

Bella L Grigorenko

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123 papers	2,552 citations	29 h-index	46 g-index
128 ext. papers	2,733 ext. citations	4.5 avg, IF	5.03 L-index

#	Paper	IF	Citations
123	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. <i>Chemical Reviews</i> , 2017 , 117, 758-788	38.1	154
122	Quantum chemistry behind bioimaging: insights from ab initio studies of fluorescent proteins and their chromophores. <i>Accounts of Chemical Research</i> , 2012 , 45, 265-75	24.3	114
121	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore. 1. Electronically Excited and Ionized States of the Anionic Chromophore in the Gas Phase. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1895-906	6.4	104
120	Molecular models predict light-induced glutamine tautomerization in BLUF photoreceptors. <i>Biophysical Journal</i> , 2008 , 94, 3872-9	2.9	103
119	Potential Energy Landscape of the Electronic States of the GFP Chromophore in Different Protonation Forms: Electronic Transition Energies and Conical Intersections. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2377-87	6.4	95
118	Intermolecular complexes of HXeOH with water: stabilization and destabilization effects. <i>Journal of the American Chemical Society</i> , 2002 , 124, 10706-11	16.4	86
117	QM/MM modeling the Ras-GAP catalyzed hydrolysis of guanosine triphosphate. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 60, 495-503	4.2	84
116	Effect of protein environment on electronically excited and ionized states of the green fluorescent protein chromophore. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 8296-303	3.4	82
115	Mechanisms of guanosine triphosphate hydrolysis by Ras and Ras-GAP proteins as rationalized by ab initio QM/MM simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 66, 456-66	4.2	76
114	Mechanism of the myosin catalyzed hydrolysis of ATP as rationalized by molecular modeling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 7057-61	11.5	64
113	Flexible effective fragment QM/MM method: validation through the challenging tests. <i>Journal of Computational Chemistry</i> , 2003 , 24, 1410-20	3.5	61
112	Modeling of Biomolecular Systems with the Quantum Mechanical and Molecular Mechanical Method Based on the Effective Fragment Potential Technique: Proposal of Flexible Fragments. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 10663-10672	2.8	60
111	Mechanism of triphosphate hydrolysis in aqueous solution: QM/MM simulations in water clusters. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 4407-12	3.4	56
110	First-principles characterization of the energy landscape and optical spectra of green fluorescent protein along the A-H proton transfer route. <i>Journal of the American Chemical Society</i> , 2013 , 135, 11541-9	16.4	55
109	Many-body potentials and dynamics based on diatomics-in-molecules: Vibrational frequency shifts in ArnHF (n=1-2,62) clusters. <i>Journal of Chemical Physics</i> , 1996 , 104, 5510-5516	3.9	55
108	Optimization of Cholinesterase-Based Catalytic Bioscavengers Against Organophosphorus Agents. <i>Frontiers in Pharmacology</i> , 2018 , 9, 211	5.6	52
107	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore: 2. Cis-Trans Isomerization in Water. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1907-14	6.4	42

