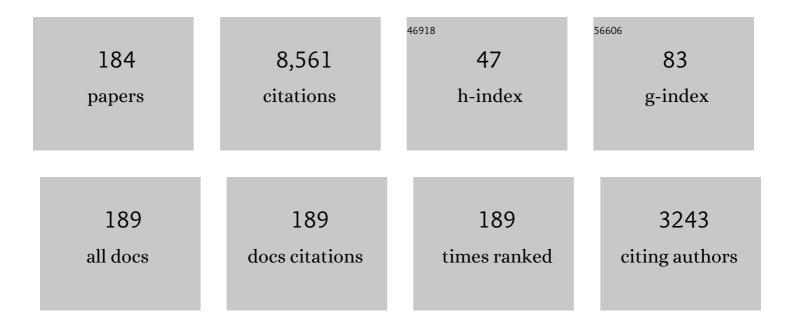
## Simon B Duckett

List of Publications by Year in descending order

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| #  | Article  | IF             | CITATIONS          |
|----|--|----------------|--------------------|
| 1  | Contrasting Photochemical and Thermal Catalysis by Ruthenium Arsine Complexes Revealed by<br>Parahydrogen Enhanced NMR Spectroscopy. European Journal of Inorganic Chemistry, 2022, 2022, .  | 1.0            | 2                  |
| 2  | SABRE hyperpolarized anticancer agents for use in <sup>1</sup> H MRI. Magnetic Resonance in Medicine, 2022, , .  | 1.9            | 2                  |
| 3  | Real-Time High-Sensitivity Reaction Monitoring of Important Nitrogen-Cycle Synthons by<br><sup>15</sup> N Hyperpolarized Nuclear Magnetic Resonance. Journal of the American Chemical<br>Society, 2022, 144, 8756-8769.  | 6.6            | 10                 |
| 4  | Zintl cluster supported low coordinate Rh( <scp>i</scp> ) centers for catalytic H/D exchange between<br>H <sub>2</sub> and D <sub>2</sub> . Chemical Science, 2022, 13, 7626-7633.   | 3.7            | 14                 |
| 5  | Reversible Hyperpolarization of Ketoisocaproate Using Sulfoxideâ€containing Polarization Transfer<br>Catalysts. ChemPhysChem, 2021, 22, 13-17.   | 1.0            | 10                 |
| 6  | Hyperpolarisation of weakly binding N-heterocycles using signal amplification by reversible exchange.<br>Chemical Science, 2021, 12, 5910-5917.  | 3.7            | 10                 |
| 7  | Î- <sup>2</sup> -Alkene Complexes of [Rh(PONOP- <sup>i</sup> Pr)(L)] <sup>+</sup> Cations (L = COD, NBD,) Tj<br>[Rh(PONOP- <sup>i</sup> Pr)(Î-H <sub>2</sub> )] <sup>+</sup> . Inorganic Chemistry, 2021, 60, 13903-13912.   | ETQq1 1<br>1.9 | 0.784314 rgE<br>11 |
| 8  | Steric and electronic effects on the <sup>1</sup> H hyperpolarisation of substituted pyridazines by signal amplification by reversible exchange. Magnetic Resonance in Chemistry, 2021, 59, 1187-1198.   | 1.1            | 4                  |
| 9  | Parawasserstoffâ€induzierte Polarisation von Aminosären. Angewandte Chemie, 2021, 133, 23688.  | 1.6            | 2                  |
| 10 | Parahydrogenâ€Induced Polarization of Amino Acids. Angewandte Chemie - International Edition, 2021,<br>60, 23496-23507.  | 7.2            | 34                 |
| 11 | Exploring the hyperpolarisation of EGTA-based ligands using SABRE. Dalton Transactions, 2021, 50, 2448-2461.   | 1.6            | 2                  |
| 12 | Bridging the Gap from Mononuclear Pd <sup>II</sup> Precatalysts to Pd Nanoparticles: Identification<br>of Intermediate Linear [Pd <sub>3</sub> (XPh <sub>3</sub> ) <sub>4</sub> ] <sup>2+</sup> Clusters as<br>Catalytic Species for Suzuki–Miyaura Couplings (X = P, As). Organometallics, 2021, 40, 3560-3570. | 1.1            | 17                 |
| 13 | Breaking bonds over many timescales: in celebration of Robin Perutz's 70th birthday. Dalton Transactions, 2020, 49, 254-255.   | 1.6            | 0                  |
| 14 | The Detection and Reactivity of Silanols and Silanes Using Hyperpolarized 29 Si Nuclear Magnetic<br>Resonance. Angewandte Chemie, 2020, 132, 2732-2736.  | 1.6            | 9                  |
| 15 | The Detection and Reactivity of Silanols and Silanes Using Hyperpolarized 29 Si Nuclear Magnetic<br>Resonance. Angewandte Chemie - International Edition, 2020, 59, 2710-2714.   | 7.2            | 12                 |
| 16 | Understanding the mechanism of cis–trans isomerism in photo-active palladium(II) complexes derived from the N,N-di-substituted benzoylthioureas. Inorganica Chimica Acta, 2020, 512, 119884.   | 1.2            | 6                  |
| 17 | The use of yttrium in medical imaging and therapy: historical background and future perspectives.<br>Chemical Society Reviews, 2020, 49, 6169-6185.  | 18.7           | 30                 |
| 18 | Remarkable Levels of <sup>15</sup> N Polarization Delivered through SABRE into Unlabeled Pyridine,<br>Pyrazine, or Metronidazole Enable Single Scan NMR Quantification at the mM Level. Journal of<br>Physical Chemistry B, 2020, 124, 4573-4580.  | 1.2            | 33                 |

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|----|--|-------------|-------------|
| 19 | Using SABRE Hyperpolarized <sup>13</sup> C NMR Spectroscopy to Interrogate Organic<br>Transformations of Pyruvate. Analytical Chemistry, 2020, 92, 9095-9103.  | 3.2         | 15          |
| 20 | A role for low concentration reaction intermediates in the signal amplification by reversible<br>exchange process revealed by theory and experiment. Physical Chemistry Chemical Physics, 2020, 22,<br>5033-5037.                              | 1.3         | 6           |
