Study of Bis- and Tris-homocubane Analogues of Group-9 Transition metals
B. Joseph, R. Prakash, K. Pathak, T. Roisnel, S. Kahlal, J.-F. Halet, S. Ghosh
New J. Chem. 2020, 44, 674–683 (DOI: 10.1039/c9nj05117a).
- 272- Ruthenium-Templated Construction of an Arylated B₄ Chain by Dihydroborane Dehydrocoupling

- C. Lenczyk, D. K. Roy, K. Oberdorf, J. Nitsch, R. D. Dewhurst, K. Radacki, J.-F. Halet, T. B. Marder, F. M. Bickelhaupt, H. Braunschweig
Chem. Eur. J. 2019, 25, 16544–16549 (DOI: 10.1002/chem.201904772).
- 271- Near Infrared Emission in Extended Pyrazinacenes Containing Seven Linearly-fused Pyrazine Units
G. J. Richards, A. Cador, S. Yamada, A. Middleton, P. A. Karr, J. Labuta, K. Ariga, F. D'Souza, S. Kahlal, J.-F. Halet, J. P. Hill
J. Am. Chem. Soc. 2019, 141, 19570–19574 (DOI: 10.1021/jacs.9b10952).
- 270- Elucidating the Electronic Structure of the Ligated Cuboctahedral Palladium Cluster $[Pd_{13}(\mu_4-C_7H_7)_6]^{2+}$
J. Wei, S. Kahlal, J.-F. Halet, J.-Y. Saillard
J. Cluster Sci. 2019, 30, 1227-1233 (DOI: 10.1007/s10876-019-01616-6).
- 269- Inorganic Niobium and Tantalum Octahedral Cluster Halide Compounds with Three-Dimensional Frameworks: A Review on Their Crystallographic and Electronic Structures
P. Lemoine, J.-F. Halet, S. Cordier
Struct. Bond. 2019, 180, 143–190 (DOI: 10.1007/430_2019_39).
- 268- Preface to 'Ligated transition-metal clusters in solid-state chemistry: The legacy of Marcel Sergent'
J.-F. Halet
Struct. Bond. 2019, 180, v-viii.
- 267- 1,4-Dimethoxybutadienediyl-Bridged Diiron Compounds in Three Oxidation Levels: Evaluation of Delocalization Effects
H. Sahnoune, V. Mahias, J.-F. Halet, C. Lapinte
Organometallics 2019, 38, 2724–2737 (DOI: 10.1021/acs.organomet.9b00174).
- 266- Mercapto-benzothiazolyl based ruthenium(II) borate complexes: Synthesis and reactivity towards various phosphines
M. Zafar, R. Ramalakshmi, A. Nanda Pradhan, K. Pathak, T. Roisnel, J.-F. Halet, S. Ghosh
Dalton Trans. 2019, 48, 7413–7424 (dx.doi.org/10.1039/C9DT00498J).
- 265- Enhanced Thermoelectric Performance through Crystal Field Engineering in Transition Metal Doped GeTe
J. Shuai, X. Tan, Q. Guoa, J. Xu, A. Gellé, R. Gautier, J.-F. Halet, F. Failamani, J. Jiang, T. Mori
Mater. Today Phys. 2019, 9, 100094 (doi.org/10.1016/j.mtphys.2019.100094).
- 264- Synthesis, Structures and Chemistry of the Metallaboranes of Group 4-9 with M_2B_5 Core having a Cross Cluster M-M Bond
R. Bag, S. Saha, R. Borthakur, B. Mondal, T. Roisnel, V. Dorcet J.-F. Halet, S. Ghosh
Inorganics 2019, 7, 27 (doi:10.3390/inorganics7030027).
- 263- Rationalising and Predicting the Structure and Bonding of Bare and Ligated Transition Metal Clusters and Nanoparticles
G. Frapper, J.-F. Halet
Computational Materials Discovery (A. R. Oganov, A. G. Kvashnin, G. Saleh, eds.), Royal Society of Chemistry, London, 2019, pp. 320–351 (doi.org/10.1039/9781788010122-00320).
- 262- Boron in Solid State Chemistry: Some Portraits of Metal Borides Taken from a Rich Structural Gallery
B. Boucher, J.-F. Halet
Handbook of Boron Science with Applications In Organometallics, Catalysis, Materials and Medicine (N. Hosmane, R. Eagling, eds.), World Science Publishers, London, Vol. 3: Boron in Materials Chemistry 2019, Chap. 5, pp. 159-188 (doi.org/10.1142/q0130-vol3).

- 261- Realizing a Stable High Thermoelectric zT of ~ 2 over a Broad Temperature Range in $\text{Ge}_{1-x-y}\text{Ga}_x\text{Sb}_y\text{Te}$ via Band Engineering and Hybrid Flash-SPS Processing
B. Srinivasan, A. Gellé, F. Gucci, C. Boussard-Pledel, B. Fontaine, R. Gautier, J.-F. Halet, M. J. Reece, B. Bureau
Inorg. Chem. Front. 2019, 3, 63–73 (DOI: 10.1039/C8QI00703A).
- 260- Detrimental Effects of Al on the Thermoelectric Performance of GeTe
B. Srinivasan, A. Gellé, J.-F. Halet, C. Boussard-Pledel, B. Bureau
Materials 2018, 11, 2237 (doi:10.3390/ma11112237).
- 259- Redox Properties of Ferrocenyl Ene-diyanyl Bridged $\text{Cp}^*(\text{dppe})\text{M}-\text{C}\equiv\text{C}-1,4-(\text{C}_6\text{H}_4)$ Complexes
R. Makhoul, J. B. G. Gluyasz, K. Vincent, H. Sahnoune, J.-F. Halet, P. J. Low, J.-R. Hamon, C. Lapinte
Organometallics 2018, 37, 4156–4171 (DOI: 10.1021/acs.organomet.8b00740).
- 258- Effect of the Processing Route on the Thermoelectric Performance of Nanostructured $\text{CuPb}_{18}\text{SbTe}_{20}$
B. Srinivasan, B. Fontaine, F. Gucci, V. Dorcet, T. G. Saunders, M. Yu, F. Chevirié, C. Boussard-Pledel, J.-F. Halet, R. Gautier, M. J. Reece, B. Bureau
Inorg. Chem. 2018, 57, 12976–12986 (DOI: 10.1021/acs.inorgchem.8b02248).
- 257- Synthesis, Characterization and Third-Order Nonlinear Optical Properties of a Dodecaruthenium Organometallic Dendrimer with a Zinc(II) Tetraphenylporphyrin Core
A. Merhi, G. Grelaud, M. Morshedi, S. Abid, K. A. Green, A. Barlow, T. Groizard, S. Kahlal, J.-F. Halet, N. H. Minh, I. Ledoux, M. P. Cifuentes, M. G. Humphrey, F. Paul, C. O. Paul-Roth
Dalton Trans. 2018, 47, 11123–11135 (DOI: 10.1039/C8DT02301H).
- 256- Structural, electronic and physical properties of solid-state rare-earth metal boride carbides
V. Babizhetskyy, J. Bauer, R. Gautier, K. Hiebl, A. Simon, J.-F. Halet
Handbook on the Physics and Chemistry of Rare Earths (HPCRE) (K.A. Gschneidner, J.-C. Bünzli, V. K. Pecharsky, eds.), Elsevier, Amsterdam, 2018, 53, chapter 302, 145–269 (doi.org/10.1016/bs.hpcr.2018.05.001).
- 255- Structural systematics of some trinuclear alkynyl and diyanyl Group 11 complexes containing dppm [$\text{dppm} = \text{CH}_2(\text{PPh}_2)_2$]
M. I. Bruce, J.-F. Halet, B. Le Guennic, B. W. Skelton, A. N. Sobolev, C. Sumbly, A. H. White
Coord. Chem. Rev. 2018, 375, 2–12 (doi.org/10.1016/j.ccr.2017.09.021).
- 254- Synthesis and characterization of diruthenaborane analogues of pentaborane(11) and hexaborane(10)
B. Joseph, S. Gomosta, S. K. Barik, S. Sinha, T. Roisnel, V. Dorcet, J.-F. Halet, S. Ghosh
J. Organomet. Chem. 2018, 865, 29–36 (doi.org/10.1016/j.jorganchem.2017.12.011) - Invited article.
- 253- Iron versus ruthenium: clarifying the electronic differences between prototypical mixed-valence organometallic butadienyldiyl-bridged molecular wires
S. Gückel, J. B. G. Gluyas, S. El-Tarhuni, A. N. Sobolev, M. W. Whiteley, J.-F. Halet, C. Lapinte, M. Kaupp, P. J. Low
Organometallics 2018, 37, 1432–1445 (DOI: 10.1021/acs.organomet.8b00099).
- 252- Impact of Coinage Metal Insertion on the Thermoelectric Properties of GeTe Solid-State Solutions
B. Srinivasan, R. Gautier, F. Gucci, B. Fontaine, J.-F. Halet, F. Chevirié, M. J. Reece, C. Boussard-Pledel, B. Bureau
J. Phys. Chem. C, 2018, 122, 227–235 (DOI: 10.1021/acs.jpcc.7b10839).
- 251- An Efficient Method for the Synthesis of Boratrane Complexes of Late Transition Metals

- K. Saha, R. Ramalakshmi, R. Borthakur, S. Gomosta, K. Pathak, V. Dorcet, T. Roisnel, J.-F. Halet, S. Ghosh*
Chem. Eur. J. 2017, 23, 18264–18275 (DOI: 10.1002/chem.201704332).
- 250- Towards the prediction of the transport properties of cluster-based molybdenum chalcogenides
R. Al Rahal Al Orabi, B. Boucher, B. Fontaine, P. Gall, C. Candolfi, B. Lenoir, P. Gougeon, J.-F. Halet, R. Gautier
J. Mater. Chem. C, 2017, 5, 12097–12104 (DOI: 10.1039/C7TC03977H).
- 249- Synthesis and structural characterization of trithiocarbonate complexes of molybdenum and ruthenium derived from CS₂
R. Ramalakshmi, B. Joseph, V. Dorcet, T. Roisnel, J.-F. Halet, S. Ghosh
J. Organomet. Chem. 2017, 849-850, 256–260 (DOI: 10.1016/j.jorganchem.2017.03.0272017) - Invited article.
- 248- First-Principles Computation of NMR Parameters in Solid State Chemistry
J. Cuny, R. Gautier, J.-F. Halet
Handbook of Solid-State Chemistry, (R. Dronskowski, S. Kikkawa A. Stein, eds.), Wiley-VCH: Weinheim, 2017, vol. 5: Theoretical Description, chap. 16, p. 607-646 (ISBN: 978-3-527-32587-0).
- 247- Cyanide linkage isomerism in cerium(III) and uranium(III) complexes. A relativistic DFT study
Y. Bouzidi, L. Belkhiri, M. Ephritikhine, J.-F. Halet, A. Boucekkine
J. Organomet. Chem. 2017, 847, 82–89 (DOI: 10.1016/j.jorganchem.2017.03.002) - Invited article.
- 246- Design, Synthesis, and Chemistry of Bis(σ)borate and Agostic Complexes of Group 7 Metals
K. Saha, R. Ramalakshmi, S. Gomosta, K. Pathak, V. Dorcet, T. Roisnel, J.-F. Halet, S. Ghosh
Chem. Eur. J. 2017, 23, 9812–9820 (DOI: 10.1002/chem.201701423).
- 245- Theoretical studies of mixed-valence organometallic species for potential utilization as quantum cellular automata
T. Groizard, S. Kahlal, J.-F. Halet
J. Organomet. Chem. 2017, 844, 35–42. (DOI: 10.1016/j.jorganchem.2017.02.021) - Invited article.
- 244- Sb Doping of Metallic CuCr₂S₄ as a Route to Highly Improved Thermoelectric Properties
A. U. Khan, R. Al Rahal Al Orabi, A. Pakdel, J.-B. Vaney, B. Fontaine, R. Gautier, J.-F. Halet, S. Mitani, T. Mori
Chem. Mater. 2017, 29, 2988–2996 (DOI: 10.1021/acs.chemmater.6b05344).
- 243- Enhancement of the Thermoelectric Properties of FeGa₃-type Structures with Group 6 Transition Metals: A Computational Exploration
B. Boucher, R. Al Rahal Al Orabi, B. Fontaine, Yu. Grin, R. Gautier, J.-F. Halet
Inorg. Chem. 2017, 56, 4229–4237 (DOI: 10.1021/acs.inorgchem.7b00251).
- 242- Small ligated organometallic palladium Pd_n clusters ($n = 4-12$): A DFT investigation
G. Manca, S. Kahlal, J.-Y. Saillard, R. Marchal, J.-F. Halet
J. Cluster Sci. 2017, 28, 853–868 (DOI: 10.1007/s10876-017-1168-2).
- 241- Nonconventional Supramolecular Self-Assemblies of Zinc(II)–Salphen Building Blocks
T. Groizard, S. Kahlal, V. Dorcet, T. Roisnel, C. Bruneau, J.-F. Halet, R. Gramage-Doria
Eur. J. Inorg. Chem. 2016, 5143–5151 (DOI: 10.1002/ejic.201600866).
- 240- Reactivity of CS₂ – Syntheses and Structures of Transition-Metal Species with Dithioformate and Methanedithiolate Ligands
C. E. Rao, S. K. Barik, K. Yuvaraj, K. Bakthavachalam, T. Roisnel, V. Dorcet, J.-F. Halet, S. Ghosh
Eur. J. Inorg. Chem. 2016, 4913–4920 (DOI: 10.1002/ejic.201600823).