106	Quantum chemical modeling of the GTP hydrolysis by the RAS-GAP protein complex. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2004 , 1700, 125-36	4	40
105	Hydrolysis of Guanosine Triphosphate (GTP) by the Ras-GAP Protein Complex: Reaction Mechanism and Kinetic Scheme. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 12838-45	3.4	37
104	A QM/MM approach with effective fragment potentials applied to the dipeptide-water structures. <i>Computational and Theoretical Chemistry</i> , 2002 , 581, 167-175		37
103	Quantum Chemistry Calculations Provide Support to the Mechanism of the Light-Induced Structural Changes in the Flavin-Binding Photoreceptor Proteins. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2293-302	6.4	36
102	Modeling of serine protease prototype reactions with the flexible effective fragment potential quantum mechanical/molecular mechanical method. <i>Theoretical Chemistry Accounts</i> , 2004 , 111, 36-48	1.9	36
101	On the Origin of Potential Barrier for the Reaction OH ⁻ + CO ₂ ⇌ HCO ₃ ⁻ in Water: Studies by Using Continuum and Cluster Solvation Methods. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 1734-1740	3.4	32
100	Modeling the role of G12V and G13V Ras mutations in the Ras-GAP-catalyzed hydrolysis reaction of guanosine triphosphate. <i>Biochemistry</i> , 2014 , 53, 7093-9	3.2	31
99	Molecular Modeling Clarifies the Mechanism of Chromophore Maturation in the Green Fluorescent Protein. <i>Journal of the American Chemical Society</i> , 2017 , 139, 10239-10249	16.4	31
98	Computer-designed active human butyrylcholinesterase double mutant with a new catalytic triad. <i>Chemico-Biological Interactions</i> , 2019 , 306, 138-146	5	30
97	Conformation-dependent chemical reaction of formic acid with an oxygen atom. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 8143-6	2.8	30
96	Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of He?Cl ₂ and Ar?Cl ₂ . <i>Chemical Physics</i> , 1997 , 219, 161-172	2.3	30
95	Ground-state structures and vertical excitations for the kindling fluorescent protein asFP595. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 18635-40	3.4	29
94	Hydrogen bonding described through diatomics-in-ionic-systems: The HF dimer. <i>Journal of Chemical Physics</i> , 1998 , 108, 4413-4425	3.9	29
93	Quantum chemical modelling in the research of molecular mechanisms of enzymatic catalysis. <i>Russian Chemical Reviews</i> , 2012 , 81, 1011-1025	6.8	26
92	Computational Challenges in Modeling of Representative Bioimaging Proteins: GFP-Like Proteins, Flavoproteins, and Phytochromes. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 6133-6149	3.4	25
91	Triple-Decker Motif for Red-Shifted Fluorescent Protein Mutants. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 1743-7	6.4	25
90	Minimum energy reaction profiles for ATP hydrolysis in myosin. <i>Journal of Molecular Graphics and Modelling</i> , 2011 , 31, 1-4	2.8	24
89	A Light-Induced Reaction with Oxygen Leads to Chromophore Decomposition and Irreversible Photobleaching in GFP-Type Proteins. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 5444-52	3.4	23

88	Computational characterization of reaction intermediates in the photocycle of the sensory domain of the AppA blue light photoreceptor. <i>Photochemistry and Photobiology</i> , 2011 , 87, 564-73	3.6	23
87	Toward Molecular-Level Characterization of Photoinduced Decarboxylation of the Green Fluorescent Protein: Accessibility of the Charge-Transfer States. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1912-20	6.4	22
86	ArHF vibrational predissociation dynamics using the diatomics-in-molecule potential energy surface. <i>Journal of Chemical Physics</i> , 1999 , 111, 2470-2477	3.9	22
85	trans and cis Chromophore structures in the kindling fluorescent protein asFP595. <i>Chemical Physics Letters</i> , 2006 , 424, 184-188	2.5	21
84	On photoabsorption of the neutral form of the green fluorescent protein chromophore. <i>Biophysical Chemistry</i> , 2009 , 145, 1-6	3.5	20
83	Quantum Chemical Simulations of the Proton Transfer in Water Wires Attached to Molecular Walls. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 2958-2965	3.4	20
82	Modeling the Complete Catalytic Cycle of Aspartoacylase. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 4221-31	3.4	20
81	Catalytic Cycle of Penicillin Acylase from Escherichia coli: QM/MM Modeling of Chemical Transformations in the Enzyme Active Site upon Penicillin G Hydrolysis. <i>ACS Catalysis</i> , 2014 , 4, 2521-2529	3.1	19
80	Biochemical evidence for the tyrosine involvement in cationic intermediate stabilization in mouse beta-carotene 15, 15-monooxygenase. <i>BMC Biochemistry</i> , 2009 , 10, 31	4.8	18
79	Amide-imide tautomerization in the glutamine side chain in enzymatic and photochemical reactions in proteins. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 23827-23836	3.6	17
78	Ab initio potential functions for the ionic states of OH. <i>Chemical Physics Letters</i> , 1997 , 276, 171-176	2.5	16
77	Hydrogen bonding at the diatomics-in-molecules level: Water clusters. <i>Journal of Chemical Physics</i> , 2000 , 113, 2638-2647	3.9	16
76	Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1. <i>Journal of Molecular Modeling</i> , 2011 , 17, 1579-86	2	15
75	Photochemical synthesis of H ₂ O ₂ from the H ₂ O...O(3P) van der Waals complex: experimental observations in solid krypton and theoretical modeling. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 11444-49	2.8	15
74	Modeling dioxygen binding to the non-heme iron-containing enzymes. <i>International Journal of Quantum Chemistry</i> , 2006 , 106, 2184-2190	2.1	15
73	On quantum mechanical--molecular mechanical (QM/MM) approaches to model hydrolysis of acetylcholine by acetylcholinesterase. <i>Chemico-Biological Interactions</i> , 2013 , 203, 51-6	5	14
72	Diatomics-in-ionic-systems and ab initio predictions for the stationary points on potential energy surfaces of the (HF) _n clusters (n=3-8). <i>Journal of Chemical Physics</i> , 1999 , 111, 4442-4452	3.9	13
71	Ab initio potential curves of the fragments and diatomics-in-molecules potential energy surfaces for the SH ₂ Kr complex. <i>Chemical Physics Letters</i> , 1999 , 301, 287-296	2.5	13

