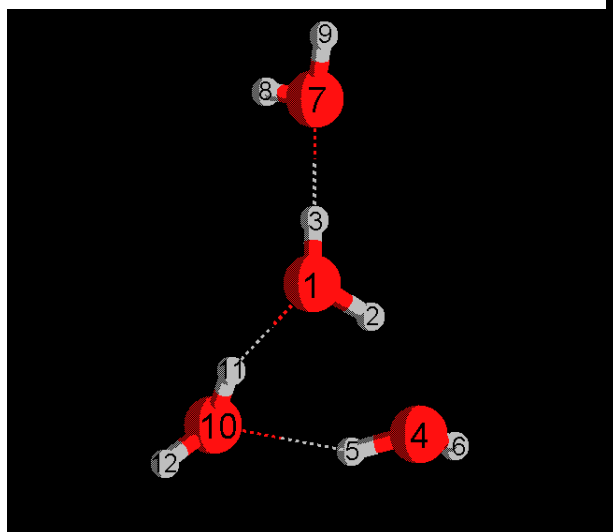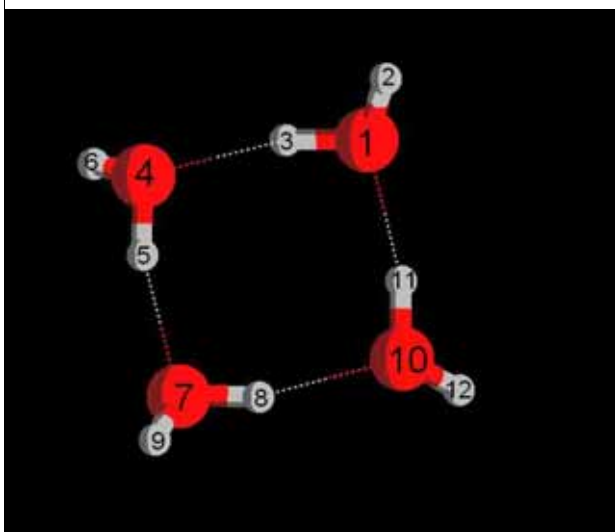Supplementary Data

The definition of the internal coordinate defined by $ZMAT in HONDO or GAMESS format.

"cyclic" tetramer internal-coordinate

$ZMAT   NZMOD=21,
    IZMAT=
    1, 1,2,
    1, 1,3,
    2, 2,1,3,
    1, 4,5,
    1, 5,6,
    2, 4,5,6,
    1, 7,8,
    1, 7,9,
    2, 8,7,9,
    1, 4,2,
    2, 2,4,5,
    2, 2,4,6,
    1, 7,5,
    2, 5,7,8,
    2, 5,7,9,
    3, 4,2,1,3,
    3, 4,5,1,3,
    3, 4,6,1,3,
    3, 7,5,4,6,
    3, 7,8,4,6,
    3, 7,9,4,6,
    $END

"branched"   internal-coordinate

$ZMAT   NZMOD=21,
    IZMAT =
    1, 1,2,
    1, 1,3,
    2, 2,1,3,
    1, 4,5,
    1, 5,6,
    2, 4,5,6,
    1, 7,8,
    1, 7,9,
    2, 8,7,9,
    1, 4,2,
    2, 2,4,5,
    2, 2,4,6,
    1, 7,3,
    2, 3,7,8,
    2, 3,7,9,
    3, 4,2,1,3,
    3, 4,5,1,3,
    3, 4,6,1,3,
    3, 7,3,1,2,
    3, 7,8,1,2,
    3, 7,9,1,2
    $END