| 21 | Parawasserstoffâ€induzierte Hyperpolarisation von Gasen. Angewandte Chemie, 2020, 132, 17940-17949.  | 1.6         | 1           |
| 22 | Optimisation of pyruvate hyperpolarisation using SABRE by tuning the active magnetisation transfer catalyst. Catalysis Science and Technology, 2020, 10, 1343-1355.  | 2.1         | 41          |
| 23 | Parahydrogenâ€induced Hyperpolarization of Gases. Angewandte Chemie - International Edition, 2020, 59,<br>17788-17797.   | 7.2         | 27          |
| 24 | A simple and cost-efficient technique to generate hyperpolarized long-lived 15N-15N nuclear spin order<br>in a diazine by signal amplification by reversible exchange. Journal of Chemical Physics, 2020, 152,<br>014201.                      | 1.2         | 9           |
| 25 | Understanding substrate substituent effects to improve catalytic efficiency in the SABRE hyperpolarisation process. Catalysis Science and Technology, 2019, 9, 3914-3922.  | 2.1         | 9           |
| 26 | Towards measuring reactivity on micro-to-millisecond timescales with laser pump, NMR probe spectroscopy. Faraday Discussions, 2019, 220, 28-44.  | 1.6         | 1           |
| 27 | Relayed hyperpolarization from <i>para</i> -hydrogen improves the NMR detectability of alcohols.<br>Chemical Science, 2019, 10, 7709-7717.   | 3.7         | 27          |
| 28 | Probing the Hydrogenation of Vinyl Sulfoxides Using <i>para</i> -Hydrogen. Organometallics, 2019, 38, 4377-4382.   | 1.1         | 9           |
| 29 | Using <i>para</i> hydrogen induced polarization to study steps in the hydroformylation reaction.<br>Dalton Transactions, 2019, 48, 2664-2675.  | 1.6         | 7           |
| 30 | Hyperpolarising Pyruvate through Signal Amplification by Reversible Exchange (SABRE). Angewandte<br>Chemie - International Edition, 2019, 58, 10271-10275.   | 7.2         | 87          |
| 31 | Hyperpolarising Pyruvate through Signal Amplification by Reversible Exchange (SABRE). Angewandte<br>Chemie, 2019, 131, 10377-10381.  | 1.6         | 52          |
| 32 | Pharmacokinetics of the SABRE agent 4,6-d2-nicotinamide and also nicotinamide in rats following oral and intravenous administration. European Journal of Pharmaceutical Sciences, 2019, 135, 32-37.  | 1.9         | 13          |
| 33 | Reaction Monitoring Using SABRE-Hyperpolarized Benchtop (1 T) NMR Spectroscopy. Analytical Chemistry, 2019, 91, 6695-6701.   | 3.2         | 39          |
| 34 | Using coligands to gain mechanistic insight into iridium complexes hyperpolarized with <i>para</i> -hydrogen. Chemical Science, 2019, 10, 5235-5245.   | 3.7         | 20          |
| 35 | <pre>Reversible photo-isomerization of <i>cis</i>-[Pd(L-i<sup>e</sup><i>S</i>,<i>O</i>)<sub>2</sub>] (HL =) IJ ETQq1 1 0.784.</pre> <i>trans</i> -[Pd(L-i <sup>e</sup> <i>S</i> , <i>O</i> ) <sub>2</sub> ] and the unprecedented formation of | 1.6 14 rgBT | Jverlock 10 |
|    | <i>trans</i> -[Pd(L-P <i>S</i> , <i>N</i> ) <sub>2</sub> ] in solution. Dalton Transactions, 2019, 48,<br>17241-17251.   |             |             |
| 36 | In Situ SABRE Hyperpolarization with Earth's Field NMR Detection. Molecules, 2019, 24, 4126.   | 1.7         | 8           |

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|----|---|-----|-----------|
| 37 | Mechanistic insight into novel sulfoxide containing SABRE polarisation transfer catalysts. Dalton<br>Transactions, 2019, 48, 15198-15206.   | 1.6 | 18        |
| 38 | Rapid <sup>13</sup> C NMR hyperpolarization delivered from <i>para</i> -hydrogen enables the low concentration detection and quantification of sugars. Chemical Science, 2019, 10, 10607-10619.               | 3.7 | 26        |
| 39 | lridium <i>α</i> â€Carboxyimine Complexes Hyperpolarized with <i>para</i> â€Hydrogen Exist in Nuclear<br>Singlet States before Conversion into Iridium Carbonates. ChemPhysChem, 2019, 20, 241-245.           | 1.0 | 17        |
| 40 | Catalyst‣ubstrate Effects on Biocompatible SABRE Hyperpolarization. ChemPhysChem, 2019, 20, 285-294.  | 1.0 | 9         |
| 41 | Direct and indirect hyperpolarisation of amines using <i>para</i> hydrogen. Chemical Science, 2018, 9, 3677-3684.   | 3.7 | 53        |
| 42 | SABRE-Relay: A Versatile Route to Hyperpolarization. Journal of Physical Chemistry Letters, 2018, 9, 1112-1117.   | 2.1 | 57        |
| 43 | Competing Pathways in the Photochemistry of<br>Ru(H) <sub>2</sub> (CO)(PPh <sub>3</sub> ) <sub>3</sub> . Organometallics, 2018, 37, 855-868.  | 1.1 | 8         |
| 44 | SignalverstÃ <b>r</b> kung durch reversiblen Austausch (SABRE): von der Entdeckung zur diagnostischen<br>Anwendung. Angewandte Chemie, 2018, 130, 6854-6866.  | 1.6 | 21        |
| 45 | Extending the Scope of <sup>19</sup> F Hyperpolarization through Signal Amplification by Reversible<br>Exchange in MRI and NMR Spectroscopy. ChemistryOpen, 2018, 7, 97-105.                                  | 0.9 | 34        |
