

Zhi Sun

List of Publications by Year in descending order

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19
papers

138
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all docs

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19
times ranked

201
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|-----|-----------|
| 1 | Cyclobutyne: Minimum or Transition State?. Journal of Organic Chemistry, 2019, 84, 5548-5553. | 3.2 | 3 |
| 2 | Alkali-Metal Trihalides: $M+X_3$ Ion Pair or MX_2 Complex?. Journal of Physical Chemistry B, 2018, 122, 3339-3353. | 2.6 | 8 |
| 3 | Vibrational frequencies, structures, and energetics of the highly challenging alkali metal trifluorides MF_3 ($M = Li, Na, K, Rb,$ and Cs). Physical Chemistry Chemical Physics, 2018, 20, 18986-18994. | 2.8 | 9 |
| 4 | Prediction and Characterization of Alkaline-Earth ($M=Be, Mg, Ca, Sr,$ and Ba) Metallacyclopentadienes and Relevant Derivatives. ChemistrySelect, 2017, 2, 1442-1453. | 1.5 | 7 |
| 5 | Thioformaldehyde S -Sulfide, Sulfur Analogue of the Criegee Intermediate: Structures, Energetics, and Rovibrational Analysis. Journal of Physical Chemistry A, 2017, 121, 998-1006. | 2.5 | 6 |
| 6 | The Hydrogen Abstraction Reaction $H_2 + OH \rightarrow H_2O + SH$: Convergent Quantum Mechanical Predictions. Journal of Physical Chemistry A, 2017, 121, 9136-9145. | 2.5 | 11 |
| 7 | Communication: The $Al + CO \rightarrow AlO + CO$ reaction: Experiment vs. theory. Journal of Chemical Physics, 2017, 147, 171101. | 3.0 | 5 |
| 8 | Experimental and Theoretical Investigation of Effects of Ethanol and Acetic Acid on Carcinogenic NDMA Formation in Simulated Gastric Fluid. Journal of Physical Chemistry A, 2016, 120, 4505-4513. | 2.5 | 1 |
| 9 | Prototypical metal-oxo bonds: the reactions of $Cr(PF_3)_6$, $Fe(PF_3)_5$, and $Ni(PF_3)_4$ with oxygen. Theoretical Chemistry Accounts, 2015, 134, 1. | 1.4 | 0 |
| 10 | The reactions of $Cr(CO)_6$, $Fe(CO)_5$, and $Ni(CO)_4$ with O_2 yield viable oxo-metal carbonyls. Journal of Computational Chemistry, 2014, 35, 998-1009. | 3.3 | 6 |
| 11 | Does the metal-metal sextuple bond exist in the bimetallic sandwich compounds $Cr_2(C_6H_6)_2$, $Mo_2(C_6H_6)_2$, and $W_2(C_6H_6)_2$? Molecular Physics, 2013, 111, 2523-2535. | 1.7 | 11 |
| 12 | The Influence of Phosphate Buffer on the Formation of N-Nitrosodimethylamine from Dimethylamine Nitrosation. Journal of Chemistry, 2013, 2013, 1-9. | 1.9 | 4 |
| 13 | Reactions of Amine and Peroxynitrite: Evidence for Hydroxylation as Predominant Reaction and New Insight into the Modulation of CO_2 . Journal of Physical Chemistry A, 2012, 116, 8058-8066. | 2.5 | 1 |
| 14 | Carbon Dioxide in the Nitrosation of Amine: Catalyst or Inhibitor?. Journal of Physical Chemistry A, 2011, 115, 7753-7764. | 2.5 | 27 |
| 15 | Theoretical investigation of reactivities of amines in the N-nitrosation reactions by N_2O_3 . Journal of Molecular Modeling, 2011, 17, 669-680. | 1.8 | 9 |
| 16 | Theoretical investigation of the isomerization and dissociation reactions of all the $HOONO_2$ isomers. Computational and Theoretical Chemistry, 2010, 959, 42-48. | 1.5 | 1 |
| 17 | Theoretical Investigation of N-Nitrosodimethylamine Formation from Nitrosation of Trimethylamine. Journal of Physical Chemistry A, 2010, 114, 455-465. | 2.5 | 13 |
| 18 | Theoretical Investigation of N-Nitrosation Mechanism of Amino Acids Mediated by N_2O_3 . , 2009, , . | | 1 |

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 19 | Theoretical investigation of the isomerization of N ₂ O ₃ and the N-nitrosation of dimethylamine by asym-N ₂ O ₃ , sym-N ₂ O ₃ , and trans-cis N ₂ O ₃ isomers. Computational and Theoretical Chemistry, 2009, 908, 107-113. | 1.5 | 15 |