

Quantum Mechanical Analysis of Bath Salt Designer Drug

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Designer drugs known by the street name “Bath Salts” have become a problem in the United States recently. According to the American Association of Poison Control Centers, in 2010 they received 304 calls referring to Bath Salt abuse. In 2011, the number of calls increased to 6,134. Bath Salts are a drug of abuse for many, but it is typically the teen age group that has been the most affected. Bath Salts are not FDA approval. There are two active ingredients in Bath Salts, Mephedrone, which can act like amphetamine and release Dopamine into the brain, and methylenedioxypyrovalerone or MDPV, which acts like cocaine by preventing dopamine from being reabsorbed into the brain’s neurons. Recently MDPV has been studied in the laboratory, where researchers have found that it is more potent than cocaine. Cocaine and MDPV have similar mechanisms of action and block dopamine transporters, preventing dopamine from being reabsorbed and leading to a high amount of dopamine in the nervous system. MDPV has a higher affinity for neurotransmitters than cocaine, and its effects could essentially be irreversible.

In this quantum mechanical research project, the molecular characteristics of MDPV and one of its 8 analogs were calculated. Some of these characteristics include: volume, dipole moment, molecular electrostatic map, HOMO-LUMO gap, and polarizability. All this was done to have a better understanding of how the MDPV molecules interact in the nervous system.

