Manuel Temprado

List of Publications by Year
in descending order

76	1,866	304743	315739
papers	citations	22 h-index	38 g-index

78	78	78	1788
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Critically Evaluated Thermochemical Properties of Polycyclic Aromatic Hydrocarbons. Journal of Physical and Chemical Reference Data, 2008, 37, 1855-1996.	4.2	384
2	Mechanism and Scope of Phosphinidene Transfer from Dibenzo-7-phosphanorbornadiene Compounds. Journal of the American Chemical Society, 2017, 139, 10822-10831.	13.7	77
3	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16. Journal of Chemical Thermodynamics, 2005, 37, 941-953.	2.0	72
4	A Retro Dielsâ€“Alder Route to Diphosphorus Chemistry: Molecular Precursor Synthesis, Kinetics of P₂ Transfer to 1,3-Dienes, and Detection of P₂ by Molecular Beam Mass Spectrometry. Journal of the American Chemical Society, 2014, 136, 13586-13589.	13.7	64
5	The Thermochemistry of 2,4-Pentanedione Revisited:â€‰ Observance of a Nonzero Enthalpy of Mixing between Tautomers and Its Effects on Enthalpies of Formation. Journal of Physical Chemistry B, 2005, 109, 12590-12595.	2.6	60
6	Oxygen Binding to [Pd(L)(Lâ€²)] (L= NHC, Lâ€² = NHC or PR3, NHC =N-Heterocyclic Carbene). Synthesis and Structure of a Paramagnetictrans-[Pd(NHC)2(Î·1-O2)2] Complex. Journal of the American Chemical Society, 2011, 133, 1290-1293.	13.7	49
7	Structure-Energy Relationship in Barbituric Acid: A Calorimetric, Computational, and Crystallographic Study. Journal of Physical Chemistry A, 2008, 112, 7455-7465.	2.5	44
8	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives. Thermochimica Acta, 2006, 441, 20-26.	2.7	36
9	Thermochemistry of 2- and 3-Acetylthiophenes:â€‰ Calorimetric and Computational Study. Journal of Physical Chemistry A, 2007, 111, 11084-11092.	2.5	34
10	Thermodynamic and Kinetic Study of Cleavage of the Nâ€“O Bond of N-Oxides by a Vanadium(III) Complex: Enhanced Oxygen Atom Transfer Reaction Rates for Adducts of Nitrous Oxide and Mesityl Nitrile Oxide. Journal of the American Chemical Society, 2013, 135, 11357-11372.	13.7	33
11	Experimental and Computational Thermochemistry of 2- and 3-Thiophenecarboxylic Acids. Journal of Physical Chemistry A, 2002, 106, 11173-11180.	2.5	32
12	Calorimetric and Computational Study of Thiacyclohexane 1-Oxide and Thiacyclohexane 1,1-Dioxide (Thiane Sulfoxide and Thiane Sulfone). Enthalpies of Formation and the Energy of the SO Bond. Journal of Organic Chemistry, 2003, 68, 1762-1770.	3.2	28
13	Thermochemistry of 1,3-Dithiacyclohexane 1-Oxide (1,3-Dithiane Sulfoxide):Â Calorimetric and Computational Study. Journal of Organic Chemistry, 2004, 69, 5454-5459.	3.2	28
14	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,Nâ€²-trimethyleneurea. Journal of Chemical Thermodynamics, 2008, 40, 386-393.	2.0	28
15	Some thermophysical properties of several solid aldehydes. Journal of Thermal Analysis and Calorimetry, 2008, 94, 257-262.	3.6	27
16	Experimental and Theoretical Study of the Structures and Enthalpies of Formation of the Synthetic Reagents 1,3-Thiazolidine-2-thione and 1,3-Oxazolidine-2-thione. Journal of Physical Chemistry A, 2009, 113, 10772-10778.	2.5	27
17	Uptake of one and two molecules of CO₂ by the molybdate dianion: a soluble, molecular oxide model system for carbon dioxide fixation. Chemical Science, 2014, 5, 1772-1776.	7.4	27
18	Experimental and Computational Thermochemical Study of 2- and 3-Thiopheneacetic Acid Methyl Esters. Journal of Physical Chemistry A, 2007, 111, 5280-5286.	2.5	26