- 239- Reactivity of cyclopentadienyl transition-metal(II) complexes with borate ligands. structural characterization of the toluene-activated molybdenum complex [Cp*Mo(CO)₂(η³-CH₂C₆H₅)]
R. Ramalakshmi, K. Maheswari, D. Sharmila, A. Paul, T. Roisnel, J.-F. Halet, S. Ghosh Dalton Trans. 2016, 45, 16317-16324 (DOI: 10.1039/C6DT02641A).
- 238- Syntheses and structures of some complexes $[\{M_3(\mu\text{-dppm})_3\}\{\mu\text{-C}\equiv\text{C}\equiv\text{C}[M'L_x]\}_n]^{(3-n)+}X^{-(3-n)}$ [M'L_x = Re(CO)₃(Bu^t₂-bpy), Ru(dppe)Cp*; dppm = CH₂(PPh₂)₂; X = PF₆, BF₄; n = 1, 2] and [Ag₆(μ-dppm)₄{C≡CC≡C[Re(CO)₃(Bu^t₂-bpy)]₄](PF₆)₂
M. I. Bruce, B. G. Ellis, J.-F. Halet, B. Le Guennic, B. K. Nicholson, H. Sahnoune, N. Scoleri, B. W. Skelton, A. N. Sobolev, C. J. Sumbly, A. H. White, N. N. Zaitseva Inorg. Chim. Acta 2016, 453, 654–666 (DOI: dx.doi.org/10.1016/j.ica.2016.09.017).
- 237- Structural and Electronic Structures of Alkaline-Earth Transition Metal Oxynitride Perovskites
E. Orisakwe, R. Marchal, B. Fontaine, R. Gautier, J.-F. Halet J. Ceram. Soc. Jpn. 2016, 124, 1056-1062 (DOI:http://dx.doi.org/10.2109/jcersj2.124.P10-1).
Eur. J. Inorg. Chem. 2016, 4913–4920 (DOI: 10.1002/ejic.201600823).
- 236- The Light at the End of the Cycle: Reductive Coupling of Diynes at Rhodium Gives Fluorescent Rhodacyclopentadienes or Phosphorescent Dibenzorhodacyclopentadienes
C. Sieck, M. G. Tay, M.-H. Thibault, R. Edkins, K. Costuas, J.-F. Halet, A. S. Batsanov, M. Hähnel, K. Fucke, A. Lorbach, A. Steffen, T. B. Marder Chem. Eur. J. 2016, 22, 10523–10532 (DOI: 10.1002/chem.201601912).
- 235- Double Insertion of Thiophene Rings in Polyynediyl Chains To Stabilize Nano-scaled Molecular Wires with [Cp*(dppe)Fe] Termini
S. Roué, H. Sahnoune, L. Toupet, J.-F. Halet, C. Lapinte Organometallics 2016, 35, 2057–2070 (DOI: 10.1021/acs.organomet.6b00209).
- 234- Structure and Bonding Patterns in Large Molecular Ligated Metal Clusters
J.-Y. Saillard, J.-F. Halet Struct. Bond. (The Chemical Bond I – 100 Years Old and Getting Stronger) 2016, 169, 157–180 (DOI: 10.1007/430_2015_210).
- 233- The Coloring Problem in the Solid-state Metal Boride Carbide ScB₂C₂. A Theoretical Analysis
S. Lassoued, B. Boucher, R. Gautier, J.-F. Halet Z. Naturforsch. B 2016, 71, 593–601 (DOI 10.1515/znb-2016-0056).
- 232- Electron-Precise 1,3-Bishomocubanes: A combined experimental and theoretical study
S. K. Barik, C. E. Rao, K. Yuvaraj, R. Jagan, S. Kahlal, J.-F. Halet, S. Ghosh Eur. J. Inorg. Chem. 2015, 5556–5562 (DOI: 10.1002/ejic.201501165).
- 231- Fe(dppe)(η⁵-C₅Me₅)-based π-conjugated complexes with NO₂ group: A theoretical analysis
H. Sahnoune, S. Gauthier, K. Green, K. Costuas, F. Paul, J.-F. Halet Aust. J. Chem. 2015, 68, 1352–1358 (DOI: 10.1071/CH15136).
- 230- Investigations in the ternary praseodymium - boron – carbon system: Solid-state phase diagram and structural chemistry
V. Babizhetskyy, A. Simon, J.-F. Halet Solid State Sci. 2015, 47, 73-77 (doi: 10.1016/j.solidstatesciences.2014.12.008).
- 229- Structural, Electronic and Magnetic Properties of Early vs Late Transition Metallaborane Clusters - A Theoretical Investigation
K. Bharathia, L. Beermaa, C. Santhia, B. S. Krishnamoorthy, J.-F. Halet J. Organomet. Chem. 2015, 792, 220-228 (doi.org/10.1016/j.jorganchem.2015.05.057).

- 228- Synthesis and chemistry of an open-cage cobalt-heteroborane cluster: A combined experimental and theoretical study
S. K. Barik, V. Dorcet, T. Roisnel, J.-F. Halet, S. Ghosh
Dalton Trans. 2015, 44, 14403-14410 (DOI: 10.1039/C5DT01511A).
- 227- The Cross-cluster M-M Bonding in Oblatonic Dimetallaboranes Unveiled by Topological Analysis
B. Boucher, J.-F. Halet, M. Kohout
Comput. Theor. Chem. 2015, 1068, 134-141 (doi.org/10.1016/j.comptc.2015.06.029).
- 226- 1,2-Diethynylbenzene Bridged [Cp*(dppe)Fe]ⁿ⁺ Units: Effect of the Steric Hindrance on the Chemical and Physical Properties
R. Makhoul, H. Sahnoune, V. Dorcet, J.-F. Halet, J.-R. Hamon, C. Lapinte
Organometallics 2015, 34, 3314-3326 (DOI: 10.1021/acs.organomet.5b00332).
- 225- In search for new bonding modes of the methylenedithiolato ligand: novel tri- and tetrametallic clusters
R. S. Anju, K. Saha, B. Mondal, T. Roisnel, J.-F. Halet, S. Ghosh
Dalton Trans. 2015, 44, 11306-11313 (DOI: 10.1039/c5dt00179j).
- 224- Prediction of high thermoelectric potential in AMN₂ layered nitrides: Electronic and vibrational properties
R. Al Rahal Al Orabi, E. Orisakwe, D. Wee, B. Fontaine, R. Gautier, J.-F. Halet, M. Fornari
J. Chem. Mater. A 2015, 3, 9945-9954 (DOI: 10.1039/C5TA00546A).
- 223- Electronic structure of modeled vs. real carbon-chain containing organometallic dinuclear complexes: similarities and differences
A. Ladjarafi, K. Costuas, H. Meghezzi, J.-F. Halet
J. Mol. Model. 2015, 21, 71-1-71-10 (DOI: 10.1007/s00894-015-2623-3).
- 222- On the Electronic Structure of Organometallic Palladium Clusters of Medium and Large Size: A Theoretical Study
R. Marchal, G. Manca, E. Furet, S. Kahlal, J.-Y. Saillard, J.-F. Halet
J. Cluster Sci. 2015, 26, 41-51 (DOI: 10.1007/s10876-014-0774-5).
- 221- Foreword to the special issue of Polyhedron dedicated to Professor Claude Lapinte
J.-F. Halet, J.-R. Hamon
Polyhedron, 2015, 86, 1 (dx.doi.org/10.1016/j.poly.2014.08.001)
- 220- Complexation of the (η⁵-Cp)Ru⁺ and (η⁵-Cp*)Ru⁺ Arenophiles on Alkynyl Naphthalene: Solvent Effect on the Regioselectivity and the Haptotropic Rearrangement
R. Makhoul, J. A. Shaw-Taberlet, H. Sahnoune, V. Dorcet, S. Kahlal, J.-F. Halet, J.-R. Hamon, C. Lapinte
Organometallics 2014, 33, 6023-6032 (dx.doi.org/10.1021/om500654d).
- 219- Experimental and theoretical studies of quadrupolar oligothiophene-cored chromophores containing dimesitylboryl moieties as π-accepting end groups: Syntheses, structures, fluorescence, one- and two-photon absorption
L. Ji, R. M. Edkins, L. J. Sewell, A. Beeby, A. S. Batsanov, K. Fucke, M. Drafz, J. A. K. Howard, O. Moutounet, F. Ibersiene, A. Boucekkine, E. Furet, Z. Liu, J.-F. Halet, C. Katan, T. B. Marder
Chem. Eur. J. 2014, 20, 13618-13635 (DOI: 10.1002/chem.201402273).
- 218- A Pentanuclear Lead(II) Complex Based on a Strapped Porphyrin with Three Different Coordination Modes
S. Le Gac, E. Furet, T. Roisnel, I. Hijazi, J.-F. Halet, B. Boitrel
Inorg. Chem. 2014, 53, 10660-10666 (dx.doi.org/10.1021/ic5017824).
- 217- Synthesis and Chemistry of Diruthenium Analogue of Pentaborane(11) Containing Dithioformate Ligand: Novel M₃E₅ Cubane Clusters
R. S. Anju, K. Saha, B. Mondal, V. Dorcet, T. Roisnel, J.-F. Halet, S. Ghosh
Inorg. Chem. 2014, 53, 10527-10535 (dx.doi.org/10.1021/ic501623f).

- 216- Proton-Controlled Regioselective Synthesis of $[\text{Cp}^*(\text{dppe})\text{Fe}-\text{C}\equiv\text{C}-1-(\eta^6\text{-C}_{10}\text{H}_7)\text{Ru}(\eta^5\text{-Cp})](\text{PF}_6)$ and Electron-Driven Haptotropic Rearrangement of the $(\eta^5\text{-Cp})\text{Ru}^+$ Arenophile
R. Makhoul, H. Sahnoune, T. Davin, S. Kahlal, V. Dorset, T. Roisnel, J.-F. Halet, J.-R. Hamon, C. Lapinte
Organometallics 2014, 33, 4792–4802 (DOI: 10.1021/om500047k).
 Addition/Correction : 2014, 33, 6267 (DOI: 10.1021/om500971t).
- 215- Synthesis and Properties of *trans*- $[\text{Cp}^*(\text{dppe})\text{Fe}-\text{C}\equiv\text{C}-\text{TTFMe}_2-\text{C}\equiv\text{C}-\text{Fe}(\text{dppe})\text{Cp}^*](\text{PF}_6)_n$ ($n = 0\text{-}3$): A Mixed-Valence Compound with Single Step Tunnelling and Multiple Step Hopping Behavior
R. Makhoul, Y. Kumamoto, A. Miyazaki, F. Justaud, F. Gendron, J.-F. Halet, J.-R. Hamon, C. Lapinte
Eur. J. Inorg. Chem. 2014, 3899–3911 (DOI:10.1002/ejic.201402022).
- 214- High-yield formation of substituted tetracyanobutadienes from reaction of ynamides with tetracyanoethylene
M. Betou, N. Kerisit, E. Meledje, Y. R. Leroux, C. Katan, J.-F. Halet, J.-C. Guillemain, Y. Trolez
Chem. Eur. J. 2014, 20, 9553–9557 (DOI: 10.1002/chem.201402653).
- 213- Theoretical Study on the Structural, Electronic and Physical Properties of Layered Alkaline-Earth-Group-4 Transition-Metal Nitrides AEMN_2
E. Orisakwe, B. Fontaine, D. Gregory, R. Gautier, J.-F. Halet
RSC Adv. 2014, 4, 31981–31987 (DOI: 10.1039/c4ra05395h).
- 212- Selenophosphine Derivatives with Pendant Electron-Rich “ $\text{Fe}(\kappa^2\text{-dppe})(\eta^5\text{-C}_5\text{Me}_5)\text{C}\equiv\text{C}$ ” Substituents
A. Tohme, H. Sahnoune, T. Roisnel, V. Dorcet, J.-F. Halet, F. Paul
Organometallics 2014, 33, 3385–3398 (DOI: 10.1021/om500211e).
- 211- Fluorescence in Rhoda- and Iridacyclopentadienes Neglecting the Spin-Orbit Coupling of the Heavy Atom: The Ligand Dominates
A. Steffen, K. Costuas, A. Boucekkine, M.-H. Thibault, A. Beeby, A. S. Batsanov, A. Charaf-Eddin, D. Jacquemin, J.-F. Halet, T. B. Marder
Inorg. Chem. 2014, 53, 7055–7069 (DOI: 10.1021/ic501115k).
- 210- Hexatriynediyl Spanning Two $\text{Cp}^*(\text{dppe})\text{M}$ Termini (M = Fe, Ru): Evidences for the Dependence of Electronic and Magnetic Couplings on the Relative Orientation of the Termini
A. Burgun, F. Gendron, C. Sumby, T. Roisnel, O. Cador, K. Costuas, J.-F. Halet, M. I. Bruce, C. Lapinte
Organometallics 2014, 33, 2613–2627 (DOI: 10.1021/om500328y).
- 209- Addition and Elimination Reactions of H_2 in Ruthenaborane Clusters: A Computational Study
H. Rabaâ, S. Ghosh, D. Sundholm, J.-F. Halet, J.-Y. Saillard
J. Organomet. Chem. 2014, 761, 1-9 (DOI: 10.1016/j.jorganchem.2014.03.001).
- 208- Beyond the icosahedron: The quest for high-nuclearity supraicosahedral metallaboranes
D. K. Roy, S. Ghosh, J.-F. Halet
J. Cluster Sci. 2014, 25, 225-237 (DOI: 10.1007/s10876-013-0682-0).
- 207- A Metal-capped Conjugated Polyynes Threaded Through a Phenanthroline-based Macrocyclic Beyond the Mechanical Bond to Interactions in Interlocked Molecular Architectures
H. Sahnoune, Z. Baranová, N. Bhuvanesh, J. A. Gladysz, J.-F. Halet
Organometallics 2013, 32, 6360-6367 (DOI: 10.1021/om400709q).
- 206- Covalent Immobilization of Redox-Active $\text{Fe}(\text{dppe})(\eta^5\text{-C}_5\text{Me}_5)$ -Based π -Conjugated Wires on Oxide-Free Hydrogen-Terminated Silicon Surfaces
K. Green, N. Gauthier, H. Sahnoune, J.-F. Halet, F. Paul, B. Fabre

