## "WALKING IN THE WOODS WITH QUANTUM CHEMISTRY - THE IMPORTANCE OF INHERENT CARBOCATION REACTIVITY IN TERPENE BIOSYNTHESIS"



Abstract: The results of quantum chemical calculations on the mechanisms of terpene-forming carbocation rearrangements will be described. Unusual phenomena, not usually associated with biological reactions, will be highlighted, e.g., concerted but highly asynchronous reaction steps in which multiple bond forming/breaking events are merged, pathways with post-transition state bifurcations, non-statistical dynamic effects.

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UNIVERSITY OF ROCHESTER
DEPARTMENT OF CHEMISTRY