| 46 | Using <sup>2</sup> H labelling to improve the NMR detectability of pyridine and its derivatives by SABRE. Magnetic Resonance in Chemistry, 2018, 56, 663-671.   | 1.1 | 13        |
| 47 | Signal Amplification by Reversible Exchange (SABRE): From Discovery to Diagnosis. Angewandte Chemie<br>- International Edition, 2018, 57, 6742-6753.  | 7.2 | 101       |
| 48 | Using <i>para</i> hydrogen to hyperpolarize amines, amides, carboxylic acids, alcohols, phosphates,<br>and carbonates. Science Advances, 2018, 4, eaao6250.   | 4.7 | 109       |
| 49 | A simple handâ€held magnet array for efficient and reproducible <scp>SABRE</scp> hyperpolarisation using manual sample shaking. Magnetic Resonance in Chemistry, 2018, 56, 641-650.                           | 1.1 | 18        |
| 50 | Achieving Biocompatible SABRE: An in vitro Cytotoxicity Study. ChemMedChem, 2018, 13, 352-359.  | 1.6 | 36        |
| 51 | Quantification of hyperpolarisation efficiency in SABRE and SABRE-Relay enhanced NMR spectroscopy.<br>Physical Chemistry Chemical Physics, 2018, 20, 26362-26371.   | 1.3 | 31        |
| 52 | Unlocking a Diazirine Long-Lived Nuclear Singlet State via Photochemistry: NMR Detection and Lifetime<br>of an Unstabilized Diazo-Compound. Journal of the American Chemical Society, 2018, 140, 16855-16864. | 6.6 | 24        |
| 53 | Quantitative In Situ Monitoring of Parahydrogen Fraction Using Raman Spectroscopy. Applied<br>Spectroscopy, 2018, 73, 000370281879864.  | 1.2 | 6         |
| 54 | Fine-tuning the efficiency of para-hydrogen-induced hyperpolarization by rational N-heterocyclic carbene design. Nature Communications, 2018, 9, 4251.  | 5.8 | 71        |

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|----|---|-----|-----------|
| 55 | Harnessing asymmetric N-heterocyclic carbene ligands to optimise SABRE hyperpolarisation. Catalysis<br>Science and Technology, 2018, 8, 4925-4933.  | 2.1 | 22        |
| 56 | Using hyperpolarised NMR and DFT to rationalise the unexpected hydrogenation of quinazoline to 3,4-dihydroquinazoline. Chemical Communications, 2018, 54, 10375-10378.  | 2.2 | 10        |
| 57 | SABRE hyperpolarization enables high-sensitivity <sup>1</sup> H and <sup>13</sup> C benchtop NMR spectroscopy. Analyst, The, 2018, 143, 3442-3450.  | 1.7 | 49        |
| 58 | Harnessing polarisation transfer to indazole and imidazole through signal amplification by reversible exchange to improve their NMR detectability. Magnetic Resonance in Chemistry, 2017, 55, 944-957.  | 1.1 | 28        |
| 59 | Following palladium catalyzed methoxycarbonylation by hyperpolarized NMR spectroscopy: a parahydrogen based investigation. Catalysis Science and Technology, 2017, 7, 2101-2109.  | 2.1 | 9         |
| 60 | A Simple Route to Strong Carbonâ€13 NMR Signals Detectable for Several Minutes. Chemistry - A<br>European Journal, 2017, 23, 10496-10500.   | 1.7 | 34        |
| 61 | Achieving High Levels of NMRâ€Hyperpolarization in Aqueous Media With Minimal Catalyst<br>Contamination Using SABRE. Chemistry - A European Journal, 2017, 23, 10491-10495.   | 1.7 | 54        |
| 62 | Coherent evolution of para hydrogen induced polarisation using laser pump, NMR probe<br>spectroscopy: Theoretical framework and experimental observation. Journal of Magnetic Resonance,<br>2017, 278, 25-38.   | 1.2 | 10        |
| 63 | Synthesis and hyperpolarisation of eNOS substrates for quantification of NO production by 1 H NMR spectroscopy. Bioorganic and Medicinal Chemistry, 2017, 25, 2730-2742.  | 1.4 | 11        |
| 64 | Delivering strong <sup>1</sup> H nuclear hyperpolarization levels and long magnetic lifetimes<br>through signal amplification by reversible exchange. Proceedings of the National Academy of Sciences<br>of the United States of America, 2017, 114, E3188-E3194. | 3.3 | 115       |
| 65 | SABRE hyperpolarisation of vitamin B3 as a function of pH. Chemical Science, 2017, 8, 2257-2266.  | 3.7 | 43        |
| 66 | Direct enhancement of nitrogen-15 targets at high-field by fast ADAPT-SABRE. Journal of Magnetic Resonance, 2017, 285, 55-60.   | 1.2 | 34        |
| 67 | Achieving High <sup>1</sup> H Nuclear Hyperpolarization Levels with Long Lifetimes in a Range of<br>Tuberculosis Drug Scaffolds. Chemistry - A European Journal, 2017, 23, 16990-16997.   | 1.7 | 18        |
| 68 | Frontispiece: Achieving High Levels of NMRâ€Hyperpolarization in Aqueous Media With Minimal Catalyst<br>Contamination Using SABRE. Chemistry - A European Journal, 2017, 23, .  | 1.7 | 0         |
| 69 | Frontispiece: Achieving High <sup>1</sup> H Nuclear Hyperpolarization Levels with Long Lifetimes in a<br>Range of Tuberculosis Drug Scaffolds. Chemistry - A European Journal, 2017, 23, .  | 1.7 | 0         |