- Organometallics** 2013, 32, 5333–5342 (DOI: 10.1021/om4006017).
- 205- Straightforward Access to New Tetrametallic Complexes with a Square Array by Oxidative Dimerisation of Organometallic Wires
A. Burgun, F. Gendron, P. A. Schauer, B. A. Skelton, P. J. Low, K. Costuas, J.-F. Halet, M. I. Bruce, C. Lapinte
Organometallics 2013, 32, 5015-5025 (DOI: 10.1021/om4003768).
- 204- Acid-base controlled stereoselective metallation of consequences overhanging carboxylic acid porphyrins: Consequences for the formation of heterobimetallic complexes
S. Le Gac, B. Najjari, V. Dorcet, T. Roisnel, L. Fusaro, M. Luhmer, E. Furet, J.-F. Halet, B. Boitrel
Chem. Eur. J. 2013, 19, 11021-11038 (DOI: 10.1002/chem.201300881).
- 203- Synthesis and Characterization of Redox-Active Mononuclear Fe(dppe)(η^5 -C₅Me₅)-Based π -Conjugated Wires
K. Green, N. Gauthier, H. Sahnoune, G. Argouarch, K. Costuas, A. Bondon, L. Toupet, B. Fabre, J.-F. Halet, F. Paul
Organometallics 2013, 32, 4366-4381 (DOI: org/10.1021/om400515g).
- 202- Theoretical Treatment of Ligated Clusters Containing Transition Metals
J.-F. Halet, J.-Y. Saillard
Comprehensive Inorganic Chemistry II (J. Reedijk, K. Poeppelmeier, eds.), Elsevier: Oxford, 2013 vol. 9: *Theory and Methods* (S. Alvarez, volume ed.), p. 869-885.
- 201- Photocatalytic Dimerization of α -Methylstyrene by a Dinuclear Ruthenium-Palladium Complex. Theoretical Aspects
K. Murata, A. Inagaki, M. Akita, J.-F. Halet, K. Costuas
Inorg. Chem. 2013, 52, 8030-8039 (dx.doi.org/10.1021/ic400666v).
- 200- Hybrid Molecular Systems Containing Tetrathiafulvalene and Iron-Alkynyl Electrophores: A Model of Nanojunction at the Molecular Model
F. Justaud, F. Gendron, Y. Ogyu, Y. Kumamoto, A. Miyazaki, L. Ouahab, K. Costuas, J.-F. Halet, C. Lapinte
Chem. Eur. J. 2013, 19, 5742–5757 (DOI: 10.1002/chem.201204227).
- 199- Geometrical, electronic structural and mechanistic studies on group-14 element-diruthenaborane cluster compounds – A theoretical investigation
B. S. Krishnamoorthy, S. Kahlal, S. Ghosh, J.-F. Halet
Theor. Chem. Acc. 2013, 132, 1356-1–1356-10 (DOI: 10.1007/s00214-013-1356-6).
- 198- Oxidative Activation of Aryldiynyl-Iron Complexes: Regio-Selective Dimerization
A. Burgun, F. Gendron, T. Roisnel, K. Costuas, J.-F. Halet, M. Bruce, C. Lapinte
Organometallics 2013, 32, 1866–1875 (dx.doi.org/10.1021/om400014g).
- 197- Theoretical Analysis of the Structure and Bonding in Electron-Rich Edge-Bridged Octahedral Tungsten Chloride Clusters
N. Nebbache, B. Fontaine, H.-J. Meyer, R. Gautier, J.-F. Halet
Solid State Sciences 2013, 19, 150–155
(dx.doi.org/10.1016/j.solidstatesciences.2013.02.024).
- 196- Charge delocalization vs localization in carbon-rich iron mixed-valence complexes: a subtle interplay between the carbon spacer and the (dppe)Cp*Fe organometallic electrophore
J.-F. Halet, C. Lapinte
Coord. Chem. Rev. 2013, 257, 1584–1613 (dx.doi.org/10.1016/j.ccr.2012.09.007).
- 195- The preparation, characterisation and electronic structures of 2,4-pentadiynyl nitrile (cyanobutadiynyl) complexes
S. Bock, S. G. Eaves, M. Parthey, M. Kaupp, B. Le Guennic, J.-F. Halet, D. S. Yufit, J. A.K. Howard, P. J. Low
Dalton Trans. 2013, 42, 4240–4243 (DOI: 10.1039/c3dt33052d).

- 194- Molecular transition-metal boron compounds. Any interest?
B. S. Krishnamoorthy, S. Kahlal, B. Le Guennic, J.-Y. Saillard, S. Ghosh, J.-F. Halet
Solid State Sciences 2012, 14, 1617–1623
 (doi.org/10.1016/j.solidstatesciences.2012.03.026).
- 193- Bonding and Electronic Structure of $\text{Cp}^*\text{Ru}_2(\text{B}_8\text{H}_{14})$, a Metalloborane Analogue of Dinuclear Pentalene Complexes
B. Boucher, S. Ghosh, J.-F. Halet, S. Kahlal, J.-Y. Saillard
J. Organomet. Chem. 2012, 721–722, 167–172.
- 192- Foreword. A Special Issue Devoted to Thomas P. Fehlner on the Occasion of his 75th Birthday
S. Ghosh, J.-F. Halet, J.-Y. Saillard
J. Organomet. Chem. 2012, 721–722, 1–2.
- 191- Structures and Stabilities of Small, Ligated $\text{Al}_n\text{L}_n^{0/2-}$ and $\text{Al}_n\text{L}_{n+2}$ Clusters (L = H, Cl) – A Theoretical Study
R. Marchal, G. Manca, S. Kahlal, P. Carbonnière, C. Pouchan, J.-F. Halet, J.-Y. Saillard
Eur. J. Inorg. Chem. 2012, 4856–4866.
- 190- Iron and Ruthenium σ -Poly-ynyls of General Formula $[\{\text{M}(\text{dppe})\text{Cp}^*\}-(\text{C}\equiv\text{C})_n\text{-R}]^{0/+}$ (M = Fe, Ru); An Experimental and Theoretical Investigation
F. Gendron, A. Burgun, B. W. Skelton, A. H. White, T. Roisnel, M. I. Bruce, J.-F. Halet, C. Lapinte, K. Costuas
Organometallics 2012, 31, 6796–6811.
- 189- Theoretical and Experimental Investigations on Hypoelectronic Heterodimetallaboranes of Group 6 Transition Metals
B. S. Krishnamoorthy, A. Thakur, K. K. V. Chakrahari, S. K. Bose, P. Hamon, T. Roisnel, S. Kahlal, S. Ghosh, J.-F. Halet
Inorg. Chem. 2012, 51, 10375–10383.
- 188- Synthesis and Characterization of Hypoelectronic Tantalaboranes. Comparison of the Geometric and Electronic Structures of $[(\text{Cp}^*\text{TaX})_2\text{B}_5\text{H}_{11}]$ (X = Cl, Br and I)
K. Geetharani, B. S. Krishnamoorthy, S. Kahlal, S. M. Mobin, J.-F. Halet, S. Ghosh
Inorg. Chem. 2012, 51, 10176–10184.
- 187- Oxidative Dimerisation of Aryldiynyl-ruthenium Complexes
M. I. Bruce, K. Costuas, F. Gendron, J.-F. Halet, M. Jevric, B. W. Skelton
Organometallics 2012, 31, 6555–6566.
- 186- Structural diversity within the series of 68-electron $\text{L}_n\text{M}_4\text{E}_2$ (M = Fe, Ru, Os, Co; E = CH, N, P, NR, PR, S) Organometallic Clusters: A Theoretical Investigation
N. Guechtouli, A. Boucekkine, J.-F. Halet, S. Kahlal, H. Meghezzi, J.-Y. Saillard
J. Cluster Sci. 2012, 23, 913–928.
- 185- Can high-hydride content hypoelectronic rhenaborane clusters take up dihydrogen? A theoretical study
M. Rochdi, J.-Y. Saillard, J.-F. Halet, S. Ghosh, H. Rabaâ
Polyhedron 2012, 43, 31–35.
- 184- Extending Metal-Capped Polyynediyl Molecular Wires by Insertion of Inorganic Metal Units
M. I. Bruce, B. Le Guennic, N. Scoleri, N. N. Zaitseva, J.-F. Halet
Organometallics 2012, 31, 4701–4706.
- 183- Structural, electronic and magnetic properties of some layered REB_2C compounds (RE = Dy, Tm, Lu)
V. Babizhetskyy, H. Mattausch, A. Simon, K. Hiebl, L. Le Pollès, R. Gautier, J.-F. Halet
J. Solid State Chem. 2012, 191, 121–128.

- 182- Translocation-coupled transmetalation at the origin of a dinuclear lead porphyrin complex: implication of an unprecedented *hanging-atop* coordination mode
S. Le Gac, B. Najjari, L. Fusaro, T. Roisnel, V. Dorcet, M. Luhmer, E. Furet, J.-F. Halet, B. Boitrel
Chem. Commun. 2012, 48, 3724–3726.
- 181- 3,5-bis(ethynyl)pyridine and 2,6-bis(ethynyl)pyridine Spaning Two Fe(Cp*)(dppe) Units: Role of the Nitrogen Atom on the Electronic and Magnetic Couplings
K. Costuas, O. Cador, F. Justaud, S. Le Stang, F. Paul, A. Monari, S. Evangelisti, L. Toupet, C. Lapinte, J.-F. Halet
Inorg. Chem. 2011, 50, 12601–12622.
- 180- Simultaneous bridge-localised and mixed-valence character in diruthenium radical cations featuring diethynylaromatic bridging ligands
M. A. Fox, B. Le Guennic, R. L. Roberts, D. A. Brue, D. S. Yufit, J. A. K. Howard, G. Manca, J.-F. Halet, F. Hartl, P. J. Low
J. Am. Chem. Soc. 2011, 133, 18433–18446.
- 179- Octahedral Niobium Cluster-Based Solid State Halides and Oxyhalides: Effects of the Cluster Condensation via Oxygen Ligand on Structural, Electronic, and Magnetic Properties
B. Fontaine, S. Cordier, R. Gautier, F. Gulo, J.-F. Halet, B. Perić, C. Perrin
New J. Chem. 2011, 35, 2245–2252.
- 178- Spectroscopic Evidence for Redox Isomerism in the 1,4-Diethynylbenzene Bridged Heterobimetallic Cation $[\{\text{Fe}(\text{dppe})\text{Cp}^*\}(\mu\text{-C}\equiv\text{CC}_6\text{H}_4\text{C}\equiv\text{C})\{\text{Mo}(\text{dppe})(\eta\text{-C}_7\text{H}_7)\}]\text{PF}_6$
E. C. Fitzgerald, A. Ladjarafi, N. J. Brown, D. Collison, K. Costuas, R. Edge, J.-F. Halet, F. Justaud, P. J. Low, H. Meghezzi, T. Roisnel, M. W. Whiteley, C. Lapinte
Organometallics, 2011, 30, 4180–4195.
- 177- New Thiocyanato and Azido Adducts of the Redox-Active $\text{Fe}(\eta^5\text{-C}_5\text{Me}_5)(\eta^2\text{-dppe})$ Center: Synthesis and Study of the Fe(II) and Fe(III) Complexes
F. Malvolti, A. M. Trujillo, O. Cador, F. Gendron, K. Costuas, J.-F. Halet, A. Bondon, L. Toupet, Y. Molard, S. Cordier, F. Paul
Inorg. Chim. Acta 2011, 374, 288–301.
- 176- New members of ternary rare-earth metal boride carbides containing finite boron-carbon chains: $\text{RE}_{25}\text{B}_{14}\text{C}_{26}$ (RE = Pr, Nd) and $\text{Nd}_{25}\text{B}_{12}\text{C}_{28}$
V. Babizhetskyy, H. Mattausch, A. Simon, R. Gautier, J.-F. Halet
J. Solid State Chem. 2011, 184, 1671–1681.
- 175- Oxidative Dimerization of Arylalkynyl-Ruthenium Complexes
M. I. Bruce, A. Burgun, F. Gendron, G. Grelaud, J.-F. Halet, B. W. Skelton
Organometallics 2011, 30, 2861–2868.
- 174- Electron-rich Iron-Ruthenium Arylalkynyl Complexes for Third-Order Nonlinear Optics. Redox-Switching between Three States
N. Gauthier, G. Argouarch, F. Paul, L. Toupet, A. Ladjarafi, K. Costuas, J.-F. Halet, M. Samoc, M. P. Cifuentes, T. C. Corkery, M. G. Humphrey
Chem. Eur. J. 2011, 17, 5561–5577.
- 173- Formation of a Dinuclear Mercury(II) Complex with a Regular Bis-Strapped Porphyrin Following a Tunable Cooperative Process
N. Motreff, S. Le Gac, M. Luhmer, E. Furet, J.-F. Halet, T. Roisnel, B. Boitrel
Angew. Chem., Int. Ed. 2011, 50, 1560–1564.
- 172- The Electronic Properties of Metal Borides and Borocarbides. Differences and Similarities
S. Lassoued, R. Gautier, J.-F. Halet
Boron Rich Solids: Sensors, Ultra High Temperature Ceramics, Thermoelectrics, Armor, Eds. N. Orlovskaya, M. Lugovy, Springer Science and Business Media V. B., 2011, pp. 95–114.

