# Dimitrios A Pantazis

## List of Publications by Year in Descending Order



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| 124 papers | 7,415 citations | 43 h-index | 84 g-index |
| 134 ext. papers | 8,386 ext. citations | 7.8 avg, IF | 6.59 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 124 | EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. *Magnetochemistry*, **2022**, 8, 36 | 3.1 | 0 |
| 123 | Electrostatic profiling of photosynthetic pigments: implications for directed spectral tuning. *Physical Chemistry Chemical Physics*, **2021**, 23, 24677-24684 | 3.6 | |
| 122 | Natural and Artificial Photosynthesis **2021**, 41-76 | | 2 |
| 121 | Isolation and reactivity of an elusive diazoalkene. *Nature Chemistry*, **2021**, 13, 587-593 | 17.6 | 18 |
| 120 | Structure-Spectroscopy Correlations for Intermediate Q of Soluble Methane Monooxygenase: Insights from QM/MM Calculations. *Journal of the American Chemical Society*, **2021**, 143, 6560-6577 | 16.4 | 6 |
| 119 | Orientational Jahn-Teller Isomerism in the Dark-Stable State of Nature's Water Oxidase. *Angewandte Chemie - International Edition*, **2021**, 60, 13493-13499 | 16.4 | 13 |
| 118 | Converged Structural and Spectroscopic Properties for Refined QM/MM Models of Azurin. *Inorganic Chemistry*, **2021**, 60, 7399-7412 | 5.1 | 3 |
| 117 | The Reactivity of the Imine Bond within Polynuclear Nickel(II) Complexes. *Crystals*, **2021**, 11, 512 | 2.3 | 1 |
| 116 | Orientational Jahn□Teller Isomerism in the Dark-Stable State of Nature's Water Oxidase. *Angewandte Chemie*, **2021**, 133, 13605-13611 | 3.6 | 2 |
| 115 | Reversible Silylium Transfer between P-H and Si-H Donors. *Angewandte Chemie - International Edition*, **2021**, 60, 2379-2384 | 16.4 | 1 |
| 114 | Arrested Substrate Binding Resolves Catalytic Intermediates in Higher-Plant Water Oxidation. *Angewandte Chemie - International Edition*, **2021**, 60, 3156-3162 | 16.4 | 14 |
| 113 | Arrested Substrate Binding Resolves Catalytic Intermediates in Higher-Plant Water Oxidation. *Angewandte Chemie*, **2021**, 133, 3193-3199 | 3.6 | 3 |
| 112 | Reversible Silylium Transfer between P-H and Si-H Donors. *Angewandte Chemie*, **2021**, 133, 2409-2414 | 3.6 | 0 |
| 111 | Chlorophyll excitation energies and structural stability of the CP47 antenna of photosystem II: a case study in the first-principles simulation of light-harvesting complexes. *Chemical Science*, **2021**, 12, 4463-4476 | 9.4 | 3 |
| 110 | Successes, challenges, and opportunities for quantum chemistry in understanding metalloenzymes for solar fuels research. *Chemical Communications*, **2021**, 57, 3952-3974 | 5.8 | 6 |
| 109 | How Can We Predict Accurate Electrochromic Shifts for Biochromophores? A Case Study on the Photosynthetic Reaction Center. *Journal of Chemical Theory and Computation*, **2021**, 17, 1858-1873 | 6.4 | 7 |
| 108 | Redox Isomerism in the S State of the Oxygen-Evolving Complex Resolved by Coupled Cluster Theory. *Chemistry - A European Journal*, **2021**, 27, 12815-12825 | 4.8 | 8 |

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| 107 | Magnetic exchange coupling in Cu dimers studied with modern multireference methods and broken-symmetry coupled cluster theory. *Theoretical Chemistry Accounts*, **2021**, 140, 1 | 1.9 | 1 |
