**Supplemental Material**

**The Examination of Molecular Structure Properties of 4,4'-oxydiphthalonitrile Compound: A combined spectral and computational analysis approaches**

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**S.1** Atom-by-atom superimposition of the calculated structure (red) with Becke, three-parameter, Lee-Yang-Parr/6-311G(d,p) over the X-ray structure (black) for the 4,4'-oxydiphthalonitrile compound. The H atoms have been omitted for clarity. (RMSE-Root mean square error=0.227).

**S.2** Correlation graph for the bond lengths of the 4,4'-oxydiphthalonitrile.

**S.3** Correlation graph for the bond angles of the 4,4'-oxydiphthalonitrile.

**S.4** Correlation graphic for experimental and theoretical wavenumbers of the 4,4'-oxydiphthalonitrile.

**S.5** Correlation graphic for experimental and theoretical 13C-NMR chemical shift values respect to CSGT approach of the 4,4'-oxydiphthalonitrile.

**S.6** Correlation graphic for experimental and theoretical 13C-NMR chemical shift valuesrespect to GIAO approach of the 4,4'-oxydiphthalonitrile.

**S.7** Correlation graphic for experimental and theoretical 13C-NMR chemical shift values respect to IGAIM approach of the 4,4'-oxydiphthalonitrile.

**S.8** Correlation graphic for experimental and theoretical 1H-NMR chemical shift values respect to CSGT approach of the 4,4'-oxydiphthalonitrile.

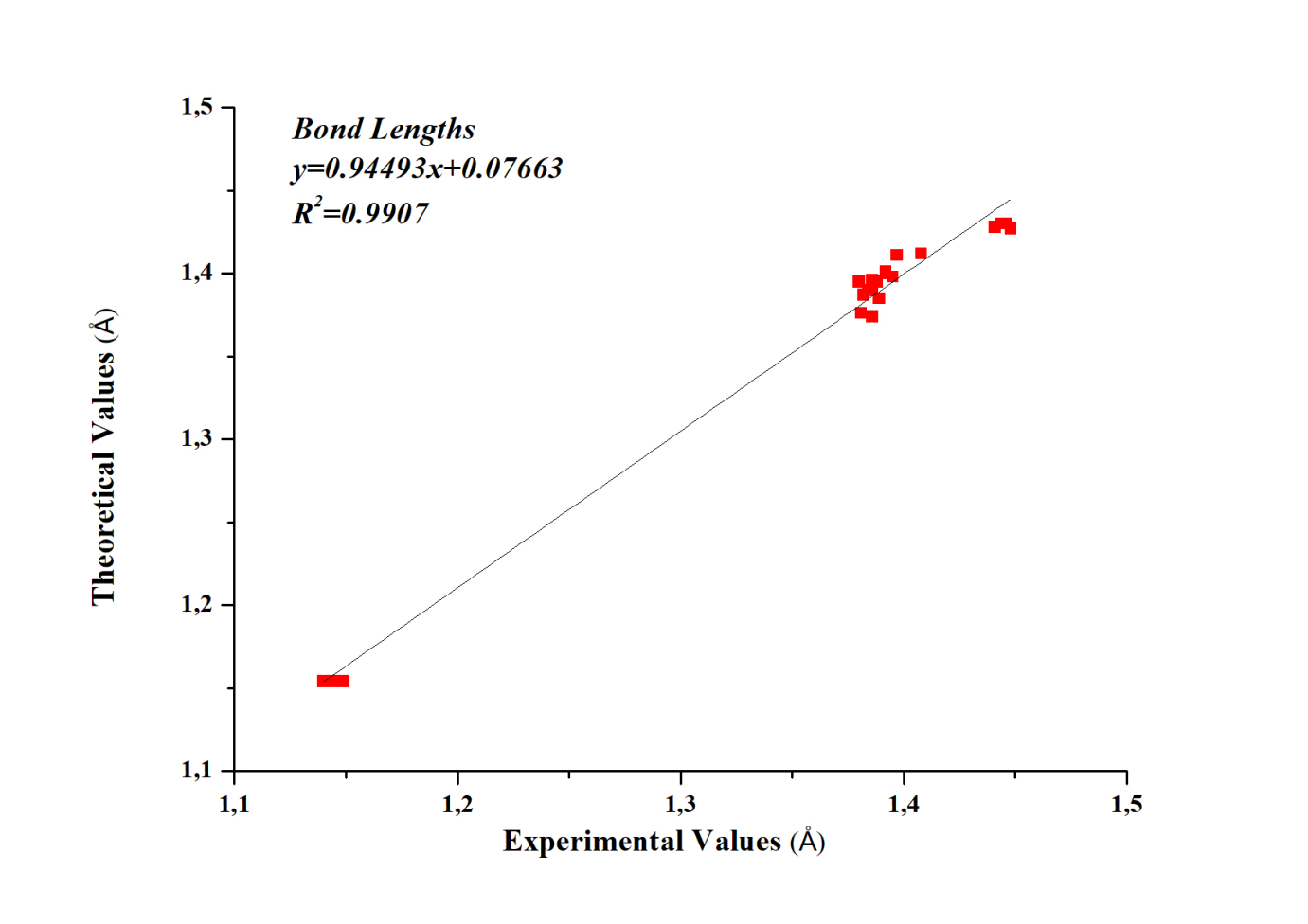
**S.9** Correlation graphic for experimental and theoretical 1H-NMR chemical shift valuesrespect to GIAO approach of the 4,4'-oxydiphthalonitrile.

