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intramolecular dynamics. iii. theoretical studies of the ch overtone spectra for benzene yongfeng zhang and fi. a. marcus arthur amos noyes laboratory of ...

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molecular dynamics (md) is a computer simulation method for studying the physical movements of atoms and molecules, and is thus a type of n-body simulation.

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vibrationally mediated photodissociation is emerging as a useful tool for studies of intramolecular dynamics in polyatomic molecules since it is a sensitive ind

THE STUDY OF INTRAMOLECULAR DYNAMICS BY NUCLEAR MAGNETIC ...

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study of intramolecular dynamics by nmr 1957 these two information sources, and taking into account additional constraints given by van der waals radii and bond-angle ...

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qualitative intramolecular quantum dynamics alexander v burenin on the importance of the born – oppenheimer approximation in intramolecular dynamics

INTRAMOLECULAR RELAXATION DYNAMICS IN SEMIFLEXIBLE ...

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the intramolecular relaxation dynamics of semiflexible dendrimers in dilute solutions are theoretically investigated in the framework of optimized rouse-zimm formalism.

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Mon, 15 May 2017 15:36:00 GMT

the ch overtone spectra for $\nu_{\text{ch}}=1, 2, \text{ and } 3$ for an intermediate sized molecule, benzene, and the related intramolecular vibrational dynamics are treated theoretically.

ON THE IMPORTANCE OF THE BORN – OPPENHEIMER APPROXIMATION ...

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on the importance of the born – oppenheimer approximation in intramolecular dynamics view the table of contents for this issue, or go to the journal homepage for more

STATISTICAL THEORY OF UNIMOLECULAR INTRAMOLECULAR DYNAMICS

Sat, 15 Apr 2017 08:55:00 GMT

field of intramolecular dynamics during the past sixty years. in a concluding section we consider possible implications for intramolecular laser selective chemistry.

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Sun, 12 Jul 2015 16:30:00 GMT

intramolecular dynamics. i. curvilinear normal modes, local modes, molecular anharmonic hamiltonian, and application to benzene yongfeng zhang, stephen j ...

INTRAMOLECULAR DYNAMICS : JOSHUA JORTNER : 9789027714923

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INTRAMOLECULAR DYNAMICS IN X₄ RHOMBIC CLUSTERS

Tue, 29 Nov 2016 09:28:00 GMT

abstract: two independent approaches are applied to study the intra-molecular dynamics in X_4 electronic ground state. first, a double minimum six-dimensional ...

INTRAMOLECULAR DYNAMICS OF HIGHLY EXCITED OCS (CONFERENCE ...

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the intramolecular dynamics of highly excited ocs has been studied within the framework of classical mechanics. one study involves the energy relaxation of ocs ...

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biomolecular systems such as multiprotein complexes or biopolymers can span several tens to several hundreds of nanometers, but the dynamics of such mesocale ...

DYNAMICS OF INTRAMOLECULAR CARBENIC REARRANGEMENTS

Thu, 13 Apr 2017 17:40:00 GMT

dynamics of intramolecular carbenic rearrangements 743 parallel observations can be made for the 1,2-c shifts of carbenes 12 and 13. with 13, $k(1,2-c) = 9.0 \sim 16 \text{ s}^{-1}$,

INTRAMOLECULAR DYNAMICS FROM EIGENSTATE-RESOLVED INFRARED ...

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244 lehmann, scoles & pate background theory dynamics from frequency-resolved spectra in this section we discuss some issues concerning the dynamical interpret

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Thu, 05 Jan 2017 18:53:00 GMT

role of surface intramolecular dynamics in the efficiency of energy transfer in ne atom collisions with a n-hexylthiolate self-assembled monolayer†

HETERO-SITE-SPECIFIC X-RAY PUMP-PROBE SPECTROSCOPY FOR ...

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the intramolecular flow of charge, energy and nuclear motion is widely encountered in molecular dynamics and underlies chemical reactivity and biological processes 1,2,3.

INTRAMOLECULAR DYNAMICS: REGULAR AND STOCHASTIC ...

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marcus, r. a. (1980) intramolecular dynamics: regular and stochastic vibrational states of molecules. in: horizons of quantum chemistry. d. reidel , dordrecht, pp ...

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title: intramolecular vibrational dynamics under high pressure conditions: collisions and intramolecular vibrational coherence: creators: yoo, hyun s.; pate, brooks h.

STUDIES OF INTRAMOLECULAR DYNAMICS - SAO/NASA ADS

Tue, 28 Apr 2015 03:04:00 GMT

abstract all four chapters of this dissertation, each of which has been or will be published, are concerned with intramolecular dynamics following photoexcitation.

INTRAMOLECULAR DYNAMICS WITHIN THE N-CAP-SH3-SH2 ...

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intramolecular dynamics within the n-cap-sh3-sh2 regulatory unit of the c-abl tyrosine kinase reveal targeting to the cellular membrane*

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marcus, r. a. (1988) intramolecular dynamics and unimolecular reactions. berichte der bunsengesellschaft für physikalische chemie, 92 (3). pp. 209-212.

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noid, d. w. and koszykowski, m. l. and marcus, r. a. (1981) intramolecular dynamics in the quasiperiodic and stochastic regimes. in: quantum mechanics in mathematics ...