|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  | | --- | |  | | |  | | --- | | **CONTROL ID:**2210996 | | **TITLE:**Calculation of the anharmonic effect of elementary reactions of high-temperature combustion reaction | | **CONTACT (NAME ONLY):**Li Yao | | **ABSTRACT STATUS:**submitted | |  | |  | | **ABSTRACT BODY:  Abstract:**Abstract Combustion plays an important role in engineering and our life. Today, about 90 percent of the energy is generated by the combustion in our world [1]. Focusing on the chemistry of combustion of fuels, it is of great significance to design the combustion chamber, control pollutants and research on alternative fuels [3-4]. The chemical kinetic mechanism of combustion of fuels is composed of a series of elementary reactions. Therefore, to better grasp the mechanism of combustion reaction, it is necessary to investigate the elementary reaction process. Being the key parameters of the chemical kinetic mechanism of the combustion reactions, the rate constant are calculated using RRKM theory, transition state theory and our own method. Most results are similar with those of accurate quantum dynamics (QD). At the same time, the RRKM theory, the intramolecular vibration theory, and the vibrational transition state theory for large molecule reaction systems, or the gas-phase reaction kinetics that are difficult to investigate by using accurate quantum dynamics and quasi classical trajectory method provide the feasibility of estimating. We investigate the anharmonic effect of the canonical and the microcanonical systems, and calculate the total number of states, the density of the states, the partition function and the rate constant. From the various calculation results, we get the following conclusions. First, the anharmonic effect is significant for the weak binding force of microscopic reaction systems. Second, the error of harmonic approximation is larger in high temperature, which is announced for the kinetic mechanism of the combustion reactions. Third, when the molecular reaction is 2000 K, the anharmonic rate constant is smaller than the harmonic rate constant ranging from 2 times to thousands times. The anharmonic effect increase with the increasing temperatures. Forth, the anharmonic effect is not only related to the intramolecular bond length and binding energy, but also with the symmetry of the molecular structure. We will focus on the developing the anharmonic model of high-temperature combustion reactions in the following days, high-temperature non-resonant correction calculation methods and apply the method and parameters to building and optimizing the kinetic mechanism of the high-temperature combustion of hydrocarbons. | | **INSTITUTIONS (ALL):**1. Department of Physics , Dalian Maritime University, Dalian, Liaoning, China. |   **SYMPOSIUM NAME:**General Papers - Oral  **CONTACT (COUNTRY ONLY):**China | |  | |  | |
|  |
|  |
|  |
| |  | | --- | | **CONTROL ID:**2209123 | | **TITLE:**Structural study of Mongolian tourmaline in the electric power saving system with infrared spectroscopy | | **CONTACT (NAME ONLY):**Ki-Seog Chang | | **ABSTRACT STATUS:**resubmitted | | **ABSTRACT BODY:  Abstract:**This Fourier Transformation Infrared (FTIR) experiment investigates the relevance of H2O and other components’ structural environments. Four element materials, tourmaline, ferrite, NaCl, and H2O, comprised the electronic power saving system. FTIR spectroscopy in the range of 3,000 to 4,000 cm-1 was used to examine the hydroxyl ions of H2O and Mongolian tourmaline. The tourmaline crystal was polar and therefore pyroelectric, electrical charges developing at the ends of the polar axis and temperature changing from the IR activation with H2O in the system. As a result, the tourmaline was shown to be related to the activation of H2O as a pyroelectric substance. | | **INSTITUTIONS (ALL):**1. Bio. & Chemical Engineering, Hongik University, Sejong, Jochiwon-eup, Korea (the Republic of). | | **SYMPOSIUM NAME:**Green Chemistry and Sustainability - Oral  **CONTACT (COUNTRY ONLY):**Korea (the Republic of) | |  | |  | |
| |  | | --- | | **CONTROL ID:**2214639 | | **TITLE:**Modified Sonogashira- and Glaser-type couplings: Reaction methodology for undergraduate research | | **CONTACT (NAME ONLY):**Matthew Mio | | **ABSTRACT STATUS:**submitted | |  | | **ABSTRACT BODY:  Abstract:**Due to their structural rigidity, conjugation and unique bond torsion, sequence-specific arylethynylene and arylbutadiyne oligomers are excellent scaffolds for the study of shape-persistent supramolecular and nanoscale systems. With the ultimate goal of improving the generation of these important architectures, new synthetic methodologies have been developed utilizing an in situ ethynylsilane deprotection reaction. While synthetic strategies for the alkynylation of aryl moieties (Sonogashira) or the homocoupling of alkynes (Glaser) traditionally involve iterative pathways, the use of an in situ ethynylsilane deprotection reaction has been shown to allow for the rapid construction, often in one pot, of complex arylethynylene and arylbutadiyne oligomers. Key to the protocol is the inclusion of a mixture of amidine base, such as 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU), CuI and substoichiometric amounts of water. The use of trimethylsilylacetylene versus bis-trimethylsilylacetylene, base toggling, inclusion of dioxygen for homocoupling, sterics of silylacetylene protection and CO insertion projects will be discussed. | | **INSTITUTIONS (ALL):**1. Chemistry and Biochemistry, University of Detroit Mercy, Berkley, MI, United States. | | **SYMPOSIUM NAME:**Organic Chemistry Research at Primarily Undergraduate Institutions - Oral  **CONTACT (COUNTRY ONLY):**United States | |
| |  | | --- | | **CONTROL ID:**2213282 | | **TITLE:**Vibrational spectroscopy of asparagine in acidic, neutral, and basic solutions | | **CONTACT (NAME ONLY):**Joong-Won Shin | | **ABSTRACT STATUS:**submitted | | **ABSTRACT BODY:  Abstract:**Fourier transform infrared spectroscopy (FTIR) utilizing attenuated total reflectance (ATR) was carried out to analyze changes in vibrational bands of asparagine (L-Asn) at 0.20 M concentration in acidic, neutral, and basic solutions in the pH range of 1 to 14. The spectra show evolution of peaks near 1730, 1680, 1260, and 1228 cm-1 at pH values below 2, suggesting protonation of the carboxylic acid on the backbone of the molecule. The appearance of peaks near 1530, 1400, and 1360 cm-1 at pH values in the 2 - 8 range implies that the amino acid adopts a zwitterionic structure. | | **INSTITUTIONS (ALL):**1. Division of Science, Governors State University, University Park, IL, United States. | | **SYMPOSIUM NAME:**General Posters – Posters  **CONTACT (COUNTRY ONLY):**United States | |
| |  | | --- | | **CONTROL ID:**2212323 | | **TITLE:**Synthesis and applications of oxaquinonacyclophane macrocycles | | **CONTACT (NAME ONLY):**Jay Wackerly | | **ABSTRACT STATUS:**submitted | |  | | **ABSTRACT BODY:  Abstract:**This presentation will feature research in our lab on the synthesis of a new class of redox active [14]oxacyclophanes that contain *p*-benzoquinones. These macrocycles can be accessed in one-pot base catalyzed reactions of 2,3-dichloronaphthoquinone and various diphenols. Modifications to the electrophile and reactions conditions were also explored to access similar structures. Subsequently, each macrocycle was investigated for its ability to act as a supramolecular host for host-guest binding. | | **INSTITUTIONS (ALL):**1. Department of Chemistry, Central College, Pella, IA, United States. | | **SYMPOSIUM NAME:**Organic Chemistry Research at Primarily Undergraduate Institutions - Oral  **CONTACT (COUNTRY ONLY):**United States | |  | |

|  |
| --- |
|  |
|  |