| 106 | Electronic properties of the S□=□5/2 Mn(II) complexes [Mn{PhC(O)NP(O)PPh2}(N,N)(NO3)], (N,N)□=□phenanthroline, neocuproine, 2,2?-bipyridine. *Polyhedron*, **2021**, 207, 115374 | 2.7 | |
| 105 | Spin-state energetics of manganese spin crossover complexes: Comparison of single-reference and multi-reference ab initio approaches. *Polyhedron*, **2021**, 208, 115399 | 2.7 | 3 |
| 104 | Characterization of a Triplet Vinylidene.. *Journal of the American Chemical Society*, **2021**, 143, 21410-21415 | 15.4 | 0 |
| 103 | Comparison of Density Functional and Correlated Wave Function Methods for the Prediction of Cu(II) Hyperfine Coupling Constants. *ChemPhysChem*, **2020**, 21, 2667-2679 | 3.2 | 8 |
| 102 | Performance of density functional theory and orbital-optimised second-order perturbation theory methods for geometries and singlet□triplet state splittings of aryl-carbenes. *Molecular Physics*, **2020**, 118, e1764644 | 1.7 | 10 |
| 101 | All-electron scalar relativistic basis sets for the elements Rb-Xe. *Journal of Computational Chemistry* , **2020**, 41, 1842-1849 | 3.5 | 28 |
| 100 | Current Understanding of the Mechanism of Water Oxidation in Photosystem II and Its Relation to XFEL Data. *Annual Review of Biochemistry*, **2020**, 89, 795-820 | 29.1 | 62 |
| 99 | Unusual P Hyperfine Strain Effects in a Conformationally Flexible Cu(II) Complex Revealed by Two-Dimensional Pulse EPR Spectroscopy. *Inorganic Chemistry*, **2020**, 59, 3666-3676 | 5.1 | 5 |
| 98 | Accurate computed spin-state energetics for Co(iii) complexes: implications for modelling homogeneous catalysis. *Dalton Transactions*, **2020**, 49, 6478-6487 | 4.3 | 11 |
| 97 | Evaluation of new low-valent computational models for the oxygen-evolving complex of photosystem II. *Chemical Physics Letters*, **2020**, 753, 137629 | 2.5 | 6 |
| 96 | Protein Matrix Control of Reaction Center Excitation in Photosystem II. *Journal of the American Chemical Society*, **2020**, 142, 18174-18190 | 16.4 | 21 |
| 95 | Accurate Computation of the Absorption Spectrum of Chlorophyll with Pair Natural Orbital Coupled Cluster Methods. *Journal of Physical Chemistry B*, **2020**, 124, 8761-8771 | 3.4 | 27 |
| 94 | Orbital Entanglement Analysis of Exchange-Coupled Systems. *Journal of Physical Chemistry Letters*, **2019**, 10, 6762-6770 | 6.4 | 12 |
| 93 | Microsolvation of the Redox-Active Tyrosine-D in Photosystem II: Correlation of Energetics with EPR Spectroscopy and Oxidation-Induced Proton Transfer. *Journal of the American Chemical Society* , **2019**, 141, 3217-3231 | 16.4 | 12 |
| 92 | Assessment of Double-Hybrid Density Functional Theory for Magnetic Exchange Coupling in Manganese Complexes. *Inorganics*, **2019**, 7, 57 | 2.9 | 11 |
| 91 | The S3 State of the Oxygen-Evolving Complex: Overview of Spectroscopy and XFEL Crystallography with a Critical Evaluation of Early-Onset Models for O□O Bond Formation. *Inorganics*, **2019**, 7, 55 | 2.9 | 19 |
| 90 | Proton Translocation via Tautomerization of Asn298 During the S-S State Transition in the Oxygen-Evolving Complex of Photosystem II. *Journal of Physical Chemistry B*, **2019**, 123, 3068-3078 | 3.4 | 20 |

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| 89 | Applications of the Density Matrix Renormalization Group to Exchange-Coupled Transition Metal Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 91-120 | 0.7 | 5 |
