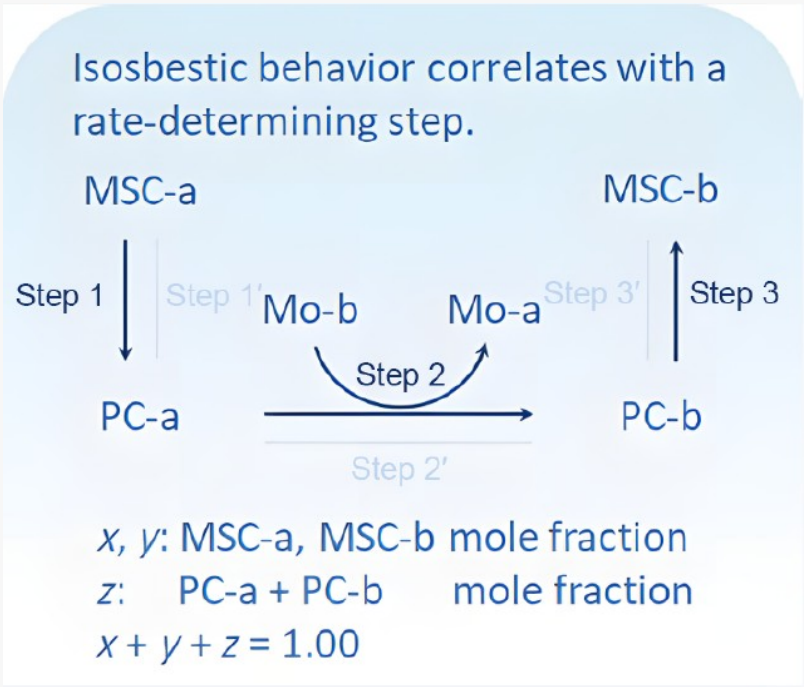
Unveiling Isosbestic Behavior in Multi-Step Transformations

CHENGDU, SICHUAN, CHINA, June 23, 2025 /EINPresswire.com/ -- Researchers challenge the traditional explanation of isosbestic behavior, using colloidal semiconductor magic-size clusters as a model system together with a multi-step pathway involving reaction intermediates



All three steps in this model can be rate-determining, which determining isosbestic behavior

Isosbestic behavior is a term that describes a specific wavelength with stable absorbance when a reaction proceeds from a reactant (R) to a product (P) and is monitored by optical absorption spectroscopy, for example. Isosbestic behavior has been viewed as a distinctive indicator that a chemical reaction happens directly without any intermediates involved. However, researchers at Sichuan University (P. R. China) challenge this traditional view. Using colloidal semiconductor magic-size clusters (MSCs) as a model system, the researchers demonstrate that relatively transparent intermediates are involved in the transformation from a reactant (MSC-a) to a product (MSC-b). The MSCs studied are small nanomaterials made of II-VI metal chalcogenide (ME) atoms with superior stability. Researchers published their results in Volume 18, Issue 6 of the journal Nano Research in June 2025.

“Isosbestic behavior has long been regarded as a spectroscopic indicator of a chemical reaction, in which a reactant transforms directly to a product without any intermediates. Room-temperature transformations of colloidal semiconductor MSCs from MSC-a (R) to MSC-b (P) can display interrupted spectral shifts in optical absorption with or without isosbestic behavior. The transformation pathway involves intermediates that are relatively transparent in optical absorption,” said Professor Kui Yu, researcher at Sichuan University and author of the study. “Isosbestic behavior is associated with a rate-determining step. This idea is noteworthy.”

The intermediates involve the precursor compounds of MSC-a and MSC-b, PC-a and PC-b, respectively. For the first time, researchers identified how a rate-determining step in a three-step pathway affects isosbestic behaviors. The first step is isomerization from MSC-a to PC-a (a configuration change with the composition maintained); when this step is rate-determining, isosbestic behavior has no distortion and the “perfect” point is called an isosbestic point. The second step is the PC-a to PC-b transformation; when this step is rate-determining, isosbestic behavior can be distorted. The third step is isomerization from PC-b to MSC-b; when this step is rate-determining, isosbestic behavior is absent.

The three-step model has been used throughout the study with consistent results to explain the isosbestic behavior observed during the MSC-a and MSC-b transformation. “Our findings provide a deeper understanding of isosbestic behavior (associated with a rate-determining step in a multi-component model with relatively transparent intermediates), and bring comprehensive insight into MSC-a to MSC-b transformations at room temperature that are assisted by intermediates (PC-a and PC-b) and monomer substitution,” said Prof. Yu.

In addition to spectral measurements, the researchers performed theoretical modeling to simulate the absorption profiles across the transformation process. These simulations confirmed that subtle changes in the relative population of intermediates could explain whether an isosbestic point remains sharp, becomes distorted, or disappears entirely. The experimental data aligned well with these predictions, reinforcing the validity of the multi-step pathway.

This refined perspective may also prove useful for interpreting spectral data in other systems—particularly in nanochemistry and materials science—where intermediate species may escape detection due to low optical activity. By associating isosbestic features with underlying kinetic steps, researchers may better map reaction dynamics even when direct observation of all components is challenging.

The traditional and standard explanation of isosbestic behavior, that a reactant (R) transforms into a product (P) directly without intermediates, has been widely accepted as a self-evident truth. However, indirect transformations via a multi-step process can be more energetically favored than direct transformations. The research team hopes their three-step pathway model involving intermediates will advance the fundamental understanding of the transformation of various matter with or without isosbestic behavior.

“Our study shines light into the probable pathway that involves intermediates that are relatively transparent, when molecules and metal clusters transform (displaying spectral shifts that are in a distinctly discontinuous pattern with and without isosbestic behavior),” said Prof. Yu.

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Reference

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About the Sichuan University
Sichuan University is one of the nation's most prestigious and historic research universities and is formally governed by China's Ministry of Education, originating in 1896 and located in Chengdu, Sichuan. Sichuan University regularly ranks within China's top 15 comprehensive universities, being a key player of the "Double First-Class" initiative with 12 major academic disciplines.

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About Professor Kui Yu from Sichuan University
Prof. Kui Yu is a leading expert in nanochemistry at Sichuan University, specializing in the fundamental understanding of the formation and transformation pathway of colloidal semiconductor magic-size clusters (MSCs) and quantum dots (QDs) for more than 15 years. She presumes the appearance of prenucleation clusters (PNCs) via chemical self-assembly, providing a different view on the nucleation and growth of QDs and on the MSC formation and transformation. She earned her Ph.D. in Chemistry from McGill University (Canada), and conducted research at Sandia National Laboratories (USA) and the National Research Council Canada before she joined Sichuan University.

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