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19	Thermodynamic and Kinetic Studies of H Atom Transfer from HMo(CO)3(Î·5-C5H5) to Mo(N[t-Bu]Ar)3 and (PhCN)Mo(N[t-Bu]Ar)3: Direct Insertion of Benzonitrile into the Moâ˜H Bond of HMo(N[t-Bu]Ar)3 forming (Ph(H)Câ•N)Mo(N[t-Bu]Ar)3. Inorganic Chemistry, 2008, 47, 9380-9389.	4.0	25
20	Thermochemistry of Bithiophenes and Thienyl Radicals. A Calorimetric and Computational Study. Journal of Physical Chemistry A, 2009, 113, 11042-11050.	2.5	25
21	Heat capacities of thiane sulfones and thiane sulfoxide. Thermochimica Acta, 2003, 406, 9-16.	2.7	24
22	Experimental and Theoretical Study of the Structures and Enthalpies of Formation of 3H-1,3-Benzoxazole-2-thione, 3H-1,3-Benzothiazole-2-thione, and Their Tautomers. Journal of Physical Chemistry A, 2010, 114, 6336-6341.	2.5	24
23	Thermodynamic, Kinetic, and Mechanistic Study of Oxygen Atom Transfer from Mesityl Nitrile Oxide to Phosphines and to a Terminal Metal Phosphido Complex. Inorganic Chemistry, 2011, 50, 9620-9630.	4.0	23
24	Two-Step Binding of O₂ to a Vanadium(III) Trisanilide Complex To Form a Non-Vanadyl Vanadium(V) Peroxo Complex. Journal of the American Chemical Society, 2012, 134, 18249-18252.	13.7	23
25	Dinuclear Gold(I) Complexes Bearing Alkyl-Bridged Bis(N-heterocyclic carbene) Ligands as Catalysts for Carboxylative Cyclization of Propargylamine: Synthesis, Structure, and Kinetic and Mechanistic Comparison to the Mononuclear Complex [Au(IPr)Cl]. Organometallics, 2020, 39, 2907-2916.	2.3	23
26	Thermophysical, crystalline and infrared studies of the 2- and 3-thiophenecarboxylic acids. Thermochimica Acta, 2003, 404, 235-244.	2.7	22
27	The energetics of naphthalene derivatives, III: phenylacetic acid and the isomeric 1- and 2-naphthylacetic acids. Molecular Physics, 2004, 102, 1909-1917.	1.7	22
28	Enthalpy of formation of methyl benzoate: calorimetry and consequencesElectronic supplementary information (ESI) available: Physical properties at T = 298.15 K of methyl benzoate. See http://www.rsc.org/suppdata/cp/b2/b202033e/. Physical Chemistry Chemical Physics, 2002, 4, 3611-3613.	2.8	21
29	Lewis acid fragmentation of a lithium aryloxide cage: generation of new heterometallic aluminiumâ€“lithium species. Chemical Communications, 2011, 47, 11757.	4.1	21
30	Thermochemistry of Furancarboxylic Acids. Journal of Physical Chemistry A, 2003, 107, 11460-11467.	2.5	20
31	Experimental and Computational Thermochemical Study and Solid-Phase Structure of 5,5-Dimethylbarbituric Acid. Journal of Physical Chemistry A, 2010, 114, 3583-3590.	2.5	20
32	Thermochemistry of 2,5-Thiophenedicarboxylic Acid. Journal of Physical Chemistry A, 2006, 110, 12477-12483.	2.5	19
33	Calorimetric and Computational Study of 1,3- and 1,4-Oxathiane Sulfones. Journal of Organic Chemistry, 2007, 72, 1143-1147.	3.2	19
34	Structural studies of cyclic ureas: 3. Enthalpy of formation of barbital. Journal of Chemical Thermodynamics, 2009, 41, 1400-1407.	2.0	19
35	Modulating Nitric Oxide Release by S-Nitrosothiol Photocleavage: Mechanism and Substituent Effects. Journal of Physical Chemistry A, 2012, 116, 7039-7049.	2.5	19
36	Synthesis of [Pt(SnBu^t₃)(IBu^t)(Î¼-H)]₂, a Coordinatively Unsaturated Dinuclear Compound which Fragments upon Addition of Small Molecules to Form Mononuclear Ptâ€“Sn Complexes. Inorganic Chemistry, 2016, 55, 307-321.	4.0	19