| 88 | Multireference Approaches to Spin-State Energetics of Transition Metal Complexes Utilizing the Density Matrix Renormalization Group. *Advanced Theory and Simulations*, **2019**, 2, 1800201 | 3.5 | 29 |
| 87 | Physical Nature of Differential Spin-State Stabilization of Carbenes by Hydrogen and Halogen Bonding: A Domain-Based Pair Natural Orbital Coupled Cluster Study. *Journal of Physical Chemistry A*, **2019**, 123, 5081-5090 | 2.8 | 11 |
| 86 | Implications of structural heterogeneity for the electronic structure of the final oxygen-evolving intermediate in photosystem II. *Journal of Inorganic Biochemistry*, **2019**, 199, 110797 | 4.2 | 13 |
| 85 | First-Principles Calculation of Transition Metal Hyperfine Coupling Constants with the Strongly Constrained and Appropriately Normed (SCAN) Density Functional and its Hybrid Variants. *Magnetochemistry*, **2019**, 5, 69 | 3.1 | 4 |
| 84 | Calcium Valence-to-Core X-ray Emission Spectroscopy: A Sensitive Probe of Oxo Protonation in Structural Models of the Oxygen-Evolving Complex. *Inorganic Chemistry*, **2019**, 58, 16292-16301 | 5.1 | 9 |
| 83 | Meeting the Challenge of Magnetic Coupling in a Triply-Bridged Chromium Dimer: Complementary Broken-Symmetry Density Functional Theory and Multireference Density Matrix Renormalization Group Perspectives. *Journal of Chemical Theory and Computation*, **2019**, 15, 938-948 | 6.4 | 25 |
| 82 | Accurate Spin-State Energetics for Aryl Carbenes. *Journal of Chemical Theory and Computation*, **2018**, 14, 4733-4746 | 6.4 | 17 |
| 81 | Exchange Coupling Interactions from the Density Matrix Renormalization Group and N-Electron Valence Perturbation Theory: Application to a Biomimetic Mixed-Valence Manganese Complex. *Journal of Chemical Theory and Computation*, **2018**, 14, 166-179 | 6.4 | 40 |
| 80 | Systematic High-Accuracy Prediction of Electron Affinities for Biological Quinones. *Journal of Computational Chemistry*, **2018**, 39, 2439-2451 | 3.5 | 6 |
| 79 | Missing Pieces in the Puzzle of Biological Water Oxidation. *ACS Catalysis*, **2018**, 8, 9477-9507 | 13.1 | 101 |
| 78 | What Can We Learn from a Biomimetic Model of Nature's Oxygen-Evolving Complex?. *Inorganic Chemistry*, **2017**, 56, 3875-3888 | 5.1 | 35 |
| 77 | Structural models of the biological oxygen-evolving complex: achievements, insights, and challenges for biomimicry. *Green Chemistry*, **2017**, 19, 2309-2325 | 10 | 55 |
| 76 | Differences in the Active Site of Water Oxidation among Photosynthetic Organisms. *Journal of the American Chemical Society*, **2017**, 139, 14340-14343 | 16.4 | 25 |
| 75 | The First State in the Catalytic Cycle of the Water-Oxidizing Enzyme: Identification of a Water-Derived Hydroxo Bridge. *Journal of the American Chemical Society*, **2017**, 139, 14412-14424 | 16.4 | 49 |
| 74 | Principles of Natural Photosynthesis. *Topics in Current Chemistry*, **2016**, 371, 23-48 | | 40 |
| 73 | Recent developments in biological water oxidation. *Current Opinion in Chemical Biology*, **2016**, 31, 113-9 | 9.7 | 87 |
| 72 | Improved Segmented All-Electron Relativistically Contracted Basis Sets for the Lanthanides. *Journal of Chemical Theory and Computation*, **2016**, 12, 1148-56 | 6.4 | 62 |