| 70 | Creating a hyperpolarised pseudo singlet state through polarisation transfer from parahydrogen under SABRE. Chemical Communications, 2016, 52, 7842-7845.   | 2.2 | 24        |
| 71 | Manganese(I) atalyzed Câ^'H Activation: The Key Role of a 7â€Membered Manganacycle in Hâ€Transfer and Reductive Elimination. Angewandte Chemie - International Edition, 2016, 55, 12455-12459.  | 7.2 | 111       |
| 72 | Long-lived states to sustain SABRE hyperpolarised magnetisation. Physical Chemistry Chemical Physics, 2016, 18, 24905-24911.  | 1.3 | 50        |

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|----|--|-----|-----------|
| 73 | Photochemical pump and NMR probe to monitor the formation and kinetics of hyperpolarized metal dihydrides. Chemical Science, 2016, 7, 7087-7093.   | 3.7 | 16        |
| 74 | Using signal amplification by reversible exchange (SABRE) to hyperpolarise <sup>119</sup> Sn and <sup>29</sup> Si NMR nuclei. Chemical Communications, 2016, 52, 14482-14485.  | 2.2 | 48        |
| 75 | Manganese(I) atalyzed Câ^'H Activation: The Key Role of a 7â€Membered Manganacycle in Hâ€Transfer and<br>Reductive Elimination. Angewandte Chemie, 2016, 128, 12643-12647.   | 1.6 | 54        |
| 76 | A Hyperpolarizable <sup>1</sup> H Magnetic Resonance Probe for Signal Detection 15â€Minutes after Spin<br>Polarization Storage. Angewandte Chemie, 2016, 128, 15871-15874.   | 1.6 | 16        |
| 77 | A Hyperpolarizable <sup>1</sup> H Magnetic Resonance Probe for Signal Detection 15â€Minutes after Spin<br>Polarization Storage. Angewandte Chemie - International Edition, 2016, 55, 15642-15645.  | 7.2 | 36        |
| 78 | Iridium Cyclooctene Complex That Forms a Hyperpolarization Transfer Catalyst before Converting to<br>a Binuclear C–H Bond Activation Product Responsible for Hydrogen Isotope Exchange. Inorganic<br>Chemistry, 2016, 55, 11639-11643.   | 1.9 | 14        |
| 79 | Solvent responsive catalyst improves NMR sensitivity via efficient magnetisation transfer. Chemical Communications, 2016, 52, 8467-8470.   | 2.2 | 11        |
| 80 | Molecular MRI in the Earth's Magnetic Field Using Continuous Hyperpolarization of a Biomolecule in<br>Water. Journal of Physical Chemistry B, 2016, 120, 5670-5677.  | 1.2 | 37        |
| 81 | Facing and Overcoming Sensitivity Challenges in Biomolecular NMR Spectroscopy. Angewandte Chemie<br>- International Edition, 2015, 54, 9162-9185.  | 7.2 | 258       |
| 82 | Detection of Ïf-alkane complexes of manganese by NMR and IR spectroscopy in solution:<br>(η <sup>5-C<sub>5</sub>H<sub>5</sub>)Mn(CO)<sub>2</sub>(ethane) and<br/>(η<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)Mn(CO)<sub>2</sub>(isopentane). Chemical Science, 2015,<br/>6, 418-424.</sup> | 3.7 | 28        |
| 83 | Deactivation of signal amplification by reversible exchange catalysis, progress towards in vivo application. Chemical Communications, 2015, 51, 9857-9859.   | 2.2 | 44        |
| 84 | Catalytic Transfer of Magnetism Using a Neutral Iridium Phenoxide Complex. Organometallics, 2015, 34, 2997-3006.   | 1.1 | 23        |
| 85 | Strategies for the Hyperpolarization of Acetonitrile and Related Ligands by SABRE. Journal of Physical Chemistry B, 2015, 119, 1416-1424.  | 1.2 | 87        |
| 86 | The reaction of an iridium PNP complex with parahydrogen facilitates polarisation transfer without chemical change. Dalton Transactions, 2015, 44, 1077-1083.  | 1.6 | 30        |
| 87 | Utilisation of water soluble iridium catalysts for signal amplification by reversible exchange. Dalton<br>Transactions, 2015, 44, 7870-7880.   | 1.6 | 49        |
| 88 | Improving the Hyperpolarization of <sup>31</sup> P Nuclei by Synthetic Design. Journal of Physical Chemistry B, 2015, 119, 5020-5027.  | 1.2 | 65        |
| 89 | Investigating pyridazine and phthalazine exchange in a series of iridium complexes in order to define their role in the catalytic transfer of magnetisation from para-hydrogen. Chemical Science, 2015, 6, 3981-3993.  | 3.7 | 43        |
| 90 | Toward Biocompatible Nuclear Hyperpolarization Using Signal Amplification by Reversible Exchange:<br>Quantitative <i>in Situ</i> Spectroscopy and High-Field Imaging. Analytical Chemistry, 2014, 86,<br>1767-1774.  | 3.2 | 105       |

| #   | Article  | IF  | CITATIONS |
|-----|--|-----|-----------|
| 91  | Hyperpolarisation through reversible interactions with parahydrogen. Catalysis Science and Technology, 2014, 4, 3544-3554.   | 2.1 | 84        |
| 92  | Photochemical studies of<br>(η <sup>5</sup> -C <sub>5</sub> H <sub>5</sub> )Ru(PPh <sub>3</sub> ) <sub>2</sub> Cl and<br>(η <sup>5</sup> -C <sub>5</sub> H <sub>5</sub> )Ru(PPh <sub>3</sub> ) <sub>2</sub> Me: formation of Si–H<br>and C–H bond activation products. Dalton Transactions, 2014, 43, 1162-1171. | 1.6 | 13        |
| 93  | Hydrogen Activation by an Aromatic Triphosphabenzene. Journal of the American Chemical Society, 2014, 136, 13453-13457.  | 6.6 | 71        |
