Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Hydrogen Storage on Volleyballene

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Table S1. Calculated tilt angles among pentagonal rings and triangular faces of the hydrogenated volleyballene.

Figure S1. Comparison between ORCA and G03 calculations of IR/Raman spectra of volleyballene.

Figure S2. Comparison of IR/Raman spectra of volleyballene and hydrogenated volleyballene.

Table S1. Calculated tilt angles between pentagonal rings and triangular faces of icosahedron like Sc_{12} cluster.

Indexes	angle (degrees)
1	22.35
2	25.27
3	27.22
4	33.35
5	35.85
6	40.33
7	41.97
8	42.21
9	43.95
10	45.28
11	48.14
12	57.37

Note: The obtained difference among tilt angles is a consequence of the C_1 symmetry displayed by the hydrogenated volleyballene.

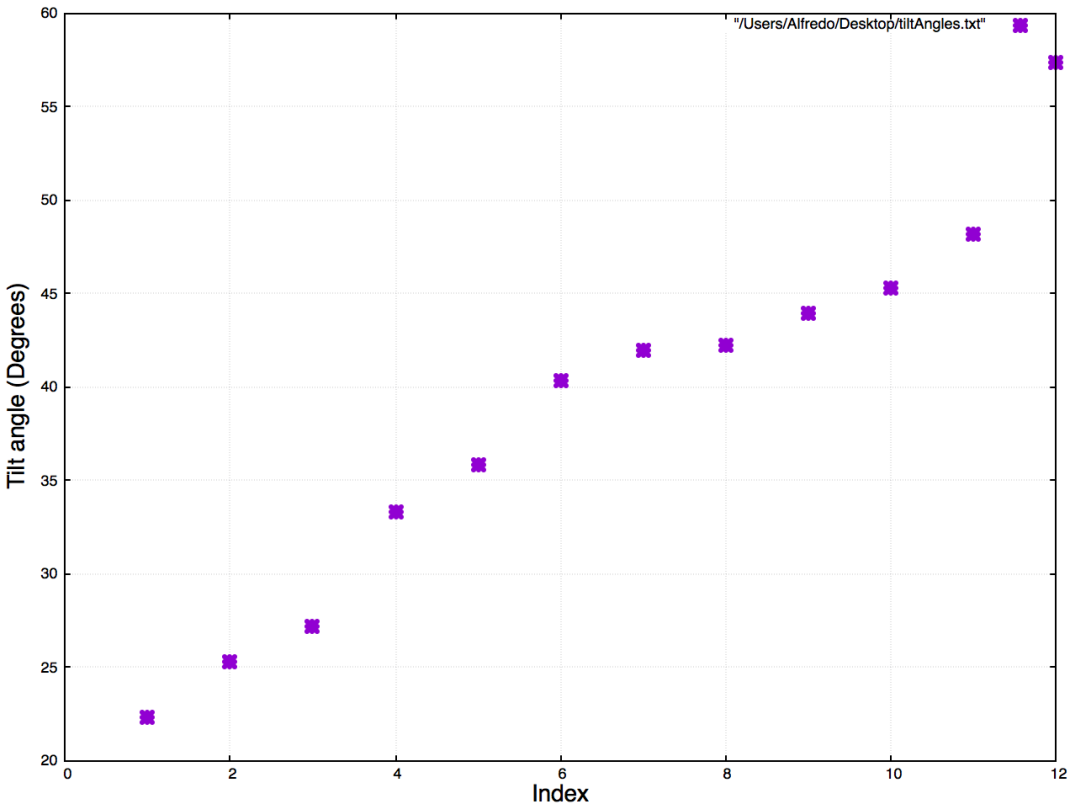
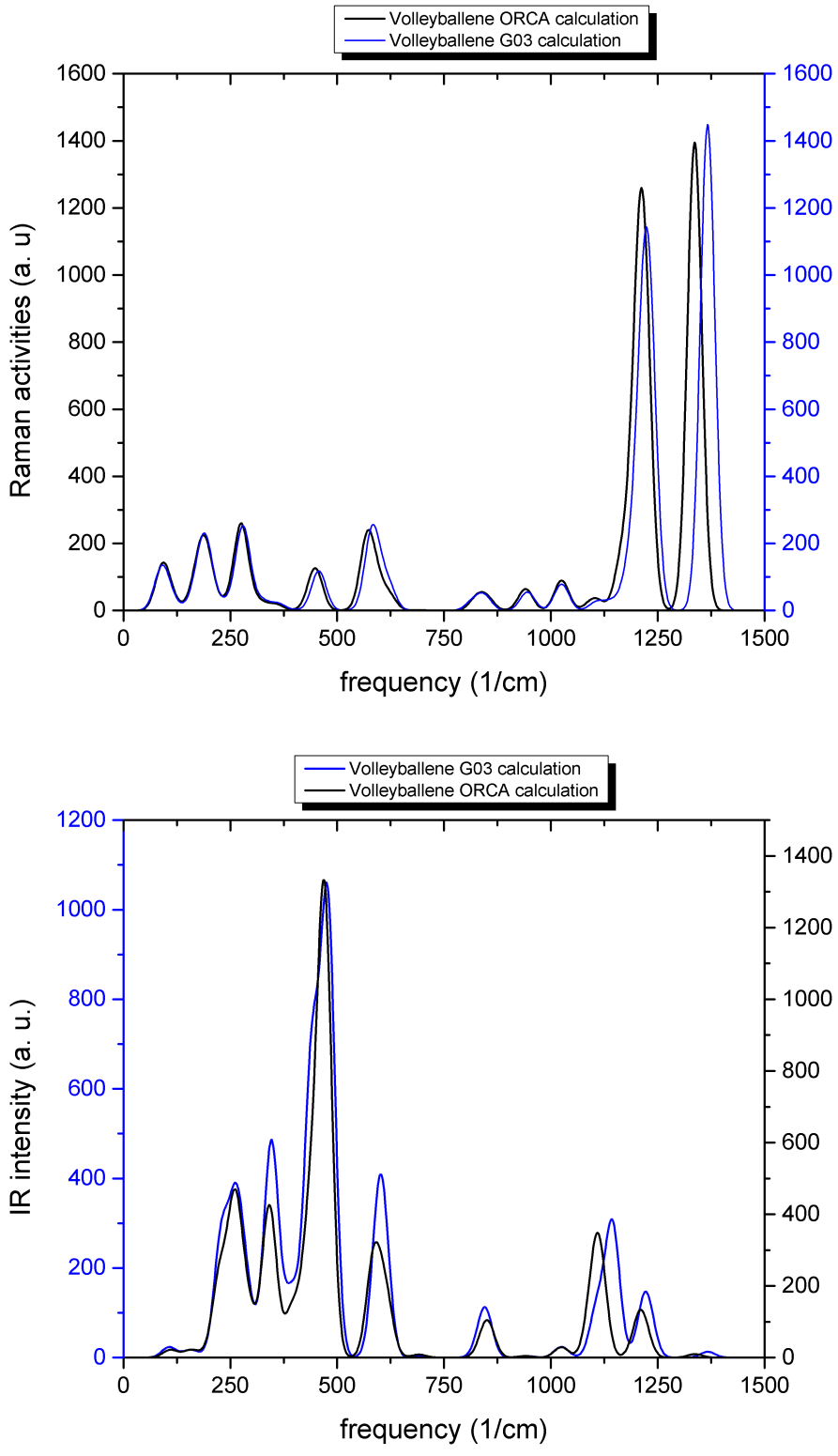
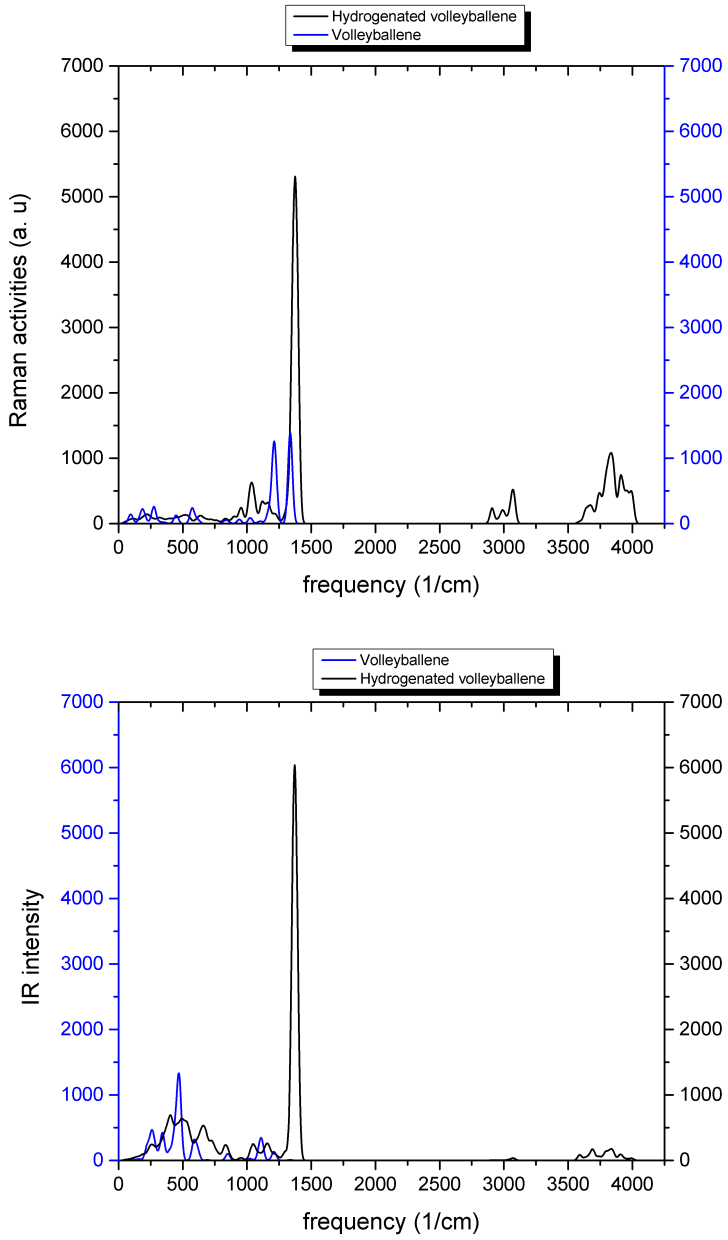


Figure S1. Comparison between ORCA/G03 calculations of IR/Raman spectra of V-ball. Both calculations are in agreement with Ref. 2.



Blue profiles correspond with the G03 calculations in ref. 2. A gaussian broadening of 20 cm^{-1} was used.

Figure S2. Comparison of calculated Raman (upper panel) and IR (lower panel) spectra of V-ball and heavy hydrogenated volleyballene ($Sc_{20}C_{60}H_{70}$) by means of DFT calculations (ORCA package). A gaussian broadening of 20 cm^{-1} was used.



Raman spectra (upper panel) show a slight shift toward large frequencies for hydrogenated volleyballene with an intense and characteristic peak located circa 1391 cm^{-1}. IR spectra (lower panel) features an intense peak located circa 1382 cm^{-1} for hydrogenated volleyballene which can be attributed to Sc-H stretching vibration. Both IR and Raman spectra feature more intense peaks in the case of hydrogenated volleyballene. Characteristic peaks after 2700 cm^{-1} are displayed by the hydrogenated structure.