- 171- Interactions Between the Redox-Active Cp*(dppe)Fe Acetylide and a TTF Derivative. A New Mixed-Valence System
A. Miyazaki, Y. Ogyu, F. Justaud, L. Ouahab, T. Cauchy, J.-F. Halet, C. Lapinte
Organometallics, 2010, 29, 4628-4638.
- 170- Exploiting Non-Innocent Ligands: New Routes to Masked Pd(0) Complexes
D. A. Smith, A. S. Batsanov, K. Costuas, R. Edge, D. C. Apperley, D. Collison, J.-F. Halet, J. A. K. Howard, P. W. Dyer
Angew. Chem., Int. Ed. 2010, 49, 7040-7044.
- 169- Characterization of a Six-Coordinate Ferrous High-Spin Heme with both Intramolecular Axial Carboxylic Acid and Pyridine
I. Hijazi, T. Roisnel, P. Even-Hernandez, E. Furet, J.-F. Halet, O. Cador, B. Boitrel
J. Am. Chem. Soc. 2010, 132, 10652-10653.
- 168- Rings and chains in solid-state metal borides and borocarbides. The electron count matters
S. Lassoued, R. Gautier, A. Boutarfaia, J.-F. Halet
J. Organomet. Chem. 2010, 695, 983-997.
- 167- Syntheses, Structures, Two-Photon Absorption Cross-Sections and Computed Second Hyperpolarisabilities of Quadrupolar A- π -A Systems Containing E-Dimesitylborylethenyl Acceptors
C. D. Entwistle, J. C. Collings, A. Steffen, L.-O. Pålsson, A. Beeby, D. Albesa-Jové, J. M. Burke, A. S. Batsanov, J. A. K. Howard, J. A. Mosely, S.-Y. Poon, W.-Y. Wong, F. Ibersiene, S. Fathallah, A. Boucekkine, J.-F. Halet, T. B. Marder
J. Mater. Chem., 2009, 19, 7532-7544.
- 166- Computational Methods: Transition Metal Cluster-Chemistry
R. Gautier, J.-F. Halet, J.-Y. Saillard
Computational Inorganic and Bioinorganic Chemistry, Eds. E. Solomon, R. A. Scott, R. B. King, John Wiley & Sons, Chichester, UK, 2009, pp. 433-452.
- 165- Experimental and Theoretical Evidences of π -d Interactions in Supramolecular Assemblies Based on TTF-CH=CH-Py Ligands Tethered to Mo₆X₈ Octahedral Molybdenum Halide Cluster Cores
G. Prabusankar, Y. Molard, S. Cordier, S. Golhen, Y. Le Gal, C. Perrin, L. Ouahab, S. Kahlal, J.-F. Halet
Eur. J. Inorg. Chem., 2009, 2153-2161 (DOI: 10.1002/ejic.200900136).
- 164- Bonding and Electron Delocalization in Ru(III) σ -Arylacetylide Radicals [trans-Cl(η^2 -dppe)₂RuC \equiv C(4-C₆H₄X)]⁺ (X = NO₂, C(O)H, C(O)Me, F, H, OMe, NMe₂): Misleading Aspects of the ESR Anisotropy
N. Gauthier, N. Tchouar, F. Justaud, G. Argouarch, M. P. Cifuentes, L. Toupet, D. Touchard, J.-F. Halet, S. Rigaut, M. G. Humphrey, K. Costuas, F. Paul
Organometallics, 2009, 28, 2253-2266 (DOI: 10.1021/om801138q).
- 163- Some transition metal complexes derived from mono- and di-ethynyl perfluorobenzenes
D. J. Armit, M. I. Bruce, M. Gaudio, N. N. Zaitseva, B. W. Skelton, A. H. White, B. Le Guennic, J.-F. Halet, M. A. Fox, P. J. Low
Dalton Trans., 2008, 6763-6775 (DOI: 10.1039/b808798a).
- 162- New examples of ternary rare-earth metal boride carbides containing finite boron-carbon chains: The crystal and electronic structure of RE₁₅B₆C₂₀ (RE = Pr, Nd)
V. Babizhetskyy, Hj. Mattausch, A. Simon, K. Hiebl, M. Ben Yahia, R. Gautier, J.-F. Halet
J. Solid State Chem. 2008, 181, 1882-1890.
- 161- DFT Calculations of Quadrupolar Solid State NMR Properties. Some Examples in Solid-State Inorganic Chemistry
J. Cuny, S. Messaoudi, V. Alonzo, E. Furet, J.-F. Halet, E. Le Fur, S. E. Ashbrook, C. J. Pickard, R. Gautier, L. Le Pollès
J. Comput. Chem. 2008, 29, 2279-2287.

- 160- Can Metal Tetraborides Exist with Divalent Metals? A Partial Answer from the Comparison of their DFT Electronic Structure with that of Rare-Earth Metal Tetraborides
M. Ben Yahia, O. Reckeweg, R. Gautier, J. Bauer, T. Schleid, J.-F. Halet, J.-Y. Saillard
Inorg. Chem. 2008, 47, 6137–6143.
- 159- Electron-Sponge Behavior, Reactivity and Electronic Structures of Cobalt-Centered Cubic $\text{Co}_9\text{Te}_6(\text{CO})_8$ Clusters
M. Bencharif, O. Cador, H. Cattey, A. Ebner, J.-F. Halet, S. Kahlal, W. Meier, Y. Mugnier, J.-Y. Saillard, P. Schwarz, F. Z. Trodi, J. Wachter, M. Zabel
Eur. J. Inorg. Chem. 2008, 1959–1968.
- 158- Ruthenium complexes of C,C'-bis(ethynyl)-1,10- and 1,12-*para*-carboranes: An investigation of electronic interactions mediated by spherical pseudo-aromatic spacers
M. A. Fox, R. L. Roberts, T. E. Baines, B. Le Guennic, J.-F. Halet, F. Hartl, D. S. Yuffit, D. Albesa-Jové, J. A. K. Howard, P. J. Low.
J. Am. Chem. Soc., 2008, 130, 3566–3578.
- 157- Beryllocene-like in solid state chemistry: The η^1, η^6 coordination of beryllium ions in graphite-analogue BeB_2C_2
K. Hofmann, X. Rocquefelte, J.-F. Halet, C. Baehtz, B. Albert
Angew. Chem., Int. Ed., 2008, 47, 2301–2303.
- 156- Syntheses, structures and redox properties of some complexes containing the $\text{Os}(\text{dppe})\text{Cp}^*$ fragment, including $\{\text{Os}(\text{dppe})\text{Cp}^*\}_2(\mu\text{-C}\equiv\text{CC}\equiv\text{C})$
M. I. Bruce, K. Costuas, T. Davin, J.-F. Halet, K. A. Kramarczuk, P. J. Low, B. K. Nicholson, G. J. Perkins, R. L. Roberts, B. W. Skelton, M. E. Smith, A. H. White
Dalton Trans., 2007, 5387–5399.
- 155- Magnetic and Nonmagnetic Octahedral Cluster Units in Molybdenum Chalcogenide Chemistry
K. Kirakci, S. Cordier, A. Shames, B. Fontaine, O. Hernandez, E. Furet, J.-F. Halet, R. Gautier, C. Perrin
Chem. Eur. J., 2007, 13, 9608–9616.
- 154- M_2B_5 or M_2B_4 ? A reinvestigation of the Mo/B and W/B system
M. Frotscher, W. Klein, J. Bauer, C.-M. Fang, J.-F. Halet, A. Senyshyn, C. Baehtz, B. Albert
Z. Anorg. Allg. Chem., 2007, 633, 2626–2630.
- 153- Linked and Fused Tungstaborane Clusters: Synthesis, Characterization and Electronic Structures of *bis*- $\{(\eta^5\text{-C}_5\text{Me}_5\text{W})_2\text{B}_5\text{H}_8\}_2$ and $(\eta^5\text{-C}_5\text{Me}_5\text{W})_2\{\text{Fe}(\text{CO})_3\}_n\text{B}_{6-n}\text{H}_{10-n}$, $n = 0, 1$
S. K. Bose, S. Ghosh, B. C. Noll, J.-F. Halet, J.-Y. Saillard, A. Vega
Organometallics, 2007, 26, 5377–5385.
- 152- Crystal structures of ternary metal boron carbides MB_2C_4 ($M = \text{Mg}, \text{Ca}; \text{La}$ and Ce) from first-principles theory
Fang, C.-M.; Bauer, J.; Saillard, J.-Y.; Halet, J.-F.
J. Solid State Chem., 2007, 80, 2465–2470.
- 151- Hypothetical hypercloso octahedral M_4N_2 clusters: A new mode of dinitrogen coordination?
F. Z. Trodi, G. Lucas, M. Bencharif, J.-F. Halet, S. Kahal, J.-Y. Saillard
J. Cluster Sci., 2007, 18, 729–740.
- 150- Molecular Clusters. A Bridge to Solid State Chemistry
T. P. Fehlner, J.-F. Halet, J.-Y. Saillard
 Cambridge University Press, Cambridge, Grande-Bretagne, ISBN-13 978-0-521-85236-4, 2007, 378 pp.
- 149- On the Electronic Structure of Distorted Cubic Rhodium Cluster Complexes Containing Bridging Germanium or Phosphorus Ligands
Zouchoune, B.; Saillard, J.-Y.; Halet, J.-F.
J. Cluster Sci., 2007, 18, 720–728.

- 148- Redox-active complexes containing Group 8 metal centres linked by C₂ bridges
M. I. Bruce, K. Costuas, B. G. Ellis, J.-F. Halet, P. J. Low, N. Ouddai, G. S. Perkins, B. K. Skelton, A. H. White
Organometallics, 2007, 26, 3735–3745.
- 147- Bismuth and lead hanging-carboxylate porphyrins: Unprecedented mononuclear dimetallic lead(II) complex
Z. Halime, M. Lachkar, T. Roisnel, E. Furet, J.-F. Halet, B. Boitrel
Angew. Chem., Int. Ed., 2007, 46, 5120–5124.
- 146- Crystal structure of the graphite intercalate LaC₆ predicted from first-principles theory
Fang, C.-M.; Bauer, J.; Saillard, J.-Y.; Halet, J.-F.
Z. Naturforsch. B, 2007, 62b, 971–976.
- 145- Synthesis, photophysical properties and crystal and molecular structures of luminescent 2,5-bis(*p*-R-phenylethynyl)thiophenes and 2,5-bis(pentafluorophenylethynyl)thiophene
J. S. Siddle, R. M. Ward, J. C. Collings, S. R. Rutter, L. Porrès, L. Applegarth, A. Beeby, A. S. Batsanov, A. L. Thompson, J. A. K. Howard, A. Boucekkine, K. Costuas, J.-F. Halet, T. B. Marder
New J. Chem., 2007, 31, 841–851.
- 144- Electron counting in carbaalane clusters with cubic aluminum core
B. Creton, S. Kahlal, M. T. Garland, Z. Lin, J.-F. Halet, J.-Y. Saillard
J. Cluster Science, 2007, 18, 271–288.
- 143- Metallaborane Reactivity. A Stoichiometric Mechanism for the Insertion of Two Alkynes into an Iridaborane Framework via a Disposable Molybdenum Chaperone
de Montigny, F.; Macias, R.; Noll, B.; Fehlner, T. P.; Costuas, K.; Saillard, J.-Y.; Halet, J.-F.
J. Am. Chem. Soc., 2007, 129, 3392–3401.
- 142- Chemical Bonding and Properties of EuPdGe and EuPtGe
Rocquefelte, X.; Gautier, R.; Halet, J.-F.; Müllmann, R.; Rosenhahn, C.; Mosel, B. D.; Kotzyba, G.; Pöttgen, R.
J. Solid State Chem., 2007, 180, 533–540.
- 141- Spin delocalization in Electron-Rich Iron(III) Piano-Stool σ -Acetylides. An Experimental (NMR) and Theoretical (DFT) Investigation
Paul, F.; da Costa, G.; Bondon, A.; Gauthier, N.; Sinbandhit, S.; Toupet, L.; Costuas, K.; Halet, J.-F.; Lapinte, C.
Organometallics, 2007, 26, 874–896.
- 140- Electron-Sponge Behavior and Electronic Structures in Cobalt-Centered Pentagonal Prismatic Co₁₁Te₇(CO)₁₀ and Co₁₁Te₅(CO)₁₅ Clusters
Cador, O.; Cattey, H.; Halet, J.-F.; Meier, W.; Mugnier, Y.; Saillard, J.-Y.; Wachter, J.; Zabel, M.; Zouchoune, B.
Inorg. Chem., 2007, 46, 501–509.
- 139- M₂B₄ vs. M₂B₅ structure type (M = Mo, W): A new DFT and crystal structure study
M. Frotscher, W. Klein, B. Albert, N. Combes, J. Bauer, C.-M. Fang, J.-F. Halet
Z. Anorg. Allg. Chem., 2006, 632, 2165.
- 138- Linear and pre-organized carboxylic acid picket(s) porphyrins as bismuth chelators
Halime, Z.; Lachkar, M.; Furet, E.; Halet, J.-F.; Boitrel, B.
Inorg. Chem., 2006, 45, 10661–10669.
- 137- Portraits of Some Representatives of Rare-Earth Metal Boride Carbide and Boride Silicide Compounds
Ben Yahia, M.; Roger, J.; Rocquefelte, X.; Gautier, R.; Bauer, J.; Guérin, R.; Saillard, J.-Y.; Halet, J.-F.
J. Solid State Chem., 2006, 179, 2779–2786.