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37	The energetics of the isomeric 1- and 2-naphthoic acids: context, quantum chemical calculations and thermochemical measurements. Molecular Physics, 2003, 101, 1311-1318.	1.7	18
38	Calorimetric and Computational Study of 1,3-Dithiacyclohexane 1,1-Dioxide (1,3-Dithiane Sulfone). Journal of Organic Chemistry, 2004, 69, 1670-1675.	3.2	18
39	Thermochemical properties of two benzimidazole derivatives: 2-Phenyl- and 2-benzylbenzimidazole. Journal of Chemical Thermodynamics, 2005, 37, 1168-1176.	2.0	18
40	Functionalization Reactions Characteristic of a Robust Bicyclic Diphosphane Framework. Inorganic Chemistry, 2013, 52, 8851-8864.	4.0	18
41	Substituent Effects on Enthalpies of Formation of Nitrogen Heterocycles:â€‰ 2-Substituted Benzimidazoles and Related Compounds. Journal of Physical Chemistry A, 2006, 110, 2535-2544.	2.5	17
42	Destabilization in the isomeric nitrobenzonitriles: an experimental thermochemical study. Journal of Chemical Thermodynamics, 2003, 35, 803-811.	2.0	16
43	Substituent and ring effects on enthalpies of formation: 2-methyl- and 2-ethylbenzimidazoles versus benzene- and imidazole-derivatives. Molecular Physics, 2004, 102, 711-721.	1.7	16
44	2- and 3-furancarboxylic acids: a comparative study using calorimetry, IR spectroscopy and X-ray crystallography. Thermochimica Acta, 2004, 420, 59-66.	2.7	16
45	Application of correlation-gas chromatography to evaluate the vaporization enthalpy of a component in an equilibrium mixture. Thermochimica Acta, 2005, 435, 49-56.	2.7	15
46	Heat capacities and enthalpies of transitions of three nitrobenzonitriles. Thermochimica Acta, 2002, 394, 25-29.	2.7	14
47	Calorimetric and Computational Study of 3-Buten-1-ol and 3-Butyn-1-ol. Estimation of the Enthalpies of Formation of 1-Alkenols and 1-Alkynols. Journal of Physical Chemistry A, 2005, 109, 7832-7838.	2.5	13
48	Calorimetric and Computational Study of 1,4-Dithiacyclohexane 1,1-Dioxide (1,4-Dithiane Sulfone). Journal of Organic Chemistry, 2006, 71, 2581-2586.	3.2	13
49	Thermophysical properties in medium temperature range of several thio and dithiocarbamates. Journal of Thermal Analysis and Calorimetry, 2008, 91, 471-475.	3.6	13
50	Experimental and Computational Studies of Binding of Dinitrogen, Nitriles, Azides, Diazoalkanes, Pyridine, and Pyrazines to M(PR3)2(CO)3 (M = Mo, W; R = Me, iPr).. Inorganic Chemistry, 2009, 48, 7891-7904.	4.0	13
51	Structural Substituent Effect in the Excitation Energy of a Chromophore: Quantitative Determination and Application to S-Nitrosothiols. Journal of Chemical Theory and Computation, 2012, 8, 3293-3302.	5.3	13
52	Experimental thermochemical study of two 2-alkylbenzimidazole isomers (alkyl=propyl and isopropyl). Journal of Chemical Thermodynamics, 2004, 36, 533-539.	2.0	12
53	Experimental and Computational Thermochemical Study of Barbituric Acids: Structureâ^'Energy Relationship in 1,3-Dimethylbarbituric Acid. Journal of Physical Chemistry A, 2011, 115, 3167-3173.	2.5	12
54	Thermophysical Study of Several Barbituric Acid Derivatives by Differential Scanning Calorimetry (DSC). Journal of Chemical & Engineering Data, 2011, 56, 263-268.	1.9	12