| 94  | Photochemical Pump and NMR Probe: Chemically Created NMR Coherence on a Microsecond Time Scale. Journal of the American Chemical Society, 2014, 136, 10124-10131.  | 6.6 | 39        |
| 95  | Computational Studies Explain the Importance of Two Different Substituents on the Chelating<br>Bis(amido) Ligand for Transfer Hydrogenation by Bifunctional Cp*Rh(III) Catalysts. Organometallics,<br>2014, 33, 3433-3442.   | 1.1 | 39        |
| 96  | Probing signal amplification by reversible exchange using an NMR flow system. Magnetic Resonance in Chemistry, 2014, 52, 358-369.  | 1.1 | 81        |
| 97  | A continuousâ€flow, highâ€throughput, highâ€pressure parahydrogen converter for hyperpolarization in a<br>clinical setting. NMR in Biomedicine, 2013, 26, 124-131.   | 1.6 | 83        |
| 98  | Activation of a (cyclooctadiene) rhodium(i) complex supported by a chiral ferrocenyl phosphine<br>thioether ligand for hydrogenation catalysis: a combined parahydrogen NMR and DFT study. Dalton<br>Transactions, 2013, 42, 11720.  | 1.6 | 9         |
| 99  | Optimization of SABRE for polarization of the tuberculosis drugs pyrazinamide and isoniazid. Journal of Magnetic Resonance, 2013, 237, 73-78.  | 1.2 | 122       |
| 100 | A hyperpolarized equilibrium for magnetic resonance. Nature Communications, 2013, 4, 2946.   | 5.8 | 126       |
| 101 | Iridium(III) Hydrido N-Heterocyclic Carbene–Phosphine Complexes as Catalysts in Magnetization<br>Transfer Reactions. Inorganic Chemistry, 2013, 52, 13453-13461.   | 1.9 | 69        |
| 102 | Utilization of SABRE-Derived Hyperpolarization To Detect Low-Concentration Analytes via 1D and 2D NMR Methods. Journal of the American Chemical Society, 2012, 134, 12904-12907.   | 6.6 | 110       |
| 103 | Detection of Unusual Reaction Intermediates during the Conversion of<br>W(N <sub>2</sub> ) <sub>2</sub> (dppe) <sub>2</sub> to W(H) <sub>4</sub> (dppe) <sub>2</sub> and of<br>H <sub>2</sub> O into H <sub>2</sub> . Journal of the American Chemical Society, 2012, 134, 18257-18265.                          | 6.6 | 8         |
| 104 | Photochemical-mediated solid-state [2+2]-cycloaddition reactions of an unsymmetrical dibenzylidene acetone (monothiophos-dba). CrystEngComm, 2012, 14, 5564.   | 1.3 | 21        |
| 105 | Application of <i>Para</i> hydrogen Induced Polarization Techniques in NMR Spectroscopy and Imaging. Accounts of Chemical Research, 2012, 45, 1247-1257.   | 7.6 | 198       |
| 106 | The theory and practice of hyperpolarization in magnetic resonance using parahydrogen. Progress in<br>Nuclear Magnetic Resonance Spectroscopy, 2012, 67, 1-48.   | 3.9 | 317       |
| 107 | Characterisation of tri-ruthenium dihydride complexes through the computation of NMR parameters.<br>Dalton Transactions, 2012, 41, 4618.   | 1.6 | 10        |
| 108 | Improving NMR and MRI Sensitivity with Parahydrogen. Topics in Current Chemistry, 2012, 338, 75-103.   | 4.0 | 16        |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 109 | Manganese Alkane Complexes: An IR and NMR Spectroscopic Investigation. Journal of the American Chemical Society, 2011, 133, 2303-2310.  | 6.6 | 84        |
| 110 | Iridium N-Heterocyclic Carbene Complexes as Efficient Catalysts for Magnetization Transfer from <i>para</i> -Hydrogen. Journal of the American Chemical Society, 2011, 133, 6134-6137.      | 6.6 | 318       |
| 111 | Selective detection of hyperpolarized NMR signals derived from para-hydrogen using the Only<br>Para-hydrogen SpectroscopY (OPSY) approach. Journal of Magnetic Resonance, 2011, 208, 49-57. | 1.2 | 53        |
| 112 | A parahydrogen based NMR study of Pt catalysed alkyne hydrogenation. Dalton Transactions, 2010, 39,<br>3495.  | 1.6 | 20        |
| 113 | Photoinduced N2 loss as a route to long-lived organometallic alkane complexes: A time-resolved IR and NMR study. Chemical Science, 2010, 1, 622.  | 3.7 | 44        |
| 114 | A theoretical basis for spontaneous polarization transfer in non-hydrogenative<br><i>para</i> hydrogen-induced polarization. Journal of Chemical Physics, 2009, 131, 194505.                | 1.2 | 188       |
| 115 | Spontaneous Transfer of <i>Para</i> hydrogen Derived Spin Order to Pyridine at Low Magnetic Field.<br>Journal of the American Chemical Society, 2009, 131, 13362-13368.                     | 6.6 | 165       |
| 116 | Reversible Interactions with para-Hydrogen Enhance NMR Sensitivity by Polarization Transfer. Science, 2009, 323, 1708-1711.   | 6.0 | 761       |
| 117 | <i>Para</i> -Hydrogen Induced Polarization without Incorporation of <i>Para</i> -Hydrogen into the<br>Analyte. Inorganic Chemistry, 2009, 48, 663-670.                                      | 1.9 | 104       |