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| 71 | A five-coordinate Mn(iv) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding. *Chemical Science*, **2016**, 7, 72-84 | 9.4 | 134 |
| 70 | Redox potential tuning by redox-inactive cations in nature's water oxidizing catalyst and synthetic analogues. *Physical Chemistry Chemical Physics*, **2016**, 18, 10739-50 | 3.6 | 29 |
| 69 | Spin State as a Marker for the Structural Evolution of Nature's Water-Splitting Catalyst. *Inorganic Chemistry*, **2016**, 55, 488-501 | 5.1 | 70 |
| 68 | Interaction of methanol with the oxygen-evolving complex: atomistic models, channel identification, species dependence, and mechanistic implications. *Chemical Science*, **2016**, 7, 6463-6476 | 9.4 | 40 |
| 67 | Alkene Insertions into a RuPR2 Bond. *Organometallics*, **2016**, 35, 3970-3980 | 3.8 | 9 |
| 66 | Ionization Energies and Aqueous Redox Potentials of Organic Molecules: Comparison of DFT, Correlated ab Initio Theory and Pair Natural Orbital Approaches. *Journal of Chemical Theory and Computation*, **2016**, 12, 2272-84 | 6.4 | 68 |
| 65 | Axial ligand effect on the catalytic activity of biomimetic Fe-porphyrin catalyst: An experimental and DFT study. *Journal of Catalysis*, **2016**, 344, 768-777 | 7.3 | 18 |
| 64 | Understanding and tuning the properties of redox-accumulating manganese helicates. *Dalton Transactions*, **2016**, 45, 18900-18908 | 4.3 | 12 |
| 63 | Characterization of Oxygen Bridged Manganese Model Complexes Using Multifrequency (17)O-Hyperfine EPR Spectroscopies and Density Functional Theory. *Journal of Physical Chemistry B*, **2015**, 119, 13904-21 | 3.4 | 19 |
| 62 | Dioxygen Activation and Catalytic Reduction to Hydrogen Peroxide by a Thiolate-Bridged Dimanganese(II) Complex with a Pendant Thiol. *Journal of the American Chemical Society*, **2015**, 137, 8644-53 | 16.4 | 44 |
| 61 | Calcium and heterometallic manganese-calcium complexes supported by tripodal pyridine-carboxylate ligands: structural, EPR and theoretical investigations. *Dalton Transactions*, **2015**, 44, 12757-70 | 4.3 | 14 |
| 60 | How Accurately Can Extended X-ray Absorption Spectra Be Predicted from First Principles? Implications for Modeling the Oxygen-Evolving Complex in Photosystem II. *Journal of the American Chemical Society*, **2015**, 137, 12815-34 | 16.4 | 22 |
| 59 | Resolving the Manganese Oxidation States in the Oxygen-evolving Catalyst of Natural Photosynthesis. *Israel Journal of Chemistry*, **2015**, 55, 1219-1232 | 3.4 | 21 |
| 58 | Artificial photosynthesis: understanding water splitting in nature. *Interface Focus*, **2015**, 5, 20150009 | 3.9 | 47 |
| 57 | Metal oxidation states in biological water splitting. *Chemical Science*, **2015**, 6, 1676-1695 | 9.4 | 225 |
| 56 | Structure, ligands and substrate coordination of the oxygen-evolving complex of photosystem II in the S2 state: a combined EPR and DFT study. *Physical Chemistry Chemical Physics*, **2014**, 16, 11877-92 | 3.6 | 66 |
| 55 | The first tyrosyl radical intermediate formed in the S2-S3 transition of photosystem II. *Physical Chemistry Chemical Physics*, **2014**, 16, 11901-10 | 3.6 | 60 |
| 54 | Oxygen-evolving Photosystem II **2014**, 1-13 | | 4 |

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| 53 | A first-principles approach to the calculation of the on-site zero-field splitting in polynuclear transition metal complexes. *Inorganic Chemistry*, **2014**, 53, 11785-93 | 5.1 | 28 |