70	Theoretical vibrational spectrum of (HF) ₂ in argon matrices. <i>Chemical Physics Letters</i> , 1996 , 250, 226-231	2.5	13
69	Unusual emitting states of the kindling fluorescent protein: appearance of the cationic chromophore in the GFP family. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 7228-34	3.4	12
68	Conformation dependence of pK _a of the chromophores from the purple asFP595 and yellow zFP538 fluorescent proteins. <i>Computational and Theoretical Chemistry</i> , 2008 , 863, 39-43		12
67	Properties of the NBr molecule in argon clusters. <i>Chemical Physics Letters</i> , 1995 , 233, 627-631	2.5	12
66	Modeling structure and excitation of biliverdin-binding domains in infrared fluorescent proteins. <i>Chemical Physics Letters</i> , 2018 , 710, 59-63	2.5	12
65	Modeling reactivation of the phosphorylated human butyrylcholinesterase by QM(DFTB)/MM calculations. <i>Journal of Theoretical and Computational Chemistry</i> , 2015 , 14, 1550051	1.8	11
64	Conformational partitioning in pH-induced fluorescence of the kindling fluorescent protein (KFP). <i>Journal of Physical Chemistry B</i> , 2011 , 115, 9195-201	3.4	11
63	Modelling trapping sites of (HF) ₂ in argon clusters. <i>Chemical Physics Letters</i> , 1997 , 270, 103-107	2.5	11
62	Diversity of mechanisms in Ras-GAP catalysis of guanosine triphosphate hydrolysis revealed by molecular modeling. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 4879-4891	3.9	10
61	Structures of the Peptide-Water Complexes Studied by the Hybrid Quantum Mechanical-Molecular Mechanical (QM/MM) Technique. <i>Structural Chemistry</i> , 2004 , 15, 3-9	1.8	10
60	Computational study of a transition state analog of phosphoryl transfer in the Ras-RasGAP complex: AlF ₃ (x) versus MgF ₃ ⁻ . <i>Journal of Molecular Modeling</i> , 2005 , 11, 503-8	2	10
59	Excited-state site effects in luminescence spectroscopy of SH radicals in krypton matrices: Experiment and simulations. <i>Journal of Chemical Physics</i> , 1999 , 110, 5836-5843	3.9	10
58	Why does mutation of Gln61 in Ras by the nitro analog NGLn maintain activity of Ras-GAP in hydrolysis of guanosine triphosphate?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015 , 83, 2091-9	4.2	9
57	MDDIM simulations of the 3σ _g (ion-pair)-σ _u ⁺ (valence) red-shifted transitions of Cl ₂ in neon matrices. <i>Chemical Physics Letters</i> , 1998 , 296, 84-92	2.5	9
56	Molecular Modeling the Reaction Mechanism of Serine-Carboxyl Peptidases. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 1168-75	6.4	9
55	QM/MM modeling of the glutathione-γ-hydroxymethyl radical reaction in water. <i>Physical Chemistry Chemical Physics</i> , 2004 , 6, 1031-1038	3.6	9
54	Thermal isomerization of the chromoprotein asFP595 and its kindling mutant A143G: QM/MM molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 13507-14	3.4	7
53	Towards quantum-based modeling of enzymatic reaction pathways: Application to the acetylcholinesterase catalysis. <i>Chemical Physics Letters</i> , 2013 , 556, 251-255	2.5	7