| 118 | A systematic approach to the generation of long-lived metal alkane complexes: combined IR and NMR study of (Tp)Re(CO)2(cyclopentane). Chemical Communications, 2009, , 1401.                | 2.2 | 27        |
| 119 | An NMR study of cobalt-catalyzed hydroformylation using para-hydrogen induced polarisation.<br>Dalton Transactions, 2009, , 2496.   | 1.6 | 29        |
| 120 | Para-hydrogen induced polarisation effects in liquid phase hydrogenations catalysed by supported metal nanoparticles. Dalton Transactions, 2009, , 5074.                                    | 1.6 | 73        |
| 121 | Parahydrogen-based NMR methods as a mechanistic probe in inorganic chemistry. Coordination Chemistry Reviews, 2008, 252, 2278-2291.   | 9.5 | 117       |
| 122 | Detection of platinum dihydride bisphosphine complexes and studies of their reactivity through para-hydrogen-enhanced NMR methods. Magnetic Resonance in Chemistry, 2008, 46, S107-S114.    | 1.1 | 8         |
| 123 | A DFT Study on the Mechanism of Palladium-Catalyzed Alkyne Hydrogenation: Neutral versus Cationic<br>Pathways. Organometallics, 2008, 27, 43-52.  | 1.1 | 23        |
| 124 | Palladium catalysed alkyne hydrogenation and oligomerisation: a parahydrogen based NMR<br>investigation. Dalton Transactions, 2008, , 4270.   | 1.6 | 20        |
| 125 | Only para-hydrogen spectroscopy (OPSY), a technique for the selective observation of para-hydrogen enhanced NMR signals. Chemical Communications, 2007, , 1183-1185.                        | 2.2 | 84        |
| 126 | Diastereoselective Oxidative Addition of Dihydrogen to IrI(CO)((R)-BINAP) and<br>[Ir(CO)2((R)-BINAP)][SbF6]. Inorganic Chemistry, 2007, 46, 1196-1204.                                      | 1.9 | 14        |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 127 | A para-Hydrogen Investigation of Palladium-Catalyzed Alkyne Hydrogenation. Journal of the American<br>Chemical Society, 2007, 129, 6513-6527.   | 6.6 | 60        |
| 128 | Low temperature in situ UV irradiation of [(η5-C5H5)Co(C2H4)2] in the NMR probe: formation of Co(iii) silyl hydride complexes. Dalton Transactions, 2007, , 2993-2996.  | 1.6 | 13        |
| 129 | Detection of Picomole Amounts of Biological Substrates by <i>para</i> -Hydrogen-Enhanced NMR<br>Methods in Conjunction with a Suitable Receptor Complex. Journal of the American Chemical Society,<br>2007, 129, 11012-11013.         | 6.6 | 38        |
| 130 | A Model Iridium Hydroformylation System with the Large Bite Angle Ligand Xantphos:  Reactivity with<br>Parahydrogen and Implications for Hydroformylation Catalysis. Inorganic Chemistry, 2006, 45,<br>7197-7209.                     | 1.9 | 67        |
| 131 | Use of the tetrahydroborate ligand as "gate-keeper―and protected hydride ligand: preparation and study of alkyl hydride and acyl hydride complexes of ruthenium(ii). Dalton Transactions, 2006, , 2661-2670.                          | 1.6 | 11        |
| 132 | Parahydrogen studies of H2addition to Ir(i) complexes containing chiral phosphine–thioether ligands:<br>implications for catalysis. Dalton Transactions, 2006, , 3350-3359.   | 1.6 | 17        |
| 133 | Contrasting photochemical and thermal reactivity of Ru(CO)2(PPh3)(dppe) towards hydrogen rationalised by parahydrogen NMR and DFT studies. Dalton Transactions, 2006, , 2072.   | 1.6 | 16        |
| 134 | Palladium-Catalyzed Hydrogenation:Â Detection of Palladium Hydrides. A Joint Study Using<br>Para-Hydrogen-Enhanced NMR Spectroscopy and Density Functional Theory. Journal of the American<br>Chemical Society, 2006, 128, 9596-9597. | 6.6 | 33        |
| 135 | Photochemical Isomerization of N-Heterocyclic Carbene Ruthenium Hydride Complexes:Â In situ<br>Photolysis, Parahydrogen, and Computational Studies. Journal of the American Chemical Society, 2006,<br>128, 7452-7453.                | 6.6 | 20        |
| 136 | Coordination Chemistry and Diphenylacetylene Hydrogenation Catalysis of Planar Chiral<br>Ferrocenylphosphane-Thioether Ligands with Cyclooctadieneiridium(l). European Journal of Inorganic<br>Chemistry, 2006, 2006, 1803-1816.      | 1.0 | 26        |
| 137 | Generation and interrogation of a pure nuclear spin state by parahydrogen-enhanced NMR spectroscopy: a defined initial state for quantum computation. Magnetic Resonance in Chemistry, 2005, 43, 200-208.                             | 1.1 | 31        |
| 138 | Parahydrogen derived illumination of pyridine based coordination products obtained from reactions involving rhodium phosphine complexes. Dalton Transactions, 2005, , 3773.   | 1.6 | 15        |
| 139 | Photochemical reactions of [CH2(η5-C5H4)2][Rh(C2H4)2]2with silanes: evidence for Si–C and C–H activation pathways. Dalton Transactions, 2005, , 744-759.  | 1.6 | 9         |
| 140 | Detection of Intermediates in Cobalt-Catalyzed Hydroformylation Using para-Hydrogen-Induced Polarization. Journal of the American Chemical Society, 2005, 127, 4994-4995.   | 6.6 | 39        |