**S.10** Correlation graphic for experimental and theoretical 1H-NMR chemical shift values respect to IGAIM approach of the 4,4'-oxydiphthalonitrile.

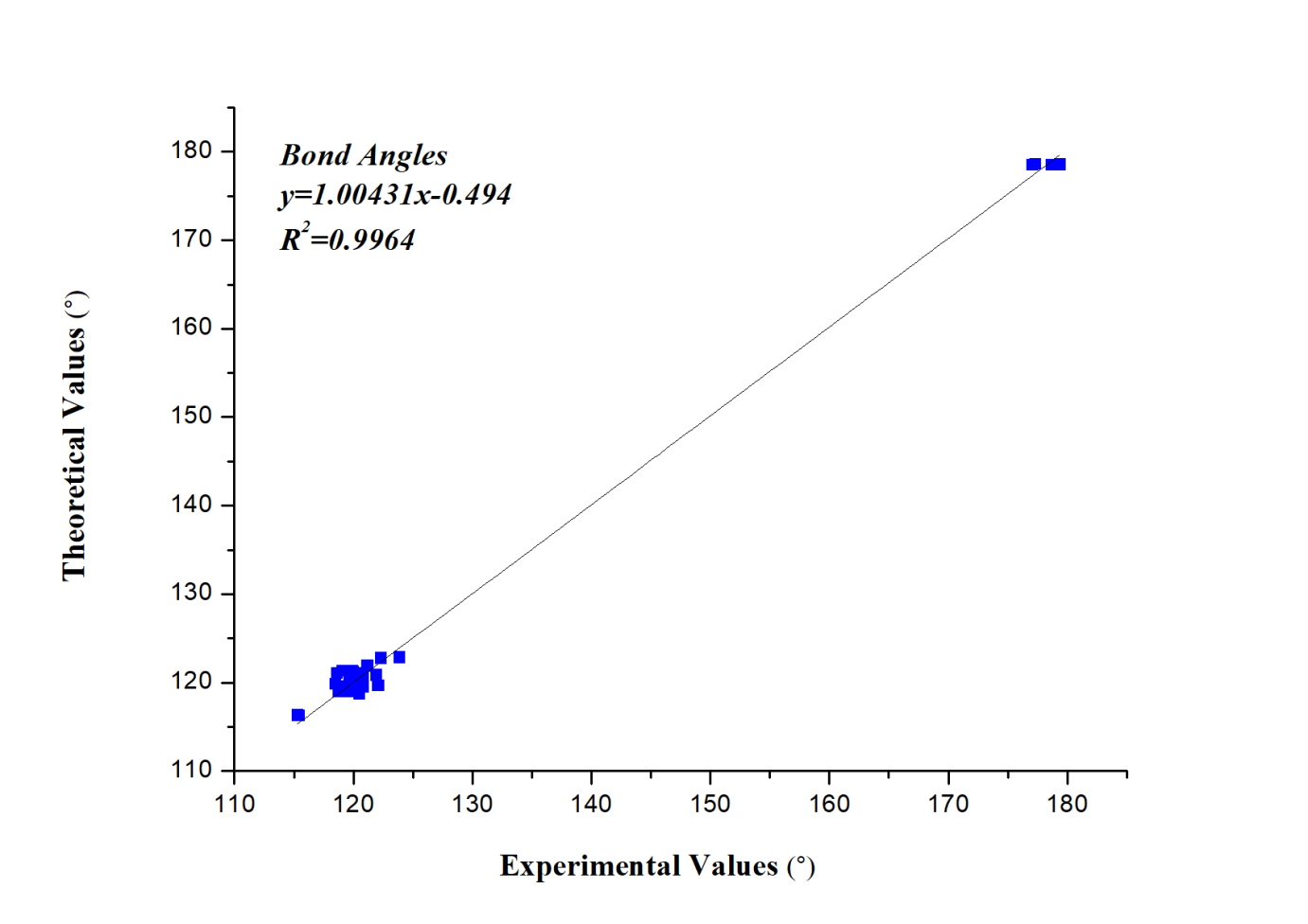
**S.11** Molecular electrostatic potential map view have been generated using Becke, three-parameter, Lee-Yang-Parr/6-311G(d,p) method of the 4,4'-oxydiphthalonitrile compound.

