

Supporting information for:
Analytic ab initio calculations of Coherent anti-Stokes Raman
Scattering (CARS)

Andreas J. Thorvaldsen, Lara Ferrighi, Kenneth Ruud,
Hans Ågren, Sonia Coriani and Poul Jørgensen

I. PERYLENE

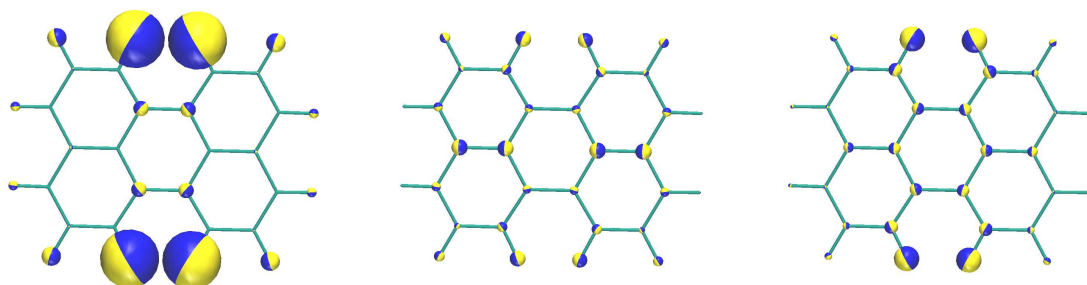


FIG. 1: Vibrational modes for perylene at the computed frequencies of: 1276, 1366 and 1564 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

II. PYRENE

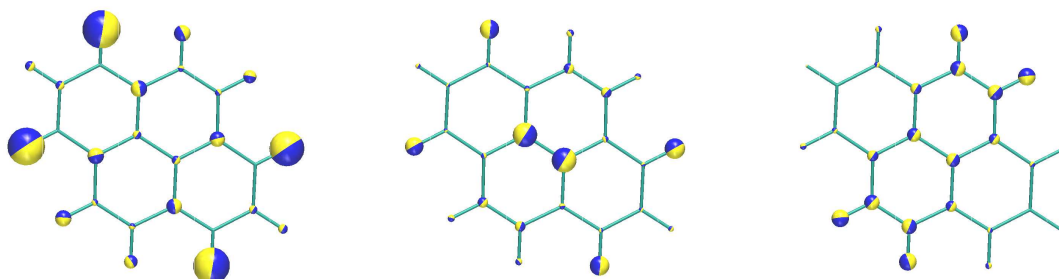


FIG. 2: Vibrational modes for pyrene at the computed frequencies of: 1228, 1395 and 1629 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

III. BENZO(A)PYRENE

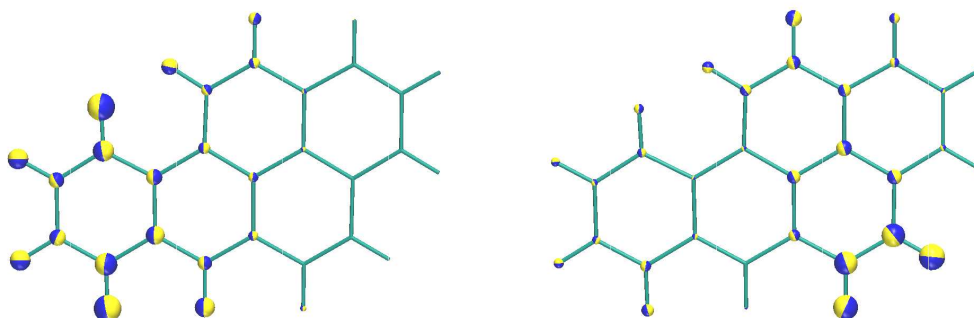


FIG. 3: Vibrational modes for benzo(a)pyrene at the computed frequencies of: 1613 and 1628 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

IV. BENZO(E)PYRENE

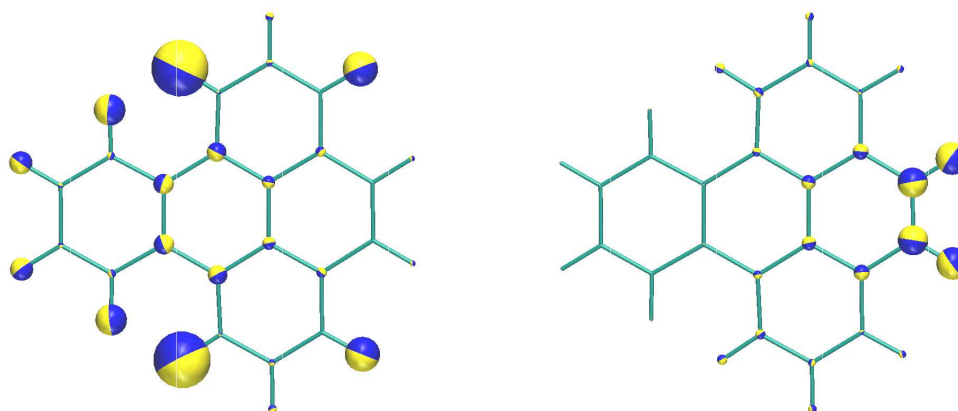


FIG. 4: Vibrational modes for benzo(e)pyrene at the computed frequencies of: 1242 and 1624 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