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55	Coordination-Mode Control of Bound Nitrile Radical Complex Reactivity: Intercepting End-on Nitrileâ^'Mo(III) Radicals at Low Temperature. Journal of the American Chemical Society, 2009, 131, 15412-15423.	13.7	11
56	Synthesis, structure, and thermochemistry of adduct formation between N-heterocyclic carbenes and isocyanates or mesitylnitrile oxide. Structural Chemistry, 2013, 24, 2059-2068.	2.0	11
57	Role of Axial Base Coordination in Isonitrile Binding and Chalcogen Atom Transfer to Vanadium(III) Complexes. Inorganic Chemistry, 2014, 53, 11185-11196.	4.0	11
58	Synthesis of novel chiral heterometallic terpene oximates: unusual generation of an aluminium enolate by a cooperative effect. Dalton Transactions, 2016, 45, 10514-10518.	3.3	10
59	Thermochemistry of 2- and 3-Thiopheneacetic Acids: Calorimetric and Computational Study. Journal of Physical Chemistry A, 2008, 112, 10378-10385.	2.5	9
60	The Puzzling Monopentamethylcyclopentadienyltitanium(III) Dichloride Reagent: Structure and Properties. Inorganic Chemistry, 2019, 58, 5314-5324.	4.0	9
61	Knowledge of a Molecule: An Experimental and Theoretical Study of the Structure and Enthalpy of Formation of Tetrahydro-2H-1,3-oxazine-2-thione. Journal of Chemical & Engineering Data, 2011, 56, 4725-4732.	1.9	8
62	Synthesis and DFT, Multinuclear Magnetic Resonance, and X-ray Structural Studies of Iminoacyl Imido Hydridotris(3,5-dimethylpyrazolyl)borate Niobium and Tantalum(V) Complexes. Organometallics, 2014, 33, 2277-2286.	2.3	8
63	Experimental and computational thermochemical study of 3-hydroxypropanenitrile. Journal of Chemical Thermodynamics, 2007, 39, 1377-1383.	2.0	7
64	Thermochemistry of methoxythiophenes: Measurement of their enthalpies of vaporization and estimation of their enthalpies of formation in the condensed phase. Journal of Chemical Thermodynamics, 2014, 73, 97-100.	2.0	7
65	Reactivity of Tuck-over Titanium Oxo Complexes with Isocyanides. Organometallics, 2018, 37, 2046-2053.	2.3	7
66	Substituent Effects on the Thermochemistry of Thiophenes. A Theoretical (G3(MP2)//B3LYP and G3) Study. Journal of Physical Chemistry A, 2012, 116, 4363-4370.	2.5	6
67	Revisiting the synthesis of trans-[Pt(dmso)2ClMe] and cis-[Pt(dmso)2Me2]: Experimental and DFT studies. Journal of Organometallic Chemistry, 2019, 896, 108-112.	1.8	5
68	Molecular Design of Cyclopentadienyl Tantalum Sulfide Complexes. Inorganic Chemistry, 2019, 58, 5593-5602.	4.0	5
69	Thermodynamic, Kinetic, Structural, and Computational Studies of the Ph₃Snâ€“H, Ph₃Snâ€“SnPh₃, and Ph₃Snâ€“Cr(CO)₃C₅Me₅ Bond Dissociation Enthalpies. Inorganic Chemistry, 2016, 55, 10751-10766.	4.0	4
70	Reactions of Sn(Si(Bu)2Me)3 with HM(CO)3C5R5 (M = Cr or Mo, R = H or CH3) and Hg. Ionic, covalent, and Î¼-CO bonding patterns between transition metals and tin. Inorganica Chimica Acta, 2018, 469, 550-560.	2.4	4
71	Thermochemical study of arene carboxylic acids. Arkivoc, 2005, 2005, 364-374.	0.5	4
72	Ligand-Directed Reactivity in Dioxygen and Water Binding to cis-[Pd(NHC)2(Î·2-O2)]. Journal of the American Chemical Society, 2018, 140, 264-276.	13.7	2

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73	N-heterocyclic carbene complexes of palladium in oxygen atom transfer reactions involving the making and breaking of N-O bonds. Inorganica Chimica Acta, 2017, 468, 285-293.	2.4	1
74	The mechanism of carboxylative cyclization of propargylamine by N-heterocyclic carbene complexes of Au(I). Journal of Organometallic Chemistry, 2021, 934, 121583.	1.8	1
75	Structural Diversity in the Reactions of Dimetallic Alkyl Titanium Oxides with Isonitriles and Nitriles. Organometallics, 2021, 40, 2610-2623.	2.3	0
76	Mechanistic Pathways for N2O Elimination from trans-R3Sn-O-Nâ•N-O-SnR3 and for Reversible Binding of CO2 to R3Sn-O-SnR3 (R = Ph, Cy). Inorganic Chemistry, 2021, 60, 12075-12084.	4.0	0