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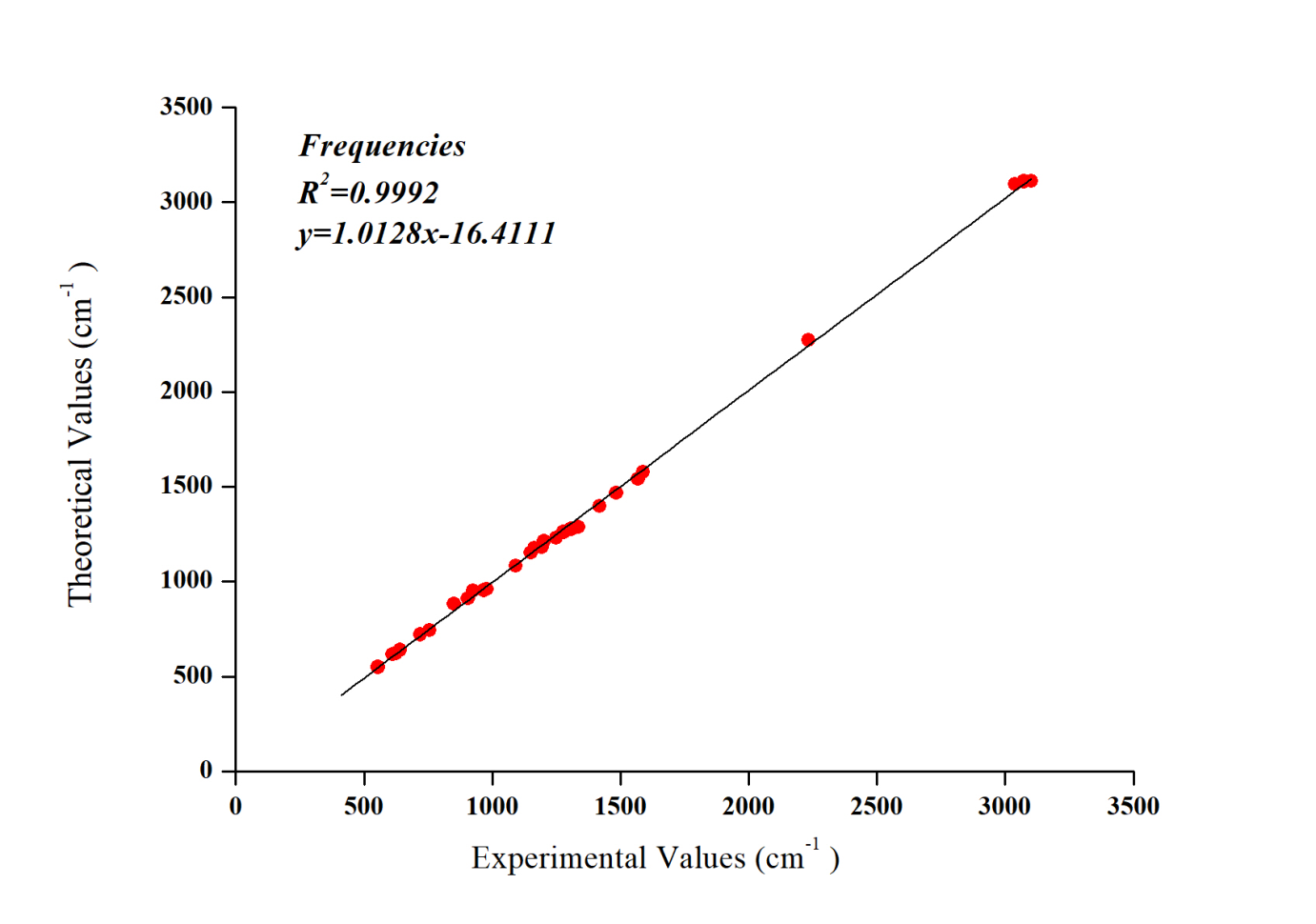
**S.1** Atom-by-atom superimposition of the calculated structure (red) with Becke, three-parameter, Lee-Yang-Parr/6-311G(d,p) over the X-ray structure (black) for the 4,4'-oxydiphthalonitrile compound. The H atoms have been omitted for clarity. (RMSE-Root mean square error=0.227).