- 136- Mn₅Si₃-type host-interstitial boron rare-earth metal silicide compounds RE₅Si₃: Crystal structures, physical properties and theoretical considerations
Roger, J.; Ben Yahia, M.; Babizhetskyy, V.; Cordier, S.; Guérin, R.; Bauer, J.; Hiebl, K.; Rocquefelte, X.; Saillard, J.-Y.; Halet, J.-F.
J. Solid State Chem., 2006, 179, 2310–2328.
- 135- Tin flux synthesis of rare-earth metal silicide compounds RESi_{1.7} (RE = Dy, Ho) : A novel ordered structure derived from the AlB₂ type
Roger, J.; Babizhetskyy, V.; Jardin, R.; Guérin, R.; Moinet, C.; Burkhardt, U.; Halet, J.-F.
Z. Kristallogr., 2006, 221, 502–510.
- 134- The ternary RE-Si-B Systems (RE = Dy, Ho, Er and Y) at 1270 K: Solid state phase equilibria and magnetic properties of the solid solution REB_{2-x}Si_x (RE = Dy and Ho)
Roger, J.; Babizhetskyy, V.; Guizouarn, T.; Hiebl, K.; Guérin, R.; Halet, J.-F.
J. Alloys Compds., 2006, 417, 72–84.
- 133- Solid state phase equilibria in the ternary Nd-Si-B system at 1270 K
Roger, J.; Babizhetskyy, V.; Jardin, R.; Halet, J.-F.; Guérin, R.
J. Alloys Compds., 2006, 415, 73–84.
- 132- Synthesis, Crystal Structures, Linear and Nonlinear Optical Properties, and Theoretical Studies of (*p*-R-Phenyl)-, (*p*-R-Phenylethynyl)-, and (*E*)-[2-(*p*-RPhenyl)ethenyl] dimesitylboranes and Related Compounds
Yuan, Z.; Entwistle, C. D.; Collings, J. C.; Albesa-Jove, D. Batsanov, A. S.; Howard, J. A. K.; Kaiser, H. M.; Kaufmann, D. E.; Poon, S.-K.; Wong, W.-Y.; Jardin, C.; Fathallah, S.; Boucekkine, A.; Halet, J.-F.; Marder, T. B.
Chem. Eur. J., 2006, 12, 2758–2771.
- 131- Iodine Substituted Tetrathiafulvalene Radical Cation Salts with [M(isoq)₂(NCS)₄]⁻ Anions where M = Cr^{III}, Ga^{III}: Role of I···S and S···S Contacts on Structural and Magnetic Properties
Hervé, K.; Cador, O.; Golhen, S.; Costuas, K.; Halet, J.-F.; Shirahata, T.; Muto, T.; Imakubo, T.; Miyazaki, A.; Ouahab, L.
Chem. Mater., 2006, 18, 790–797.
- 130- Bonding and Substituent Effects in Electron-Rich Mononuclear Ruthenium σ -Arylacetylides of Formula [(η^2 -dppe)(η^5 -C₅Me₅)Ru(C \equiv C-C₆H₄-X)][PF₆]ⁿ (n = 0, 1)
Paul, F.; Ellis, B. G.; Bruce, M. I.; Toupet, L.; Roisnel, T.; Costuas, K.; Halet, J.-F.; Lapinte, C.
Organometallics, 2006, 25, 649–665.
- 129- Synthesis and Crystal and Electronic Structures of the Na₂(Sc₄Nb₂)(Nb₆O₁₂)₃ Octahedral Niobium Cluster Oxide. Structural Correlations between A_nBM₆L₁₂(Z) Series and Chevrel Phases
Cordier, S.; Kirakci, K.; Fontaine, B.; Halet, J.-F.; Gautier, R.; Perrin, C.
Inorg. Chem., 2006, 45, 883–893.
- 128- Structural chemistry, magnetism and electrical properties of binary Gd silicides and Ho₃Si₄
Roger, J.; Babizhetskyy, V.; Hiebl, K.; Halet, J.-F.; Guérin, R.
J. Alloys Compds., 2006, 407, 25–35.
- 127- Structural Preference versus Metal within the MB₂C₂ (M = Mg, Sc, Ca, Y, Ln) Phases: The Coloring Problem Revisited by DFT Calculations
Rocquefelte, X.; Boulfelfel, S.-E.; Ben Yahia, M.; Bauer, J.; Saillard, J.-Y.; Halet, J.-F.
Angew. Chem., Int. Ed., 2005, 44, 7542–7545. **Angew. Chem.**, 2005, 117, 7714–7717.
- 126- Electronic interactions in bridged bis(cluster) assemblies – a comparison of *para*-CB₁₀H₁₀C, *para*-C₆H₄ and C₄ bridges
Le Guennic, B.; Costuas, K.; Halet, J.-F.; Nervi, C.; Paterson, M. A. J.; Fox, M. A.; Roberts, R. L.; Albesa-Jove, D.; Puschmann, H.; Howard, J. A. K.; Low, P. J.
C. R. Chimie, 2005, 8, 1883–1896.

- 125- Skeletal Isomerism in Mixed Transition-Metal/Main-Group *Closo* Clusters
Guechtouli, N.; Lucas, G.; Boucekkine, A.; Halet, J.-F.; Kahlal, S.; Lokbani-Azzouz, N. S.; Meghezzi, H.; Saillard, J.-Y.
C. R. Chimie, 2005, 8, 1863–1872.
- 124- Electron-Rich Piano-Stool Iron σ -Acetylides. Electronic Structure of Arylalkynyl Fe(III) Radical Cations
Paul, F.; Toupet, L.; Thépot, J.-Y.; Costuas, K.; Halet, J.-F.; Lapinte, C.
Organometallics, 2005, 24, 5464–5478.
- 123- Electron Transfer and Electron Exchange between [Cp*(dppe)Fe]ⁿ⁺ (n = 0, 1) Building Blocks Mediated by the 9,10-bis(Ethynyl)anthracene Bridge
de Montigny, F.; Argouarch, G.; Costuas, K.; Halet, J.-F.; Roisnel, T.; Toupet, L.; Lapinte, C.
Organometallics, 2005, 24, 4558–4572.
- 122- Iron versus Ruthenium – Dramatic Changes in Electronic Structure Result from Replacement of one Fe by Ru in [{Cp*(dppe)Fe}-CC-CC-{Fe(dppe)Cp*}]ⁿ⁺ (n = 0, 1, 2)
Bruce, M. I.; Costuas, K.; Davin, T.; Ellis, B. G.; Halet, J.-F.; Lapinte, C.; Low, P. J.; Smith, M. E.; Skelton, B. W.; Toupet, L.; White, A. H.
Organometallics, 2005, 24, 3864–3881.
- 121- Bridging Phosphanes: Exotic or Versatile Binucleating Ligands?
Leca, F.; Lescop, C.; Rodriguez, E.; Costuas, K.; Halet, J.-F.; Réau, R.
Angew. Chem., Int. Ed., 2005, 44, 4362–4365.
- 120- Theoretical aspects of the bonding in acetylide-bridged organometallic dinuclear complexes
Ouddaï, N.; Costuas, K.; Bencharif, M.; Saillard, J.-Y., Halet, J.-F.
Comptes-Rendus-Chimie, 2005, 8, 1336–1350.
- 119- Crystal structures, physical properties and NMR experiments on the ternary rare-earth metal silicide boride compounds RE₅Si₂B₈ (RE = Y, Sm, Gd, Tb, Dy, Ho)
Roger, J.; Babizhetskyy, V.; Cordier, S.; Bauer, J.; Hiebl, K.; Le Pollès, L.; Ashbrook, S. E.; Halet, J.-F.; Guérin, R.
J. Solid State Chem., 2005, 178, 1851–1863.
- 118- Structural Chemistry and Physical Properties of the Rare Earth Silicide Dy₃Si₄
Roger, J.; Guizouarn, T.; Hiebl, K.; Halet, J.-F.; Guérin, R.
J. Alloys Compds., 2005, 394, 28–34.
- 117- B₅C₅ Anionic Molecules Trapped in a Solid Matrix: The Crystal and Electronic Structures of the Rare Earth Metal Boride Carbide LaBC
Babizhetskyy, V.; Mattausch, H.; Simon, A.; Gautier, R.; Bauer, J.; Halet, J.-F.
Z. Anorg. Allg. Chem., 2005, 631, 1041–1046.
- 116- Boron–silicon solid solution: synthesis and crystal structure of a carbon-doped boron-rich SiB_n (n~30) compound
Roger, J.; Babizhetskyy, V.; Halet, J.-F.; Guérin, R.
J. Solid State Chem., 2004, 177, 4167–4174.
- 115- Some ruthenium complexes containing cyanocarbon ligands: syntheses, structures and electronic communication in binuclear systems
Bruce, M. I.; Buntine, M. A.; Costuas, K.; Ellis, B. G.; Halet, J.-F.; Low, P. J.; Skelton, B. W.; White, A. H.
J. Organomet. Chem., 2004, 689, 3308–3326.
- 114- Luminescent Heterometallic Branched Alkynyl Complexes of Rhenium(I)-Palladium(II) - Potential Building Blocks for Heterometallic Metallodendrimers
Chong, S. H.-F.; Lam, S. C.-F.; Yam, V. W.-W.; Zhu, N.; Cheung, K.-K.; Fathallah, S.; Costuas, K.; Halet, J.-F.
Organometallics, 2004, 23, 4924–4933.

- 113- Bonding analysis of square-antiprismatic and fused square-antiprismatic copper(I)-selenium clusters
Zouchoune, Z.; Halet, J.-F.; Saillard, J.-Y.
J. Cluster Sci., 2004, 15, 267–276.
- 112- Synthesis, Photophysics, Electrochemistry and Transient Absorption Studies of Luminescent Copper(I) and Silver(I) Diynyl Complexes. X-ray Crystal Structures of $[\text{Cu}_3(\mu\text{-dppm})_3(\mu_3\text{-}\eta^1\text{-C}\equiv\text{CC}\equiv\text{CPh})_2]\text{PF}_6$ and $[\text{Cu}_3(\mu\text{-dppm})_3(\mu_3\text{-}\eta^1\text{-C}\equiv\text{CC}\equiv\text{CH})_2]\text{PF}_6$
Yam, V. W.-W.; Lo, W.-Y.; Lam, S. C.-F.; Cheung, K.-K.; Zhu, N.; Fathallah, S.; Messaoudi, S.; Le Guennic, B.; Kahlal, S.; Halet, J.-F.
J. Am. Chem. Soc., 2004, 126, 7300–7310.
- 111- Synthesis and Characterization of Hypoelectronic Rhenaboranes. Analysis of the Geometric and Electronic Structures of Species Following Neither Borane nor Metal Cluster Electron Counting Paradigms
Le Guennic, B.; Jiao, H.; Kahlal, S.; Saillard, J.-Y.; Halet, J.-F.; Ghosh, S.; Shang, M.; Beatty, A. M.; Rheingold, A. L.; Fehlner, T. P.
J. Am. Chem. Soc., 2004, 126, 3203–3217 (doi.org/10.1021/ja039770b).
- 110- Electron-Rich Piano-Stool Iron σ -Acetylides. Theoretical and Phenomenological Investigation of Electronic Substituent Effects in Fe(II) Acetylides
Costuas, K.; Paul, F.; Toupet, L.; Halet, J.-F.; Lapinte, C.
Organometallics, 2004, 23, 2053–2068.
- 109- $\text{Gd}_5\text{Si}_2\text{B}_8$: A Ternary Rare-Earth-Metal Silicide Boride Compound
Babizhetskyy, V.; Roger, J.; Députier, S.; Guérin, R.; Jardin, R.; Bauer, J.; Hiebl, K.; Jardin, C.; Saillard, J.-Y.; Halet, J.-F.
Angew. Chem., Int. Ed., 2004, 43, 1979–1983; **Angew. Chem.**, 2004, 116, 2013–2016.
- 108- A Novel Layered Niobium Oxychloride Based on Nb_2 Pairs and Nb_6 Octahedral Clusters: Synthesis, Crystal and Electronic Structures of $\text{Nb}_{10}\text{Cl}_{16}\text{O}_7$
Cordier, S.; Roisnel, T.; Gulo, F.; Le Guennic, B.; Gautier, R.; Halet, J.-F.; Perrin, C.
Inorg. Chem., 2003, 42, 8320–8327.
- 107- Chemistry of the 1,3,5,7-octatetraynediyl carbon rod end-capped by two electron-rich ($\eta^5\text{-C}_5\text{Me}_5$)($\mu^2\text{-dppe}$)Fe groups
Coat, F.; Paul, F.; Lapinte, C.; Toupet, L.; Costuas, K.; Halet, J.-F.
J. Organomet. Chem., 2003, 683, 368–378.
- 106- Electro-Switchable Photoluminescence Activity: Synthesis, Spectroscopy, Electrochemistry, Photophysics, and X-ray Crystal and Electronic Structures of $[\text{Re}(\text{bpy})(\text{CO})_3(\text{C}\equiv\text{C}-\text{C}_6\text{H}_4-\text{C}\equiv\text{C})\text{Fe}(\eta^5\text{-C}_5\text{Me}_5)(\mu^2\text{-dppe})][\text{PF}_6]_n$ ($n = 0, 1$)
Wong, K. M.-H.; Lam, S. C.-F.; Ko, C.-C.; Zhu, N.; Yam, V. W.-W.; Roué, S.; Lapinte, C.; Fathallah, S.; Costuas, K.; Kahlal, S.; Halet, J.-F.
Inorg. Chem., 2003, 42, 7086–7097.
- 105- First-Principles Study of Ternary Rare-Earth Metal Borocarbide Compounds Containing Finite Linear BC_2 Units
Jardin, C.; Hillebrecht, H.; Bauer, J.; Halet, J.-F.; Saillard, J.-Y.; Gautier, R.
J. Solid State Chem., 2003, 176, 609–614.
- 104- Structural trends and electronic structure of the rare-earth oxomolybdates RMO_5O_8 ($\text{R} = \text{La, Ce, Pr, Nd, Sm, Eu, and Gd}$) containing chains of bioctahedral Mo_{10} clusters
Gougeon, P.; Gall, P.; Gautier, R.; Halet, J.-F.
Acta Crystallogr., 2003, B59, 472–478.
- 103- Electronic Bonding and Electronic Structure in Consanguineous and Conjugal Iron and Rhenium sp Carbon Chain Complexes $[\text{MC}_4\text{M}]^{\text{n}+}$: Computational Analyses of the Effect of the Metal
Jiao, H.; Costuas, K.; Gladysz, J. A.; Halet, J.-F.; Guillemot, M.; Toupet, L.; Paul, F.; Lapinte, C.
J. Am. Chem. Soc., 2003, 125, 9511–9522.

