

## Rovibrational Energies and Spectroscopic Constants for Buckyball Dimer

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### INTRODUCTION

After being discovered by Kroto and co-authors<sup>1</sup> in 1985, the C<sub>60</sub> molecule (buckyballs) and other stable fullerenes have opened a completely new field of material research. The dimerization of C<sub>60</sub> and other forms<sup>2</sup> has attracted considerable interest from both experimental and theoretical scientists. Apart from (C<sub>60</sub>)<sub>2</sub> and (C<sub>70</sub>)<sub>2</sub> fullerene dimers, many other stable larger ones (C<sub>76</sub>, C<sub>78</sub>, C<sub>83</sub>, etc.) exist.<sup>3</sup> In this work, we have built Binding Energies Curves (BECs) from interactions between C<sub>60</sub>, C<sub>70</sub> and C<sub>84</sub> fullerenes. In this way, different dimers were studied, such as (C<sub>60</sub>)<sub>2</sub>, (C<sub>70</sub>)<sub>2</sub> and (C<sub>84</sub>)<sub>2</sub>. Cross-dimers, such as C<sub>60</sub>C<sub>70</sub>, C<sub>70</sub>C<sub>84</sub>, etc., were studied as well. We have also calculated the rovibrational energies and spectroscopic constants from the BEC by solving the Nuclear Schrödinger Equation and Dunham method as well.

### METHODS

Firstly, all BECs (rigid scan) were obtained at the  $\omega$ B97XD/6-31G(d) level of calculation as implemented in the G09 suite of programs and calculated as following:

$$E_b = E_{Dimer} - (E_{monomer,1} + E_{monomer,2}),$$

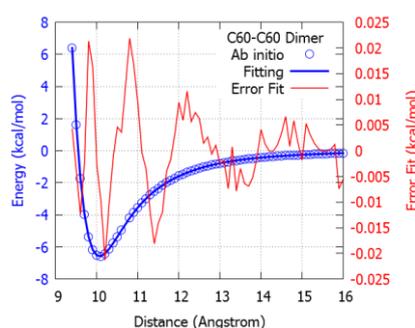
where,  $E_{Dimer}$ , and  $E_{monomer,i}$  are the total energies of dimers and monomer  $i$ , respectively. We have evaluated the effect of inclusion of BSSE correction.

The rovibrational energies  $E_{v,J}$  were obtained by solving the Nuclear Schrodinger Equation using the Discrete Variable Representation (DVR) method. We have employed the generalized Rydberg of sixth degree (Ryd 6) to represent the effective potential for the nuclei in motion. To ensure the consistency of this approach, the spectroscopic constants care also determined by the Dunham method.

### RESULTS AND DISCUSSION

The calculated BEC for the (C<sub>60</sub>)<sub>2</sub> is depicted in the Figure 1. From this Figure, it is possible to

extract the dissociation energy and the center to center (C<sub>60</sub>)<sub>2</sub> dimer distance, which is  $De_{(C60)2} = 6.54$  kcal/mol and  $R_e = 10.06$  Å, respectively. There is a close agreement between our results for the center-to-center (C<sub>60</sub>)<sub>2</sub> distance and the experimental one ( $R_e = 9.91$  Å).<sup>4</sup>



**Figure 1.** BEC (blue line) of the C60C60 dimer and its error fits (red line).

The spectroscopic constants obtained using the Dunham method for the (C<sub>60</sub>)<sub>2</sub> dimer are:  $\omega_e = 27.32$  cm<sup>-1</sup>,  $\omega_e x_e = 9.24 \times 10^{-2}$  cm<sup>-1</sup>, and  $B_e = 4.61 \times 10^{-4}$  cm<sup>-1</sup>. The results obtained using DVR and Dunham are in excellent agreement, thus indicating the good quality of our results and the suitability of both approaches to treat these systems.

### CONCLUSIONS

In this work we have calculated the rovibrational and spectroscopic constants for dimers and cross-dimers formed by C<sub>60</sub>, C<sub>70</sub> and C<sub>84</sub>. The current theoretical predictions are expected to be useful in the future experimental investigations.

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<sup>1</sup> H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl, and R.E. Smalley, *Nature* **318**, 162 (1985).<sup>2</sup> H.W. Kroto, *Nature* **329**, 529 (1987).<sup>3</sup> H.W. Kroto and D.R.M. Walton, *Chem. Phys. Lett.* **214**, 353 (1993).<sup>4</sup> M.R. Pederson and A.A. Quong, *Phys. Rev. Lett.* **74**, 2319 (1995).