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Progesterone Receptor Antagonist, Mifepristone, Inhibits Amphibian Ovulation

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In full-grown ovarian follicles of amphibians gonadotropin induces the production of a maturation-inducing steroid which is progesterone in the ovaries of *Xenopus laevis*. Progesterone binds to a cell surface receptor to initiate oocyte maturation. In addition, progesterone may also bind to a nuclear receptor to induce oocyte ovulation. In this study we hypothesized that different types of progesterone receptors might be involved in the processes of oocyte maturation and ovulation in *Xenopus laevis*. To test this hypothesis we examined the effects of a classical progesterone receptor antagonist, mifepristone, on oocyte maturation and ovulation in *Xenopus laevis* follicles. Ovarian tissue fragments were primed with human chorionic gonadotropin (hCG) for 30 minutes in a modified Barth's solution and then incubated with progesterone alone or in the presence of varying concentrations of mifepristone over a period of 36 hours. We found that mifepristone inhibited both hCG- and progesterone-induced ovulation in a dose-dependent manner, but had no effect on hCG- and progesterone-stimulated maturation. In fact, mifepristone by itself at low concentrations had a stimulatory effect on maturation. Immunocytochemistry of ovarian tissue sections using antisera against the classical progesterone receptor yielded a positive signal in the nuclei of follicle cells (granulosa and theca) as well as in the cytoplasm of oocytes. We suggest that the nuclear progesterone receptor of follicle cells might be involved in the transduction pathway for progesterone-induced ovulation. The role of the cytoplasmic oocyte progesterone receptor in either oocyte maturation or ovulation of *Xenopus laevis* is still unknown and merits further investigation.

Key words; progesterone, mifepristone, amphibian, ovulation

Effects of Donor Substitution on Vibronic Instability in Oxomolybdenum Dichalcogenolenes

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Dithiolene distortions have long been suggested to play a critical role in in electronically buffering the Mo active site of pyranopterin molybdenum enzymes against the large changes in charge that accompany Mo(IV)/Mo(V) and Mo(V)/Mo(VI) redox processes. In this work, we quantify the nature of dithiolene/diselenolene fold angle conformers via a combination of spectroscopy, bonding calculations, and the application of a vibronic coupling model. The structure of Tp*MoO(bds) (**1**) (bds = benzene-1,2- diselenolate, Tp* = hydrotris(3,5-dimethyl-1-pyrazolyl) borate) is very similar to its dithiolene analogue Tp*MoO(bdt) (**2**) (bdt = benzene-1,2-dithiolate), but possesses longer Mo-E (E = Se, S) bonds (Mo-Se: 2.61 Å; Mo-S: 2.13 Å) and a greater metal- ligand envelope fold angle (**1**: 26.2°; **2**: 21.3^{O}). Importantly, multifrequency EPR spectroscopy has revealed, for the first time, the presence of fold-angle conformers for the diselenolene ligand in **1**. The “fold up” and “fold down” conformers are populated in an approximate 80:20 ratio at room temperature. Resonance Raman spectroscopy and electronic structure calculations also provide strong evidence for the presence of these conformers in solution. We have employed a simple two-state vibronic coupling model to understand the electronic origin of the extremely soft ground state double potential well. These new results will be discussed in terms of the potential for fold angle conformers to modulate electron and atom transfer reactivity in pyranopterin molybdenum enzymes.

Key words: Molybdenum, Magnetic Circular Dichroism, Diselenolene, Electronic Structure.

Pathways to Solar Nanotechnology Using Aluminum Phosphide Clusters

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We continue our interest in the clusters of semiconductor materials in this investigation of the physical and chemical properties of AlmPn cluster ($1 \leq m \leq 15$, $1 \leq n \leq 15$). Aluminum phosphide material, usually alloyed with other binary materials, has applications in devices such as light-emitting diodes, besides its use as a pesticide. The goal of this research is to reveal the trends seen in the properties of these clusters that may have implications for technological applications. We used the hybrid ab-initio methods of quantum chemistry, particularly the DFT- B3LYP model, and the Many Body Perturbation Theory (MBPT)/MP2 model, to derive the optimal geometries for the clusters of interest. We compare the calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for the various clusters. The optimized geometries that we obtained are various combinations of triangles,
squares, rectangles, pentagons and hexagons. For the very small clusters, C2v and D2v symmetries dominate. Our results reveal many abrupt changes in structure and spectroscopy, as a cluster is built up from its constituents. The values of HUMO-LUMO gap decrease as the cluster size increases. We also investigate the effects of crystal symmetries corresponding to the bulk structures. Overall, we conclude that for the clusters that we examined, MP2 can be considered a very suitable and economical model. Furthermore, DFT methods are also fairly reliable in predicting polarizability values.