| 141 | A Parahydrogen Study of Catalytic Hydrogenation by Diphosphane-Substituted Triruthenium Clusters.<br>European Journal of Inorganic Chemistry, 2004, 2004, 4381-4387.  | 1.0 | 11        |
| 142 | Hydrogenation Studies Involving Halobis(phosphine)–Rhodium(i) Dimers: Use of Parahydrogen<br>Induced Polarisation To Detect Species Present at Low Concentration. Chemistry - A European Journal,<br>2004, 10, 2459-2474.             | 1.7 | 42        |
| 143 | Roles of a tetrahydroborate ligand in a facile route to ruthenium(ii) ethyl hydride complexes, and a kinetic study of ethane reductive elimination. Dalton Transactions, 2004, , 3788-3797.   | 1.6 | 10        |
| 144 | New perspectives in hydroformylation : a para-hydrogen study. Chemical Communications, 2004, ,<br>1826-1827.  | 2.2 | 32        |

| #   | Article  | IF  | CITATIONS |
|-----|--|-----|-----------|
| 145 | A combined parahydrogen and theoretical study of H2 activation by 16-electron d8 ruthenium(0) complexes and their subsequent catalytic behaviour. Dalton Transactions, 2004, , 3616.   | 1.6 | 31        |
| 146 | Applications of the parahydrogen phenomenon in inorganic chemistry. Dalton Transactions, 2004, , 2601.   | 1.6 | 70        |
| 147 | New insights into catalytic hydrogenation by phosphido-substituted triruthenium clusters:<br>confirmation of intact cluster catalysis by parahydrogen NMR. Dalton Transactions, 2004, , 2108-2114.   | 1.6 | 21        |
| 148 | The reaction of M(CO)3(Ph2PCH2CH2PPh2) (M = Fe, Ru) with parahydrogen: probing the electronic structure of reaction intermediates and the internal rearrangement mechanism for the dihydride products. Dalton Transactions, 2004, , 3218-3224.   | 1.6 | 39        |
| 149 | Direct reaction of photogenerated diarylcarbenes at square-planar rhodium(i). Dalton Transactions, 2004, , 2746-2749.  | 1.6 | 10        |
| 150 | Implementation of NMR quantum computation with parahydrogen-derived high-purity quantum states.<br>Physical Review A, 2004, 70, .  | 1.0 | 25        |
| 151 | Platinum Bis(tricyclohexylphosphine) Silyl Hydride Complexes. Organometallics, 2004, 23, 5744-5756.  | 1.1 | 68        |
| 152 | Preparing High Purity Initial States for Nuclear Magnetic Resonance Quantum Computing. Physical<br>Review Letters, 2004, 93, 040501.   | 2.9 | 74        |
| 153 | Detection and Reactivity of Pd((C8H14)PCH2CH2P(C8H14))(CHPhCH2Ph)(H) as Determined by Parahydrogen-Enhanced NMR Spectroscopy. Journal of the American Chemical Society, 2004, 126, 16708-16709.  | 6.6 | 26        |
| 154 | The Study of Inorganic Systems by NMR Spectroscopy in Conjunction with Parahydrogenâ€Induced Polarisation. European Journal of Inorganic Chemistry, 2003, 2003, 2901-2912.   | 1.0 | 55        |
| 155 | Catalytic Hydrogenation by Triruthenium Clusters: A Mechanistic Study with Parahydrogen-Induced Polarization. Chemistry - A European Journal, 2003, 9, 1045-1061.  | 1.7 | 41        |
| 156 | Nucleophilic attack on η3-allyl and η2-tetrahydroborate complexes of ruthenium(ii). Dalton<br>Transactions, 2003, , 2603-2614.   | 1.6 | 19        |
| 157 | Dipyridylketone binding and subsequent C–C bond insertion reactions at cyclopentadienylrhodium.<br>Chemical Communications, 2003, , 2332-2333.   | 2.2 | 24        |
| 158 | Exchange Processes in Complexes with Two Ruthenium (η2-Silane) Linkages: Role of the Secondary<br>Interactions between Silicon and Hydrogen Atoms. Organometallics, 2002, 21, 5347-5357.   | 1.1 | 75        |
| 159 | Ruthenium Dihydride Complexes:Â NMR Studies of Intramolecular Isomerization and Fluxionality<br>Including the Detection of Minor Isomers by Parahydrogen-Induced Polarization. Inorganic Chemistry,<br>2002, 41, 2960-2970.  | 1.9 | 40        |
| 160 | NMR characterisation of unstable solvent and dihydride complexes generated at low temperature by in-situ UV irradiation. Chemical Communications, 2002, , 2836-2837.   | 2.2 | 26        |
| 161 | Activation of H2 by halocarbonyl bis-phosphine and bis-arsine iridium(i) complexes. The use of parahydrogen induced polarisation to detect species present at low concentration and investigate their reactivityBased on the presentation given at Dalton Discussion No. 4, 10–13th January 2002, Kloster Banz, Germany Dalton Transactions RSC. 2002 743-751. | 2.3 | 16        |
| 162 | Separation and characterisation of products of the reaction between propionamide and formaldehyde. Chromatographia, 2002, 55, 307-316.   | 0.7 | 2         |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 163 | NMR Studies of Ru3(CO)10(PMe2Ph)2and Ru3(CO)10(PPh3)2and Their H2Addition Products:Â Detection of<br>New Isomers with Complex Dynamic Behavior. Journal of the American Chemical Society, 2001, 123,<br>9760-9768.  | 6.6 | 43        |