| 52 | Electronic structural flexibility of heterobimetallic Mn/Fe cofactors: R2lox and R2c proteins. *Journal of the American Chemical Society*, **2014**, 136, 13399-409 | 16.4 | 31 |
| 51 | Photosynthesis. Electronic structure of the oxygen-evolving complex in photosystem II prior to O-O bond formation. *Science*, **2014**, 345, 804-8 | 33.3 | 363 |
| 50 | All-electron basis sets for heavy elements. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 363-374 | 7.9 | 26 |
| 49 | Convergence of QM/MM and Cluster Models for the Spectroscopic Properties of the Oxygen-Evolving Complex in Photosystem II. *Journal of Chemical Theory and Computation*, **2013**, 9, 3832-42 | 6.4 | 50 |
| 48 | Ammonia binding to the oxygen-evolving complex of photosystem II identifies the solvent-exchangeable oxygen bridge (Ebxo) of the manganese tetramer. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 15561-6 | 11.5 | 130 |
| 47 | Biological water oxidation. *Accounts of Chemical Research*, **2013**, 46, 1588-96 | 24.3 | 407 |
| 46 | On the magnetic and spectroscopic properties of high-valent Mn3CaO4 cubanes as structural units of natural and artificial water-oxidizing catalysts. *Journal of the American Chemical Society*, **2013**, 135, 5726-39 | 16.4 | 81 |
| 45 | Two interconvertible structures that explain the spectroscopic properties of the oxygen-evolving complex of photosystem II in the S2 state. *Angewandte Chemie - International Edition*, **2012**, 51, 9935-40 | 16.4 | 293 |
| 44 | Zwei ineinander umwandelbare Strukturen erklEen die spektroskopischen Eigenschaften des Wasser oxidierenden Enzyms des Photosystems II im S2-Zustand. *Angewandte Chemie*, **2012**, 124, 10074-10079 | 3.6 | 25 |
| 43 | All-electron scalar relativistic basis sets for the 6p elements. *Theoretical Chemistry Accounts*, **2012**, 131, 1 | 1.9 | 79 |
| 42 | A Hierarchy of Methods for the Energetically Accurate Modeling of Isomerism in Monosaccharides. *Journal of Chemical Theory and Computation*, **2012**, 8, 2630-45 | 6.4 | 49 |
| 41 | Effect of Ca2+/Sr2+ substitution on the electronic structure of the oxygen-evolving complex of photosystem II: a combined multifrequency EPR, 55Mn-ENDOR, and DFT study of the S2 state. *Journal of the American Chemical Society*, **2011**, 133, 3635-48 | 16.4 | 190 |
| 40 | Theoretical evaluation of structural models of the S2 state in the oxygen evolving complex of Photosystem II: protonation states and magnetic interactions. *Journal of the American Chemical Society*, **2011**, 133, 19743-57 | 16.4 | 249 |
| 39 | Detailed ab initio first-principles study of the magnetic anisotropy in a family of trigonal pyramidal iron(II) pyrrolide complexes. *Inorganic Chemistry*, **2011**, 50, 7460-77 | 5.1 | 120 |
| 38 | The electronic structures of the S(2) states of the oxygen-evolving complexes of photosystem II in plants and cyanobacteria in the presence and absence of methanol. *Biochimica Et Biophysica Acta - Bioenergetics*, **2011**, 1807, 829-40 | 4.6 | 75 |
| 37 | What is not required to make a single molecule magnet. *Faraday Discussions*, **2011**, 148, 229-38; discussion 299-314 | 3.6 | 265 |
| 36 | All-Electron Scalar Relativistic Basis Sets for the Actinides. *Journal of Chemical Theory and Computation*, **2011**, 7, 677-684 | 6.4 | 187 |