52	Minimum energy reaction profiles for the hydrolysis reaction of the cyclic guanosine monophosphate in water: Comparison of the results of two QM/MM approaches. <i>Computational and Theoretical Chemistry</i> , 2012 , 983, 88-94	2	7
51	A new hybrid approach for modeling reactions in molecular clusters: Application for the hydrogen bonded systems. <i>Journal of Chemical Physics</i> , 2000 , 112, 513-521	3.9	7
50	Mechanisms of ATP to cAMP Conversion Catalyzed by the Mammalian Adenylyl Cyclase: A Role of Magnesium Coordination Shells and Proton Wires. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 451-460	3.4	7
49	Theoretical vibrational spectroscopy of intermediates and the reaction mechanism of the guanosine triphosphate hydrolysis by the protein complex Ras-GAP. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 166, 68-72	4.4	6
48	Modeling of the glycine tripeptide cyclization in the Ser65Gly/Tyr66Gly mutant of green fluorescent protein. <i>Mendeleev Communications</i> , 2019 , 29, 187-189	1.9	6
47	Improving the Design of the Triple-Decker Motif in Red Fluorescent Proteins. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 10602-10609	3.4	6
46	Opening the Arg-Glu salt bridge in myosin: computational study. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 4804-7	3.6	6
45	Modeling properties of the HF dimer in argon clusters. <i>International Journal of Quantum Chemistry</i> , 1997 , 62, 55-65	2.1	6
44	Towards quantitative diatomics-in-molecules model for the water molecule. <i>Chemical Physics</i> , 1998 , 232, 321-328	2.3	6
43	Computational Modeling Reveals the Mechanism of Fluorescent State Recovery in the Reversibly Photoswitchable Protein Dreiklang. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 8901-8909	3.4	5
42	All-atom structures and calcium binding sites of the bacterial photosynthetic LH1-RC core complex from <i>Thermochromatium tepidum</i> . <i>Journal of Molecular Modeling</i> , 2014 , 20, 2287	2	5
41	Modeling of the mechanism of hydrolysis of succinylcholine in the active site of native and modified (Asp70Gly) human butyrylcholinesterase. <i>Russian Chemical Bulletin</i> , 2010 , 59, 55-60	1.7	5
40	An analysis of stationary points on the (HF) _n potential surfaces (n=8) predicted by the diatomics-in-ionic-systems model. <i>Computational and Theoretical Chemistry</i> , 2000 , 498, 47-60		5
39	Effect of argon atoms on charge distributions in small lithium clusters. <i>Physical Review B</i> , 1994 , 50, 18666-18669		5
38	ORGANOPHOSPHORUS NEUROTOXINS 2020 ,		5
37	Stalling chromophore synthesis of the fluorescent protein Venus reveals the molecular basis of the final oxidation step. <i>Chemical Science</i> , 2021 , 12, 7735-7745	9.4	5
36	Interplay between Locally Excited and Charge Transfer States Governs the Photoswitching Mechanism in the Fluorescent Protein Dreiklang. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 757-770	3.4	5
35	Modeling of calcium binding in the light-harvesting complex of photosynthetic reaction center of the <i>Thermochromatium tepidum</i> bacterium. <i>Moscow University Chemistry Bulletin</i> , 2011 , 66, 80-82	0.5	4

34	Simulated ^{18}O kinetic isotope effects in enzymatic hydrolysis of guanosine triphosphate. <i>Biochemistry (Moscow)</i> , 2009 , 74, 1044-8	2.9	4
33	Theoretical characterization of the 1,3-diazaazulene molecule and its derivatives. <i>Computational and Theoretical Chemistry</i> , 2008 , 855, 40-44		4
32	Investigation of matrix-isolated species: spectroscopy and molecular modelling. <i>Russian Chemical Reviews</i> , 2007 , 76, 1085-1092	6.8	4
31	Emission of SH radicals in solid krypton: mixed quantum-classical molecular dynamics simulations. <i>Chemical Physics Letters</i> , 2001 , 338, 317-322	2.5	4
30	Analysis of proton wires in the enzyme active site suggests a mechanism of c-di-GMP hydrolysis by the EAL domain phosphodiesterases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016 , 84, 1670-1680	4.2	4
29	Molecular Modeling Reveals the Mechanism of Ran-RanGAP-Catalyzed Guanosine Triphosphate Hydrolysis without an Arginine Finger. <i>ACS Catalysis</i> , 2021 , 11, 8985-8998	13.1	3
28	Effect of solvation water shells on enzyme active sites in zinc-dependent hydrolases. <i>Structural Chemistry</i> , 2019 , 30, 481-488	1.8	3
27	Tuning Electrostatic Gating of Semiconducting Carbon Nanotubes by Controlling Protein Orientation in Biosensing Devices. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 20184-20189	16.4	3
26	Molecular model of LH1 light-harvesting complex of the photosynthetic center of Thermochromatium tepidum bacteria. <i>Moscow University Chemistry Bulletin</i> , 2013 , 68, 80-82	0.5	2
25	Optical transitions in the light-harvesting complexes of bacterial photosynthetic centers. <i>Moscow University Chemistry Bulletin</i> , 2014 , 69, 152-154	0.5	2
24	Modeling the mechanism of hydrolysis of cyclic guanosine monophosphates in aqueous solution. <i>Moscow University Chemistry Bulletin</i> , 2011 , 66, 229-231	0.5	2
23	Implementation of a molecular dynamics approach with rigid fragments to simulation of chemical reactions in biomolecular systems. <i>Moscow University Chemistry Bulletin</i> , 2007 , 62, 177-179	0.5	2
22	QM/MM Approaches Shed Light on GFP Puzzles. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2021 , 271-292	0.7	2
21	Computational characterization of the all-atom structure and the calcium binding sites of the LH1RC core complex from Thermochromatium tepidum. <i>Journal of Theoretical and Computational Chemistry</i> , 2016 , 15, 1650020	1.8	2
20	Theoretical characterization of the photochemical reaction $\text{CO}_2 + \text{O}(^3\text{P}) \rightarrow \text{CO} + \text{O}_2$ related to experiments in solid krypton. <i>Chemical Physics Letters</i> , 2020 , 746, 137303	2.5	1
19	Structure of the Brain γ -Acetylase Biosynthetic Enzyme NAT8L Revealed by Computer Modeling. <i>ACS Chemical Neuroscience</i> , 2020 , 11, 2296-2302	5.7	1
18	Modeling hydrolysis of the cyclic dimeric guanosine monophosphate by phosphodiesterases. <i>Moscow University Chemistry Bulletin</i> , 2016 , 71, 12-15	0.5	1
17	The structure of the enzyme-substrate complex of the phosphodiesterase catalytic domain with cyclic diguanosine monophosphate. <i>Moscow University Chemistry Bulletin</i> , 2014 , 69, 1-4	0.5	1