V. BENZO(GHI)PERYLENE

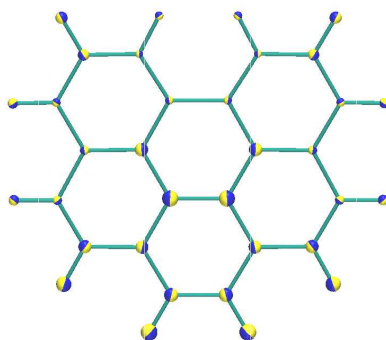


FIG. 5: Vibrational mode for benzo(ghi)perylene at the computed frequency of 1598 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

VI. CHRYSENE

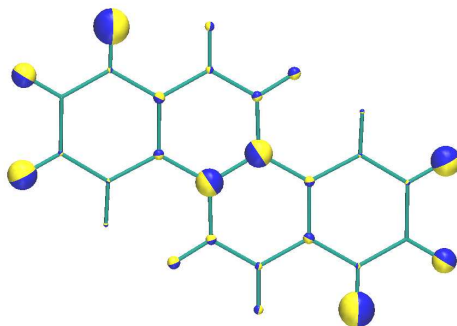


FIG. 6: Vibrational mode for chrysene at the computed frequency of 1363 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

VII. CORONENE

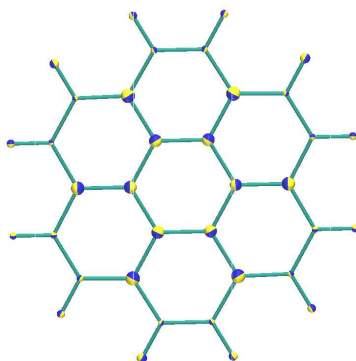


FIG. 7: Vibrational mode for coronene at the computed frequency of 1347 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

VIII. ANTHRACENE

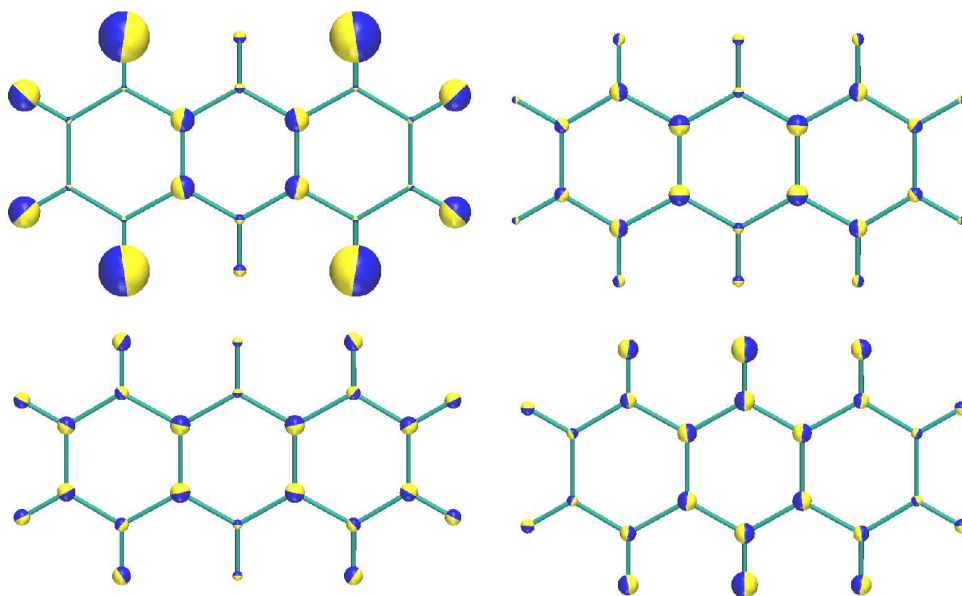


FIG. 8: Vibrational modes for anthracene at the computed frequencies of: 1253 and 1400 cm^{-1} in the top row, 1554 and 1627 cm^{-1} in the bottom row. The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

IX. TETRACENE

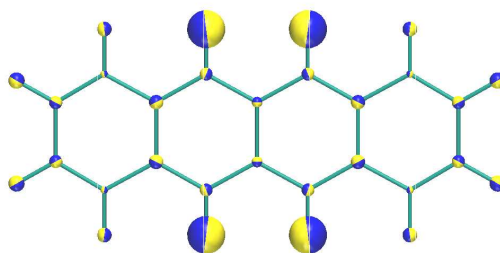


FIG. 9: Vibrational mode for tetracene at the computed frequency of 1387 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.

X. 1,2-BENZANTHRACENE

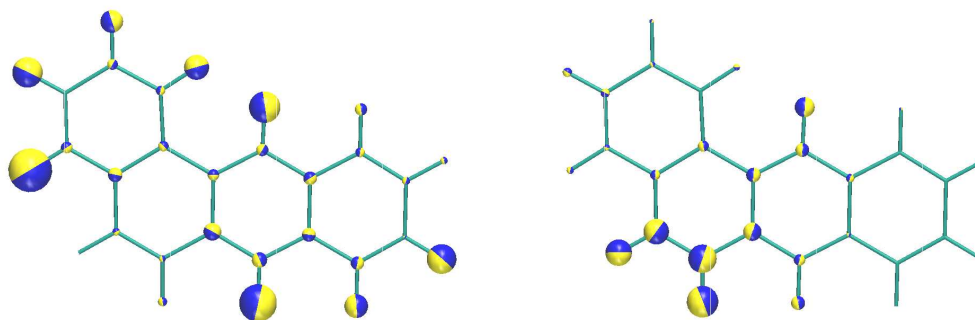


FIG. 10: Vibrational modes for 1,2-benzanthracene at the computed frequencies of 1411 and 1620 cm^{-1} . The sizes of the spheres define the magnitude of the vibrational amplitude and the different colours the positive and negative directions of the motion.