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| 35 | Effect of Ca2+/Sr2+Substitution on the Electronic Structure of the Oxygen-Evolving Complex of Photosystem II: A Combined Multifrequency EPR,55Mn-ENDOR, and DFT Study of the S2State. *Journal of the American Chemical Society*, **2011**, 133, 14149-14149 | 16.4 | 7 |
| 34 | Benzonitrile Adducts of Terminal Diarylphosphido Complexes: Preparative Sources of Ru?PR2 *Organometallics*, **2011**, 30, 6458-6465 | 3.8 | 19 |
| 33 | C-H bond activation of benzene by unsaturated -cyclopropene and -benzyne complexes of niobium. *Journal of the American Chemical Society*, **2010**, 132, 14239-50 | 16.4 | 35 |
| 32 | Activation of a water molecule using a mononuclear Mn complex: from Mn-aquo, to Mn-hydroxo, to Mn-oxyl charge compensation. *Energy and Environmental Science*, **2010**, 3, 924-938 | 35.4 | 49 |
| 31 | Dealing with Complexity in Open-Shell Transition Metal Chemistry from a Theoretical Perspective: Reaction Pathways, Bonding, Spectroscopy, And Magnetic Properties. *Advances in Inorganic Chemistry*, **2010**, 62, 301-349 | 2.1 | 33 |
| 30 | Theoretical magnetochemistry of dinuclear manganese complexes: broken symmetry density functional theory investigation on the influence of bridging motifs on structure and magnetism. *Dalton Transactions*, **2010**, 39, 4959-67 | 4.3 | 93 |
| 29 | Concerted [2+2] cycloaddition of alkenes to a ruthenium-phosphorus double bond. *Angewandte Chemie - International Edition*, **2010**, 49, 3367-70 | 16.4 | 20 |
| 28 | A new quantum chemical approach to the magnetic properties of oligonuclear transition-metal complexes: application to a model for the tetranuclear manganese cluster of photosystem II. *Chemistry - A European Journal*, **2009**, 15, 5108-23 | 4.8 | 106 |
| 27 | Density functional theory. *Photosynthesis Research*, **2009**, 102, 443-53 | 3.7 | 174 |
| 26 | Magnetic and spectroscopic properties of mixed valence manganese(III,IV) dimers: a systematic study using broken symmetry density functional theory. *Inorganic Chemistry*, **2009**, 48, 7251-60 | 5.1 | 98 |
| 25 | Trinuclear terpyridine frustrated spin system with a Mn(IV)3O4 core: synthesis, physical characterization, and quantum chemical modeling of its magnetic properties. *Inorganic Chemistry*, **2009**, 48, 10281-8 | 5.1 | 50 |
| 24 | All-Electron Scalar Relativistic Basis Sets for the Lanthanides. *Journal of Chemical Theory and Computation*, **2009**, 5, 2229-38 | 6.4 | 227 |
| 23 | C Coupling Constants, JCC, Are Reliable Probes for C Agostic Structures. *Organometallics*, **2009**, 28, 940-943 | 3.8 | 23 |
| 22 | Structure of the oxygen-evolving complex of photosystem II: information on the S(2) state through quantum chemical calculation of its magnetic properties. *Physical Chemistry Chemical Physics*, **2009**, 11, 6788-98 | 3.6 | 114 |
| 21 | All-Electron Scalar Relativistic Basis Sets for Third-Row Transition Metal Atoms. *Journal of Chemical Theory and Computation*, **2008**, 4, 908-19 | 6.4 | 832 |
| 20 | On the Origin of and Agostic Distortions in Early-Transition-Metal Alkyl Complexes. *Organometallics*, **2008**, 27, 1128-1134 | 3.8 | 51 |
| 19 | A re-evaluation of the two-step spin crossover in the trinuclear cation [Co3(dipyridylamido)4Cl2]+. *Dalton Transactions*, **2008**, 608-14 | 4.3 | 21 |