- 16 Computer modeling of components of photoreceptor systems. *Russian Chemical Bulletin*, **2014**, 63, 1703-1709 1
- 15 Quantum mechanical/molecular mechanical analysis of mechanisms of enzyme action. Human acetylcholinesterase. *Russian Chemical Bulletin*, **2011**, 60, 2196-2204 1.7 1
- 14 Algorithms of the flexible effective fragment method used for modeling of transformations in enzyme active sites. *Moscow University Chemistry Bulletin*, **2010**, 65, 355-357 0.5 1
- 13 The role of magnesium in hydrolysis of triphosphates in water: Quantum mechanical/molecular mechanical modeling. *Moscow University Chemistry Bulletin*, **2007**, 62, 123-127 0.5 1
- 12 Structure of the enzyme-substrate complex for guanosine triphosphate hydrolysis by elongation factor EF-Tu: Comparison of quantum mechanics/molecular mechanics and molecular dynamics results. *Moscow University Chemistry Bulletin*, **2008**, 63, 321-323 0.5 1
- 11 Modeling photophysical properties of the bacteriophytochrome-based fluorescent protein IFP1.4. *Journal of Chemical Physics*, **2021**, 154, 065101 3.9 1
- 10 Protonation States of Molecular Groups in the Chromophore-Binding Site Modulate Properties of the Reversibly Switchable Fluorescent Protein rsEGFP2. *Journal of Physical Chemistry Letters*, **2021**, 12, 8263-8271 6.4 1
- 9 Mechanism of Metallo- β -Lactamase Inhibition by Oxacephalosporin Antibiotic. *Moscow University Chemistry Bulletin*, **2018**, 73, 155-157 0.5 0
- 8 Tuning Electrostatic Gating of Semiconducting Carbon Nanotubes by Controlling Protein Orientation in Biosensing Devices. *Angewandte Chemie*, **2021**, 133, 20346-20351 3.6 0
- 7 Modeling the spectra of matrix-isolated molecules. *Journal of Structural Chemistry*, **1997**, 38, 207-211 0.9
- 6 Mechanisms of enzymatic hydrolysis of nucleoside triphosphates by quantum and molecular mechanics. *Russian Journal of General Chemistry*, **2008**, 78, 696-703 0.7
- 5 Study and modeling of mechanisms of cholinesterasis reactions in order to improve their catalytic properties in the neutralization reactions of organophosphorous compounds **2020**, 134-174
- 4 Study and modeling of mechanisms of cholinesterasis reactions in order to improve their catalytic properties in the neutralization reactions of organophosphorus compounds **2020**, 140-180
- 3 Human cholinesterases **2020**, 69-126
- 2 Human cholinesterases **2020**, 63-120
- 1 Modeling Structures and Spectra of Trapped Species in Low-Temperature Matrices **2011**, 447-468