- 102- Stereoselective Isomerisation of P-Heterocycles Triggered by Coordination: Synthesis of the First P,N-Chelates Featuring a Phospholene Moiety
Leca, F.; Sauthier, M.; Le Guennic, B.; Lescop, C.; Toupet, L.; Halet, J.-F.; Réau, R.
Chem. Commun., 2003, 1774–1775.
- 101- Preparation and Molecular Structure of $\text{Hg}\{\text{C}\equiv\text{CC}\equiv\text{C}[\text{Ru}(\text{dppe})\text{Cp}^*]\}_2$ – An Unusual Case of Non-linearity in a Molecular Rod
Bruce, M. I.; Halet, J.-F.; Le Guennic, B.; Skelton, B. W.; White, A. H.
Inorg. Chim. Acta, 2003, 350, 175–181.
- 100- Skeletal Isomerism in Mixed Transition-Metal (M)/Main-Group (E) Clusters Exhibiting an Octahedral M_4E_2 Core
Lokbani-Azzouz, N. S.; Boucekkine, A.; Halet, J.-F.; Saillard, J.-Y.
J. Cluster Sci., 2003, 14, 49–60.
- 99- Electronic Structure of Ruthenium Cumulene Complexes $[\text{Cl}(\text{PH}_3)_4\text{RuC}_n\text{H}_2]^+$ ($n = 1-8$) and of Their Reduced States. Bonding and Properties of the Cationic, Neutral and Anionic Series with Respect to the Cumulenic Chain Length
Auger, N.; Touchard, D.; Rigaut, S.; Halet, J.-F.; Saillard, J.-F.
Organometallics, 2003, 22, 1638–1844.
- 98- Redox-Switchable Molecular Quadratic Hyperpolarizabilities with Electron-rich Iron σ -aryl Acetylides
Paul, F.; Costuas, K.; Ledoux, I.; Deveau, S.; Zyss, J.; Halet, J.-F.; Lapinte, C.
Organometallics, 2002, 21, 5229–5235.
- 97- Electronic Structure, Electrical and Magnetic Properties of $\text{RMO}_8\text{O}_{14}$ Compounds ($\text{R} = \text{La}, \text{Ce}, \text{Pr}, \text{Nd}, \text{Sm}$) Containing Bicapped Mo_8 Clusters
Gautier, R.; Andersen, O. K.; Gougeon, P.; Halet, J.-F.; Canadell, E.; Martin, J. D.
Inorg. Chem., 2002, 41, 4689–4699.
- 96- Electron Probe Microanalysis of the Ternary Gd-B-C System
Ruiz, D.; Garland, M. T.; Saillard, J.-Y.; Halet, J.-F.; Bohn, M.; Bauer, J.
Solid State Sciences, 2002, 4, 1173–1178.
- 95- Preparation of Buta-1,3-diynyl Complexes of Platinum(II) and Their Use in the Construction of Neutral Molecular Squares: Syntheses and Structural Characterisation of $\text{cyclo-}\{\text{Pt}(\mu\text{-C}\equiv\text{CC}\equiv\text{C})(\text{dppe})\}_4$ and Related Chemistry
Bruce, M. I.; Costuas, K.; Halet, J.-F.; Hall, B. C.; Low, P. J.; Nicholson, B. K.; Skelton, B. W.; White, A. H.
J. Chem. Soc., Dalton Trans., 2002, 383–398.
- 94- Electronic Structures of Electron-Rich Octahedrally-Condensed Transition Metal Chalcogenide Clusters
Gautier, R.; Furet, E.; Halet, J.-F.; Lin, Z.; Saillard, J.-Y.; Xu, Z.
Inorg. Chem., 2002, 41, 796–804.
- 93- New Charge Transfer Salts Based on Bis(ethylenedithio)tetrathiafulvalene (ET) and Ferro- or Antiferromagnetic Oxalato-Bridged Dinuclear Anions: Synthesis, Structures and Magnetism of $[\text{ET}]_5[\text{MM}'(\text{C}_2\text{O}_4)(\text{NCS})_8]$ with $\text{MM}' : \text{Cr}^{\text{III}}\text{Fe}^{\text{III}}, \text{Cr}^{\text{III}}\text{Cr}^{\text{III}}$
Triki, S.; Bérézovsky, F.; Sala Pala, J.; Gomez-Garcia, C. J.; Coronado, E.; Costuas, K.; Halet, J.-F.
Inorg. Chem., 2001, 40, 5127–5132.
- 92- A DFT Investigation of the Polytopal Rearrangement of Square-Based Pyramidal Clusters : C_5H_5^+ , P_5^+ and Sb_5^+
Suad Lokbani-Azzouz, N.; Costuas, K.; Halet, J.-F.; Saillard, J.-Y.
J. Mol. Struct. (THEOCHEM), 2001, 571, 1–6.
- 91- The Structure and Possible Catalytic Sites of Mo_3S_9 as a Model of Amorphous Molybdenum Trisulfide: A Computational Study
Jiao, H.; Li, Y.-W.; Delmon, B.; Halet, J.-F.

- J. Am. Chem. Soc.**, 2001, 123, 7334–7339.
- 90- Bonding Analysis of Inorganic Transition-Metal Cubic Clusters. 6. Copper(I)-Dithiolato Species and Related Compounds
Garland, M. T.; Halet, J.-F.; Saillard, J.-Y.
Inorg. Chem., 2001, 40, 3342–3350.
- 89- Structures and Energies of 10-Azatriquinacene and its Hydrogen Adducts: A Computational Study
Jiao, H.; Halet, J.-F.; Gladysz, J. A.
J. Org. Chem., 2001, 66, 3902-3905.
- 88- The Stability of Tetraoxobutane Revisited: Perturbation Theory and Density Functional Scheme
Jiao, H.; Frapper, G.; Halet, J.-F.; Saillard, J.-Y.
J. Phys. Chem. A, 2001, 105, 5945-5947.
- 87- Synthesis, Characterization, Structural and Theoretical Analysis of a New Rare-Earth Metal Borocarbide: Lu₃BC₃
Oeckler, O.; Jardin, C.; Mattausch, H.; Simon, A.; Halet, J.-F.; Saillard, J.-Y.; Bauer, J.
Z. Anorg. Allg. Chem., 2001, 627, 1389-1394.
- 86- An Unprecedented Phosphine Coordination Mode: A Symmetrically μ_2 -Bridging Phosphole in a Binuclear Palladium(I) Complex
Sauthier, M.; Le Guennic, B.; Deborde, V.; Toupet, L.; Halet, J.-F.; Réau, R.
Angew. Chem., Int. Ed., 2001, 40, 228-231.
- 85- Reactions of NiCp₂ with an Ru₅ cluster: X-ray Structures of two Nickel-Ruthenium Clusters Containing a C₂ Ligand
Adams, C. J.; Bruce, M. I.; Halet, J.-F.; Kahlal, S.; Skelton B. W.; White, A. H.
J. Chem. Soc., Dalton Trans., 2001, 414-422.
- 84- Synthesis, Characterization, Structural and Theoretical Analysis of Gd₄B₃C₄: A Novel Type of Rare Earth Metal Borocarbide Containing two Different Boron-Carbon Arrangements
Jardin, C.; Oeckler, O.; Mattausch, H.; Simon, A.; Halet, J.-F.; Saillard, J.-Y.; Bauer, J.
Inorg. Chem., 2000, 39, 5895-5900.
- 83- Organometallic Mixed-Valence Systems. Two-Center and Three-Center Compounds with *meta* Connections around a Central Phelylene Ring
Weyland, T.; Costuas, K.; Toupet, L.; Halet, J.-F.; Lapinte, C.
Organometallics, 2000, 19, 4228-4239.
- 82- Syntheses and Reactions of Some Cluster Complexes Containing C₄ Ligands with Iron and Cobalt Carbonyls
Bruce, M. I.; Low, P. J.; Zaitseva, N.; Kahlal, S.; Halet, J.-F.; Skelton B. W.; White, A. H.
J. Chem. Soc., Dalton Trans., 2000, 2939-2951.
- 81- Structural, Electronic and Magnetic Properties of Ternary Rare-Earth Metal Borocarbides R₅B₂C₅ (R = Y, Ce-Tm) Containing BC₂ "Molecules"
Bidaud, E.; Hiebl, K.; Hoffmann, R.-D.; Pöttgen, R.; Jardin, C.; Bauer, J.; Gautier, R.; Gougeon, P.; Saillard, J.-Y.; Halet, J.-F.
J. Solid State Chem., 2000, 154, 286-295.
- 80- Linear and Nonlinear Optical Properties of Three-Coordinate Organoboron Compounds
Yuan, Z.; Collings, J. C.; Taylor, N. J.; Marder, T. B.; Jardin, C.; Halet, J.-F.
J. Solid State Chem., 2000, 154, 5-12.
- 79- Boron Carbon "Ligands" Stabilized in Rare Earth Metal Solid State Compounds: A Theoretical Approach
Halet, J.-F.

Contemporary Boron Chemistry, Davidson, M. G.; Hugues, A. K.; Marder, T. B.; Wade, K., Eds. Royal Society of Chemistry: Cambridge, 2000, p. 514-521.