| 164 | Direct Comparison of Hydrogenation Catalysis by Intact versus Fragmented Triruthenium Clusters.<br>Angewandte Chemie - International Edition, 2001, 40, 3874-3877.  | 7.2 | 41        |
| 165 | Addition of H2 to a cationic iridium(I) complex: a study using parahydrogen NMR. Dalton Transactions RSC, 2000, , 2251-2253.  | 2.3 | 6         |
| 166 | Characterisation and kinetic behaviour of H2Rh(PPh3)2(μ-Cl)2Rh(PPh3)(alkene) and related binuclear complexes detected during hydrogenation studies involving parahydrogen induced polarisation. Chemical Communications, 2000, , 685-686.                       | 2.2 | 23        |
| 167 | Observation of New Intermediates in the Reaction of Dihydrogen with Iridium, Rhodium, and Mixed<br>Metal A-Frame Complexes with Parahydrogen-Induced Polarization. Organometallics, 2000, 19,<br>2985-2993.   | 1.1 | 31        |
| 168 | Activation of H2 by halogenocarbonylbis(phosphine)rhodium(I) complexes. The use of parahydrogen<br>induced polarisation to detect species present at low concentration. Journal of the Chemical Society<br>Dalton Transactions, 1999, , 3949-3960.              | 1.1 | 19        |
| 169 | Applications of the parahydrogen phenomenon: A chemical perspective. Progress in Nuclear Magnetic<br>Resonance Spectroscopy, 1999, 34, 71-92.   | 3.9 | 222       |
| 170 | Kinetic and mechanistic examination of NBu4[IrH2(CO)2I2] and NBu4[RhH2(CO)2I2] via para-hydrogen enhanced NMR spectroscopy. Chemical Communications, 1999, , 889-890.   | 2.2 | 12        |
| 171 | New products in an old reaction: isomeric products from H2 addition to Vaska's complex and its analogues. Chemical Communications, 1999, , 1717-1718.   | 2.2 | 22        |
| 172 | NMR detection of thermal and photochemical dihydrogen addition products of mono- and tri-nuclear ruthenium complexes containing carbonyl and triphenylphosphine ligands through para-hydrogen induced polarisation. Chemical Communications, 1999, , 1223-1224. | 2.2 | 19        |
| 173 | Structure and dynamics in metal phosphine complexes using advanced NMR studies with para-hydrogen induced polarisation. Journal of the Chemical Society Dalton Transactions, 1999, , 1429.  | 1.1 | 44        |
| 174 | Reaction of iodocarbonylbis(trimethylphosphine)rhodium(I) with parahydrogen leads to the<br>observation of five characterisable H2 addition products. Journal of the Chemical Society Dalton<br>Transactions, 1998, , 3363-3366.                                | 1.1 | 11        |
| 175 | Parahydrogen enhanced NMR studies on thermally and photochemically generated products from [IrH3(CO)(PPh3)2]. Chemical Communications, 1998, , 923-924.   | 2.2 | 17        |
| 176 | Luminescent Iridium(I) Diethyldithiocarbamate Complexes:  Synthesis, Structure, and Reactivity<br>Including Stereoselective Hydrogen Oxidative Addition. Journal of the American Chemical Society,<br>1997, 119, 7716-7725.                                     | 6.6 | 36        |
| 177 | NMR studies on ligand exchange at [IrH2Cl(CO)(PPh3)2] and [IrH2Cl(PPh3)3] by para-hydrogen induced polarisation. Chemical Communications, 1996, , 2395.   | 2.2 | 21        |
| 178 | Definitive Evidence for a Pairwise Addition of Hydrogen to a Platinum Bis(phosphine) Complex Using<br>Parahydrogen-Induced Polarization. Organometallics, 1996, 15, 2863-2865.  | 1.1 | 41        |
| 179 | Equilibria between isomers of ruthenium dihydride complexes: detection of minor isomers by parahydrogen induced polarisation. Chemical Communications, 1996, , 383.   | 2.2 | 20        |
| 180 | Dalton communications. Rapid characterisation of rhodium dihydrides by nuclear magnetic resonance spectroscopy using indirect two-dimensional methods and para-hydrogen. Journal of the Chemical Society Dalton Transactions, 1995, , 3427.                     | 1.1 | 28        |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 181 | Observation of New Intermediates in Hydrogenation Catalyzed by Wilkinson's Catalyst, RhCl(PPh3)3,<br>Using Parahydrogen-Induced Polarization. Journal of the American Chemical Society, 1994, 116,<br>10548-10556.                                | 6.6 | 170       |
| 182 | Activation of H2by chlorocarbonylbis(trimethylphosphine)rhodium(I) labilizes CO and produces the<br>new binuclear complex H(Cl)Rh(PMe3)2(Âμ-H)(Âμ-Cl)RH(PMe3)(CO). Journal of the Chemical Society<br>Chemical Communications, 1993, , 1185-1187. | 2.0 | 13        |
| 183 | Observation of H2 oxidative addition to chlorocarbonylbis(triphenylphosphine)rhodium(I) using parahydrogen induced polarization. Journal of the American Chemical Society, 1993, 115, 5292-5293.  | 6.6 | 49        |
| 184 | More than INEPT: parahydrogen and INEPT + give unprecedented resonance enhancement to carbon-13<br>by direct proton polarization transfer. Journal of the American Chemical Society, 1993, 115, 1156-1157.  | 6.6 | 72        |