| 18 | 1,2-Diphosphinobenzene as a synthon for the 1,2,3-triphospha- and 2-arsa-1,3-diphosphaindenyl anions and a stable organo derivative of the P8 unit of Hittorf's phosphorus. *Chemical Communications*, **2008**, 856-8 | 5.8 | 30 |

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| 17 | Promotion of phosphaalkyne cyclooligomerisation by a Sb(v) to Sb(iii) redox process. *Dalton Transactions*, **2008**, 3753-8 | 4.3 | 10 |
| 16 | Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. *Journal of Chemical Theory and Computation*, **2008**, 4, 1449-59 | 6.4 | 363 |
| 15 | A Highly Reactive Ruthenium Phosphido Complex Exhibiting Ru P Bonding. *Organometallics*, **2007**, 26, 1473-1482 | 3.8 | 45 |
| 14 | Critical Role of the Correlation Functional in DFT Descriptions of an Agostic Niobium Complex. *Journal of Chemical Theory and Computation*, **2007**, 3, 1329-36 | 6.4 | 51 |
| 13 | Evidence for a SN2-type pathway for phosphine exchange in phosphine-phosphenium cations, [R2P--PR'3]+. *Chemistry - A European Journal*, **2007**, 13, 6967-74 | 4.8 | 33 |
| 12 | A new reaction pathway in organophosphorus chemistry: competing S(N)2 and AE' pathways for nucleophilic attack at a phosphorus-carbon cage compound. *Angewandte Chemie - International Edition*, **2006**, 45, 3628-31 | 16.4 | 21 |
| 11 | A main-group analogue of housene: the subtle influence of the inert-pair effect in group 15 clusters. *Angewandte Chemie - International Edition*, **2006**, 45, 6685-9 | 16.4 | 31 |
| 10 | A New Reaction Pathway in Organophosphorus Chemistry: Competing SN2 and AE? Pathways for Nucleophilic Attack at a Phosphorus Carbon Cage Compound. *Angewandte Chemie*, **2006**, 118, 3710-3713 | 3.6 | 14 |
| 9 | A Main-Group Analogue of Housene: The Subtle Influence of the Inert-Pair Effect in Group 15 Clusters. *Angewandte Chemie*, **2006**, 118, 6837-6841 | 3.6 | 16 |
| 8 | Cationic phosphorus-carbon-pnictogen cages isolobal to [C5R5]+. *Chemical Communications*, **2006**, 1375-7 | 3.8 | 30 |
| 7 | Experimental and theoretical investigations of new dinuclear palladium complexes as precatalysts for the amination of aryl chlorides. *Journal of the American Chemical Society*, **2006**, 128, 6376-90 | 16.4 | 141 |
| 6 | Synthesis and Computational Studies of Palladium(I) Dimers Pd2X2(PtBu2Ph)2(X = Br, I): Phenyl versus Halide Bridging Modes. *Organometallics*, **2006**, 25, 5990-5995 | 3.8 | 18 |
| 5 | A three-state model for the polymorphism in linear tricobalt compounds. *Journal of the American Chemical Society*, **2006**, 128, 4128-35 | 16.4 | 68 |
| 4 | Structure and bonding in the isoelectronic series CnHnP5-n+: is phosphorus a carbon copy?. *Dalton Transactions*, **2004**, 2080-6 | 4.3 | 31 |
| 3 | Theoretical Study on the Mechanism of Reaction of Ground-State Fe Atoms with Carbon Dioxide. *Collection of Czechoslovak Chemical Communications*, **2004**, 69, 13-33 | | 11 |
| 2 | On the nature of the bonding in 1:1 adducts of O2. *Inorganic Chemistry*, **2003**, 42, 7734-6 | 5.1 | 22 |
| 1 | Ab Initio Quantum Chemical Study of the Coordination Preferences and Catalytic Role of Cu+ Ions in the Dehydration Reactions of Hydroxyformaldoxime Conformers and the Oxidation of HCN to Hydroxyformaldoxime by Hydrogen Peroxide. *Journal of Physical Chemistry A*, **2002**, 106, 1425-1440 | 2.8 | 9 |