- 78- Synthesis, X-ray structure and Molecular Orbital Study of a radical cation salt of a S-position isomer of an EDT-TT derivative: $C.l_3$ where C = 7-dimethylsulfanyl-2,3(dithiabutane-1,4-diyl)tetrathiafulvalene
Le Moustarder, S.; Hudhomme, P.; Illien, B.; Halet, J.-F.; Gorgues, A.; Riou, A.
Mol. Cryst. Liq. Cryst., 2000, 338, 61-74.
- 77- A DFT Investigation of the Molecular and Electronic Structures of 19-Electron Transition-Metal sandwich Complexes
Ogliaro, F.; Halet, J.-F.; Astruc, D.; Saillard, J.-Y.
New J. Chem., 2000, 24, 257-259
- 76- Oxidation Chemistry of Metal-Bonded C_4 Chains - A Combined Chemical, Spectroelectrochemical and Computational Study
Bruce, M. I.; Low, P. J.; Costuas, K.; Halet, J.-F.; Best, S. P.; Heath, G. A.
J. Am. Chem. Soc., 2000, 122, 1949-1962.
- 75- Synthesis, Physical Properties, and Theoretical Study of $R_{16}Mo_{21}O_{56}$ Compounds (R = La, Ce, Pr and Nd) Containing Biocuboctahedral Mo_{10} Clusters and Single Mo Atoms
Gall, P.; Gautier, R.; Halet, J.-F.; Gougeon, P.
Inorg. Chem., 1999, 38, 4455-4461.
- 74- Synthesis, Structural Evolution, and Theoretical and Physical Studies of the Novel Compounds $M_2Mo_9S_{11}$ (M = K, Rb) and Related Metastable Materials $Cu_xM_{1.8}Mo_9S_{11}$ (x = 0 or 2) Containing Biocuboctahedral Mo_9 Clusters
Picard, S.; Halet, J.-F.; Gougeon, P.; Potel, M.
Inorg. Chem., 1999, 38, 4422-4429.
- 73- Bonding Analysis in Inorganic Transition-Metal Cubic Clusters. 5. Main-Group-Atom-Centered Hexacapped $M_8(\mu_8-E)(\mu_4-E)_6L_8$ Species
Gautier, R.; Ogliaro, F.; Halet, J.-F.; Saillard, J.-Y.; Baerends, E. J.
Eur. J. Inorg. Chem., 1999, 1161-1168.
- 72- Different Ways to Distort a Tetracapped Tetrahedron on Route to Forming an E_4M_4 Cubane: The case of $[E_4(Pd(PPh_2Me)_2)_4][Ph_2EX_2]_2$ (E = Sb, X = Cl; E = Bi, X = Br)
Stark, J. L.; Harms, B.; Guzmán-Jimenez, I.; Whitmire, K. H.; Gautier, R.; Halet, J.-F.; Saillard, J.-Y.
J. Am. Chem. Soc., 1999, 121, 4409-4418.
- 71- Reactions of $M(C\equiv C\equiv CR)(CO)_3Cp$ [M = Mo, W; R = H, $Fe(CO)_2Cp$, $M(CO)_3Cp$] with Cobalt Carbonyls: Formation of Clusters Containing C_4 Ligands
Bruce, M. I.; Halet, J.-F.; Kahlal, S.; Low, P. J.; Skelton, B. W.; White, A.H.
J. Organomet. Chem., 1999, 578, 155-168.
- 70- Hexacapped Cubic Transition Metal Clusters and Derivatives: A Theoretical Approach
Gautier, R.; Halet, J.-F.; Saillard, J.-Y.
Metal Clusters in Chemistry, Braunstein, P.; Oro, L.; Raithby, P. R. Eds, Wiley-VCH: Weinheim, 1999, vol. 3, p. 1643-1663.
- 69- Bonding Analysis in Inorganic Transition-Metal Cubic Clusters. 4. The Distorted $Pd_9(\mu_3\eta^5, \eta^2-As_2)_4(PPh_3)_8$ Architecture
Gautier, R.; Halet, J.-F.; Saillard, J.-Y.
Eur. J. Inorg. Chem., 1999, 673-678.
- 68- Cluster Chemistry: Migration of a Phenyl Group from Coordinated dpmm to an Acetylide on an Ru_3 Cluster. X-Ray Structure and Theoretical Study of $Ru_3(\mu-H)(\mu_3-PPhCH_2PPh_2)(\mu_3-PhC_2Bu^t)(CO)_6$

- Bruce, M. I.; Humphrey, P. A.; Skelton, B. W.; White, A.H.; Costuas, K.; Halet, J.-F.*
J. Chem. Soc., Dalton Trans., 1999, 479-486.
- 67- [(Cp*)(dppe)Fe(III)]⁺ Units Bridged through 1,3-Diethynylbenzene and 1,3,5-Triethynylbenzene Spacers: Ferromagnetic Metal-Metal Exchange Interaction
Weyland, T.; Costuas, K.; Mari, A.; Halet, J.-F.; Lapinte, C.
Organometallics, 1998, 17, 5569-5579.
- 66- Rare Earth Metal Borocarbides: Examples of Coordination Compounds in Solid State Chemistry
Bauer, J.; Halet, J.-F.; Saillard, J.-Y.
Coord. Chem. Rev., 1998, 178-179, 723-753.
- 65- Detailed Structural and Theoretical Studies of the Bonding in Edge-Bridged Halide and Oxyhalide Octahedral Niobium and Tantalum Clusters
Ogliaro, F.; Cordier, S.; Halet, J.-F.; Perrin, C.; Saillard, J.-Y.; Sergent, M.
Inorg. Chem., 1998, 37, 6199-6207.
- 64- First 17-18-19-Electron Triads of Stable Isostructural Organometallic Complexes. The 17-Electron Complexes [Fe(C₅R₅)(arene)]²⁺ (R = H or Me), a Novel Family of Strong Oxidants: Isolation, Characterization, Electronic Structure, and Redox Properties
Ruiz, J.; Ogliaro, F.; Saillard, J.-Y.; Halet, J.-F.; Varret, F.; Astruc, D.
J. Am. Chem. Soc., 1998 120, 11693-11705.
- 63- On the origin of the anomalous electrical resistivity and magnetic susceptibility of LnMo₅O₈ (Ln = rare earth)
Koo, H.-J.; Whangbo, M.-H. McCarroll, W. H.; Greenblatt, M.; Gautier, R.; Halet, J.-F.; Gougeon, P.
Solid State Commun., 1998, 108, 539-544.
- 62- Five-Coordinate Hydrogen in Hydrido Rhodium Cluster Compounds: A Theoretical Analysis
Gautier, R.; Halet, J.-F.
J. Organomet. Chem., 1998, 565, 217-224.
- 61- Bonding Analysis in Inorganic Transition Metal Cubic Clusters. 3. Metal-Centered Tetracapped M₉(μ₄-E)₄L_n Species with a Tetragonal Distortion
Zouchoune, B.; Ogliaro, F.; Halet, J.-F.; Saillard, J.-Y.; Eveland, J. R.; Whitmire, K. H.
Inorg. Chem., 1998, 37, 865-875.
- 60- New Experimental and Theoretical Studies on Condensed Molybdenum Chalcogenide Cluster Compounds
Gautier, R.; Gougeon, P.; Halet, J.-F.; Potel, M.; Saillard, J.-Y.
J. Alloys Compds., 1997, 262-263, 311-315.
- 59- Boron Carbon Chains Stabilized in Rare Earth Metallic Frameworks. A Bonding Analysis
Bauer, J.; Boucekkine, G.; Frapper, G.; Halet, J.-F.; Saillard, J.-Y.; Zouchoune, B.
J. Solid State Chem., 1997, 133, 190-194.
- 58- Can carbon monoxide polymerize? A theoretical investigation of polyketone
Frapper, G.; Cui, C.-X.; Halet, J.-F.; Saillard, J.-Y.; Kertesz, M.
J. Chem. Soc., Chem. Commun., 1997, 2011-2012.
- 57- Electron Count versus Structural Arrangement in Clusters Based on Cubic Transition Metal Core with Bridging Main Group Elements
Halet, J.-F.; Saillard, J.-Y.
Struct. Bond., 1997, 87, 81-109.
- 56- Theoretical Aspects of the Bonding in Organometallic Clusters Containing Exposed Dicarbon (C₂) Entities. 2. High Nuclearity Systems
Frapper, G.; Halet, J.-F.; Bruce, M. I.

- Organometallics**, 1997, 16, 2590-2600.
- 55- Di- and Tri-metallic π -Acetylide Complexes Connected Through a Phenyl Ring in the Fe(Cp*)(dppe) Series
Weyland, T.; Lapinte, C.; Frapper, G.; Calhorda, M. J.; Halet, J.-F.; Toupet, L.
Organometallics, 1997, 16, 2024-2031.
- 54- Reaction of a Dicarbon-Ru₅ Cluster with CO: X-ray Structures of Ru₅(μ_4 -C₂)(μ -PPh₂)₂(μ -SMe)₂(CO)₁₃ and Ru₄(μ_4 -C₂)(μ -PPh₂)₂(μ -SMe)₂(CO)₁₀
Adams, C. J.; Bruce, M. I.; Skelton, B. W.; White, A. H.; Frapper, G.; Halet, J. F.
J. Chem. Soc., Dalton Trans., 1997, 371-375.
- 53- Analogies entre chimie des solides et chimie moléculaire. Exemples en chimie de coordination
Halet, J.-F.
L'Actualité Chimique, Décembre 1996, 86-91.
- 52- Boron Carbon Chains Stabilized in Rare Earth Metallic Frameworks
Ansel, D.; Bauer, J.; Bonhomme, F.; Boucekkine, G.; Frapper, G.; Gougeon, P.; Halet, J.-F.; Saillard, J.-Y.; Zouhoune, B.
Angew. Chem., 1996, 108, 2245-2248; **Int. Ed. Engl.**, 1996, 35, 2098-2101.
- 51- Crystal Structure of Ce₁₀B₉C₁₂
Gougeon, P.; Halet, J.-F.; Ansel, D.; Bauer, J.
Z. Kristallogr. NCS, 1996, 211, 825.
- 50- Crystal Structure of La₁₅B₁₄C₁₉
Gougeon, P.; Halet, J.-F.; Ansel, D.; Bauer, J.
Z. Kristallogr. NCS, 1996, 211, 823-824.
- 49- Crystal Structure of Ce₅B₄C₅
Gougeon, P.; Halet, J.-F.; Ansel, D.; Bauer, J.
Z. Kristallogr. NCS, 1996, 211, 822.
- 48- Synthesis, Crystal Structure and Physical Properties of New Quaternary Sulfides with the BaCu₂S₂ Type
Mouallem-Bahout, M.; Potel, M.; Halet, J.-F.; Padiou, J.; Carel, C.; Retat-Savel'eva, M.
Eur. J. Solid State Inorg. Chem., 1996, 33, 483-493.
- 47- Theoretical Aspects of the Bonding in Organometallic Clusters Containing Exposed Dicarbon (C₂) Entities. 1. Tetrametallic Systems
Frapper, G.; Halet, J.-F.
Organometallics, 1995, 14, 5044-5053.
- 46- Synthesis, Characterization, X-ray Structure and Molecular Analysis of [NEt₄]₂ [(OC)₅MoAsMo₃(CO)₉(μ_3 -OR)₃Mo(CO)₃] (R = Me, Et). X-ray Structure of [NEt₄]₂ [(OC)₅MoAsMo₃(CO)₉(μ_3 -OMe)₃Mo(CO)₃]·0.6thf
Van Hal, J. W.; Whitmire, K. H.; Zouhoune, B.; Halet, J.-F.; Saillard, J.-Y.
Inorg. Chem., 1995, 34, 5455-5460.
- 45- Limitations of the Polyhedral Skeletal Electron Pair Theory in Organometallic Cluster Chemistry. Examples in Tri- and Tetrametallic Systems
Halet, J.-F.
Coord. Chem. Rev., 1995, 143, 637-678.
- 44- Origin of the Unexpected sp vs sp² Hybridization of Carbon in the MB₂C (M = Th, U) Solid-State Phases: An Ab initio Study of the [H₂BCBH₂]⁴⁻ Model and Isoelectronic Species
Frapper, G.; Halet, J.-F.; Saillard, J.-Y.; Volatron, F.

- J. Phys. Chem.**, 1995, 99, 12164-12169.
- 43- Physical Properties and Electronic Structure of Ternary Barium Copper Sulfides
Ouammou, A.; Mouallem-Bahout, M.; Peña, O.; Halet, J.-F.; Saillard, J.-Y.; Carel, C.
J. Solid State Chem., 1995, 117, 73-79.
- 42- Bonding Analysis in Inorganic Transition Metal Cubic Clusters. 2. Metal-Centered Hexacapped $M_9(\mu_4-E)_6L_8$ Species.
Furet, E.; Le Beuze, A.; Halet, J.-F.; Saillard, J.-Y.
J. Am. Chem. Soc., 1995, 117, 4936-4944.
- 41- Promoter Effect of Chloride Ions on the Ruthenium Catalyzed Hydroesterification of Ethylene with Methyl Formate. Design and Evaluation of New Poly- and Mono-nuclear Catalyst Precursors
Lugan, N.; Lavigne, G.; Soulié, J.-M.; Fabre, S.; Kalck, P.; Saillard, J.-Y.; Halet, J.-F.
Organometallics, 1995, 14, 1712-1731.
- 40- Preparation and Characterization of Cobaltaboranes Containing Cobalt Carbonyl Fragments
Jun C. S.; Halet, J.-F.; Rheingold, A. L.; Fehlner, T. P.
Inorg. Chem., 1995, 34, 2101-2107.
- 39- Rare Earth Boron Carbide MBC Compounds Containing Monodimensional Branched Zigzag Chains of Non-Metal Atoms: Theoretical Aspects
Witkar, F.; Kahlal, S.; Halet, J.-F.; Saillard, J.-Y.; Bauer, J.; Rogl, P.
Inorg. Chem., 1995, 34, 1248-1256.
- 38- Localization of the Halogen Atoms in Superconducting $YBa_2Cu_3O_{6.7}X_y$ (X = F, Cl, Br) Phases
Mokhtari, M.; Perrin, C.; Sergent, M.; Furet, E.; Halet, J.-F.; Saillard, J.-Y.; Ressouche, E.; Burlet, P.
Solid State Commun., 1995, 93, 487-492.
- 37- Molecular Orbital Approach of Skeletal Isomerism and Polyhedral Rearrangements in Some Organometallic Clusters
Saillard, J.-Y.; Garland, M.-T.; Kahlal, S.; Halet, J.-F.
The Synergy Between Dynamics and Reactivity at Clusters and Surfaces, Farrugia, L. J. (Editor), Kluwer Academic Publishers (the Netherlands) 1995, 285-295.
- 36- Electronic Structure of the Superconducting Rare-Earth-Metal Nickel Boron Carbide Compounds
Halet, J.-F.
Inorg. Chem., 1994, 33, 4173-4178.
- 35- Bonding Analysis of Electron-Rich Bridged Mixed Main-Group/Transition Metal Tetrahedral M_2E_2 Organometallic Clusters
Kahlal, S.; Halet, J.-F.; Saillard, J.-Y.; Whitmire, K. H.
J. Organomet. Chem., 1994, 478, 1-8.
- 34- Crystal and Electronic Structure of the Novel Layered Rare Earth Boride Carbide $Gd_2B_3C_2$
Witkar, F.; Halet, J.-F.; Saillard, J.-Y.; Rogl, P.; Bauer, J.
Inorg. Chem., 1994, 33, 1297-1305.
- 33- Bonding Analysis in Inorganic Transition Metal Cubic Clusters. 1. Noncentered Hexacapped $M_8(\mu_4-E)_6L_n$ ($n \leq 8$) Species
Furet, E.; Le Beuze, A.; Halet, J.-F.; Saillard, J.-Y.
J. Am. Chem. Soc., 1994, 116, 274-280.
- 32- Electronic Structure of Layered MB_2C Rare Earth Borocarbide Compounds
Witkar, F.; Kahlal, S.; Halet, J.-F.; Saillard, J.-Y.; Bauer, J.; Rogl P.
J. Am. Chem. Soc., 1994, 116, 251-261.

- 31- Preparation, X-Ray crystal Structure and Spectral Investigation of the Pentamerized TTF Ion-Radical Salt: $(\text{TTF})_5[\text{Pt}(\text{CN})_4]_2 \cdot (\text{CH}_3\text{CN})_2$
Ouahab, L.; Fettouhi, M.; Halet, J.-F.; Yartsev, V. M.; Garrigou-Lagrange, C.; Delhaes, P.; Sourisseau, C.
New J. Chem., 1993, 17, 399-408.
- 30- Framework Expansion versus Edge Opening in a 50-Electron Phosphido Bridged Triruthenium Cluster. A Case Study
Lugan, N.; Fabre, P.-L.; de Montauzon, D.; Lavigne, G.; Bonnet, J.-J.; Saillard, J.-Y.; Halet, J.-F.
Inorg. Chem., 1993, 32, 1363-1369.
- 29- New Polymetallic Ruthenium Carbonyl Halide Complexes: Exotic Combinations of Electron Deficient Skeletons with Electron Rich Anions
Lavigne, G.; Lugan, N.; Soulié, J.-M.; Kalck, P.; Lerouge, O.; Saillard, J.-Y.; Halet, J.-F.
J. Am. Chem. Soc., 1992, 114, 10669-10670.
- 28- Structural Preferences Among the Rare Earth Dicarbides: The Electronic Structure of LaC_2 and ThC_2
Long, J. R.; Halet, J.-F.; Saillard, J.-Y.; Hoffmann, R.; Meyer, H.-J.
New J. Chem., 1992, 16, 839-846.
- 27- Preparation, X-ray Crystal Structures, EH Band Calculations and Physical Properties of $(\text{TTF})_6(\text{H})(\text{XMo}_{12}\text{O}_{40})(\text{NEt}_4)$ ($\text{M} = \text{W}$ or Mo , $\text{X} = \text{P}$ or Si): Evidence of Electron Transfer between Organic Donors and Polyoxometalates
Ouahab, L.; Bencharif, M.; Mhanni, A.; Pelloquin, D.; Halet, J.-F.; Pena, O.; Padiou, J.; Grandjean, D.; Garrigou-Lagrange C.; Amiell, J.; Delhaes P.
Chem. Mater., 1992, 4, 666-674.
- 26- Preparation and Properties of Tetrathia- and Tetraselena-Fulvalene Salts of $[\text{M}_6\text{O}_{19}]^{2-}$ ($\text{M} = \text{Mo}$ or W)
Triki S.; Ouahab L.; Halet J.-F.; Pena O.; Padiou J.; Grandjean D.; Garrigou-Lagrange C.; Delhaes P.
J. Chem. Soc., Dalton Trans., 1992, 1217-1227.
- 25- An Orbital Analysis of Hydrogen Pairing in Non-Stoichiometric Transition Metal Hydrides
Halet J.-F.; Saillard J.-Y.; Koudou C.; Minot C.; Nomikou Z.; Hoffmann R.; Demangeat C.
Chem. Mater., 1992, 4, 153-161.
- 24- Theoretical Aspects of the Bonding in Transition Metal Carbonyl Clusters with Interstitial Main Group Atoms
Halet J.-F.
Topics in Physical Organometallic Chemistry, Ed. Gielen M., Freund Publishing House : Londres, 1992, Vol. 4., p. 221-288.
- 23- Cluster Containing Ynamine Ligands. 4. The Synthesis and Characterizations of $\text{ReMn}(\text{CO})_8(\mu\text{-MeC}_2\text{NMe}_2)$ and $\text{ReMn}(\text{CO})_7(\mu\text{-MeCC}(\text{NMe}_2)\text{C}(\text{NMe}_2)\text{CMe})$ and the Development of a Bonding Model for the Coordination of Ynamines to $\text{M}_2(\text{CO})_8$
Adams R.D.; Chen G.; Chen L.; Yin, J.; Halet J.-F.
J. Cluster Sci., 1991, 2, 83-103.
- 22- Theoretical Analysis of the Different Coordination Modes of Diatomic Entities in Tetrametallic Butterfly-Type Clusters
Kahlal S.; Halet J.-F.; Saillard J.-Y.
New J. Chem., 1991, 15, 843-851.

- 21- Cluster Core Isomerisation from Planar to Tetrahedral: Steric Control by the Ligands of Cluster Geometry. Synthesis and Crystal Structure of $[\text{Pt}_2\text{Mo}_2(\mu\text{-C}_5\text{H}_4\text{CH}_3)_2(\text{CO})_6(\text{PCy}_3)_2]$
Braunstein P.; de Meric de Bellefon C.; Bouaoud S.-E.; Grandjean D.; Halet J.-F.; Saillard J.-Y.
J. Am. Chem. Soc., 1991, 113, 5282-5292.
- 20- On the Possible Existence of a Heteronuclear Octahedral *Hypercloso* Cluster: Can N_2 or an Alkyne Be Complexed Through a M_4L_n Square
Kahlal S.; Halet J.-F.; Saillard J.-Y.
Inorg. Chem., 1991, 30, 2567-2569.
- 19- Capping Considerations in Main Group/Transition Metal Clusters: Synthetic, Structural and Theoretical Discussions of $[\text{E}_2\text{Co}_4(\text{CO})_{10}(\mu\text{-CO})]^{1-/-2-}$ (E = Sb or Bi)
Albright T. A.; Ae Yee K.; Saillard J.-Y.; Kahlal S.; Halet J.-F.; Leigh J.S.; Whitmire K. H.
Inorg. Chem., 1991, 30, 1179-1190.
- 18- Electronic Structure of the New Transition Metal Borocarbide Sc_2BC_2
Halet J.-F.; Saillard J.-Y.; Bauer J.
J. Less-Common Met., 1990, 158, 239-250.
- 17- Electronic Structure of the Non-Classical Trimetallic Alkyne Cluster Complex $\text{Os}_3(\text{CO})_9(\mu\text{-H})_2(\mu_3\text{-HC}_2\text{NET}_2)$
Nomikou Z.; Halet J.-F.; Hoffmann R.; Tanner J. T.; Adams R. D.
Organometallics, 1990, 9, 588-595.
- 16- Intramolecular Conversion of an Azoalkane Ligand in two Nitrene Ligands on a Triiron Cluster
Wucherer E. J.; Tasi M.; Hansert B.; Powell A. K.; Garland M.-T.; Halet J.-F.; Saillard J.-Y.; Vahrenkamp H.
Inorg. Chem., 1989, 28, 3564-3572.
- 15- Electronic Structure of a New Ternary Chalcogenide: NbNiTe_5
Halet J.-F.; Hoffmann R.; Tremel W.; Liimatta E. W.; Ibers J. A.
Chem. Mater., 1989, 1, 451-459.
- 14- Adsorption of Organo-Rhodium Species on Metal Oxide Surfaces: Theoretical Aspects
Halet J.-F.; Hoffmann R.
J. Am. Chem. Soc., 1989, 111, 3548-3559.
- 13- Synthèse directe de phényl-pyruvates chrome tricarbonyle: influences de la substitution sur la nature cétonique ou énolique des produits isolés et du groupement $\text{Cr}(\text{CO})_3$ sur l'équilibre tautomère
Le Bihan J.-Y.; Sénéchal-Tocquer M.-C.; Sénéchal D.; Gentric D.; Caro B.; Halet J.-F.; Saillard J.-Y.; Jaouen G.; Top S.
Tetrahedron, 1988, 44, 3565-3574.
- 12- Effect of Cavity Size on the Charge Distribution in Carbido Metal Carbonyl Clusters and its Possible Catalytic Implications
Halet J.-F.; Evans D. G.; Mingos D. M. P.
J. Am. Chem. Soc., 1988, 110, 87-90.
- 11- Molecular Orbital Analysis of Dicarbido Transition Metal Cluster Compounds
Halet J.-F.; Mingos D. M. P.
Organometallics, 1988, 7, 51-58.
- 10- Structure and Electron Counting of Tetrahedral and Butterfly M_2E_2 Clusters: an MO Analysis of $(\text{L}_n\text{M})_2(\text{PM}^n\text{L}_5)_2$
Halet J.-F.; Saillard J.-Y.
J. Organomet. Chem., 1987, 327, 365-377.

- 9- Structure and Electron Counting in M_4E_2 Organometallic Clusters
Halet J.-F.; Saillard J.-Y.
Nouv. J. Chim., 1987, 11, 315-320.
- 8- ^{13}C NMR and EHMO Studies on Seyferth's $[Co_3(CO)_9CCO]^+$ Cluster: to Bend or not to Bend?
D'Agostino M. F.; Mlekuz M.; Kolis J. W.; Sayer G. S.; Rodger C. A.; Halet J.-F.; Saillard J.-Y.; McGlinchey M. J.
Organometallics, 1986, 5, 2345-2350.
- 7- Electron Counting in Square Pyramidal Organo-Transition Metal Carbides: Can a Carbon Atom be a Vertex of a Closo Octahedral M_5C ?
Halet J.-F.; Saillard J.-Y.; Lissillour R.; McGlinchey M. J.; Jaouen G.
Organometallics, 1986, 5, 139-145.
- 6- Clusters de métaux de transition : quelques perspectives offertes par la théorie PSEP
Halet J.-F.; Jaouen G.; McGlinchey M. J.; Saillard J.-Y.
L'Actualité Chimique, Avril 1985, 23-44.
- 5- Six- and Five- Vertex Organometallic Clusters
Halet J.-F.; Hoffmann R.; Saillard J.-Y.
Inorg. Chem., 1985, 24, 1695-1700.
- 4- Slipped vs. Zig-Zag TCNQ Stack upon Steric Control in Conducting 1:4 Diphosphonium-TCNQ Salts
Batail P.; Ouahab L.; Halet J.-F.; Padiou J.; Le Quan M.; Le Quan R.-M.
Synt. Met., 1985, 10, 415-425.
- 3- Molecular Orbital Study of Heterometallic M_3C_2 Organo-Transition Metal Clusters: Orientation of the Alkyne Moiety
Halet J.-F.; Saillard J.-Y.; Lissillour R.; McGlinchey M. J.; Jaouen G.
Inorg. Chem., 1985, 24, 218-224.
- 2- Analyse structurale du phényl-pyruvate d'éthyle obtenu sous forme énolique par activation benzylque à l'aide de l'entité $Cr(CO)_3$
Halet J.-F.; Saillard J.-Y.; Caro B.; Le Bihan J.-Y.; Top S.; Jaouen G.
J. Organomet. Chem., 1984, 264, C37-C40.
- 1- Conducteurs organiques : nouveaux complexes d'ions radicaux entre sels de diphosphonium et le tétracyanoquinométhane (TCNQ)
Le Quan M.; Le Quan R.-M.; Batail P.; Halet J.-F.; Ouahab L.
Tetrahedron Letters, 1983, 24, 3107-3108.

A soumettre :

- 000- Synthesis and Characterization of a Cyclic Alkyl Amino Carbene (cAAC) Stabilized Borylene: Exploring the Origin of its Deep Red Color
G. Vijaykumar, D. Bocéno, J.-F. Halet, S. K. Mandal
 (soumis pour publication le xx 2017).
- 000- Theoretical studies of transition metal borane clusters
B. S. Krishnamoorthy, J.-F. Halet
J. Cluster Sci. (soumis pour publication le XX 2013).
- 000- Structural, Electronic and Magnetic Properties of Early vs Late Transition Metallaborane Clusters - A Theoretical Investigation
B. S. Krishnamoorthy, J.-F. Halet

- 000- C-H Activation of Arenes and Heteroarenes by Group 5-8 Dimetallaboranes: An Experimental and Theoretical Investigation
B. S. Krishnamoorthy, K. Yuvaraj, J.-F. Halet, S. Ghosh
- 000- Density Functional Theory and High-Field Multifrequency EPR Study of Pseudo-octahedral Vanadium(III) Complexes with O and N Ligands
B. S. Krishnamoorthy, B. Le Guennic, M. Geoffroy, J.-F. Halet
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J. Singh, B. S. Krishnamoorthy, J.-F. Halet, H. L. Singh
- 000- Electronic structure of ternary metal carbon-borides MB₂C phases
Fang, C.-M.; Boulfelfel, S.-E.; Le Guennic, B.; G.; Frapper, G.; Le Pollès, L.; Gautier, R.; Bauer, J.; Saillard, J.-Y. ; Halet, J.-F.
- 000- Magnetic properties of β -UB₂C from first-principles theory
Fang, C.-M.; Saillard, J.-Y. ; Halet, J.-F.
- 000- First-principles investigations on binary boron-rich compounds in the W-B system
Fang, C.-M.; N. Combes, R. Gautier, Bauer, J.; Halet, J.-F.; Frotscher, M.; Albert, B.

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