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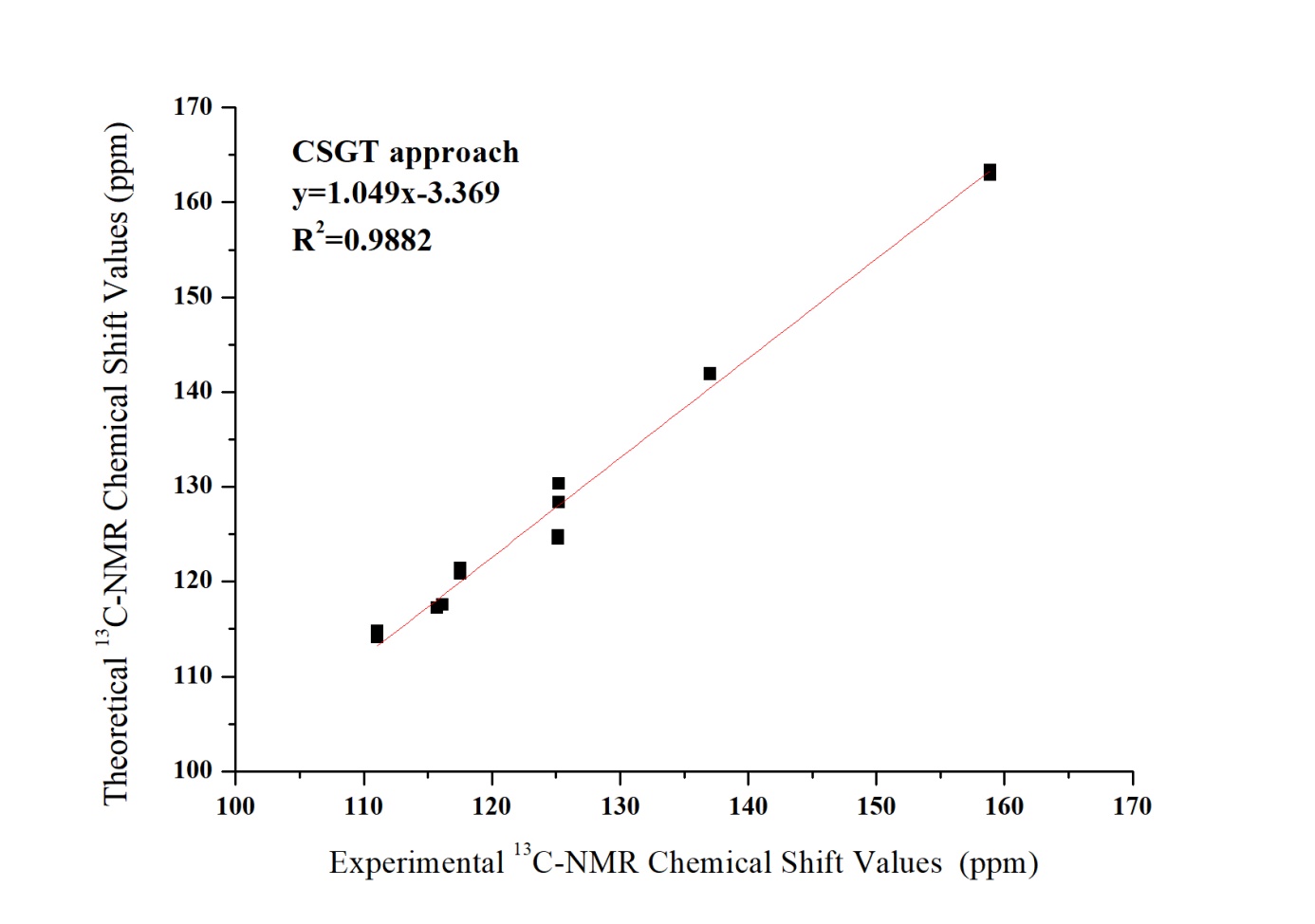
**S.2** Correlation graph for the bond lengths of the 4,4'-oxydiphthalonitrile

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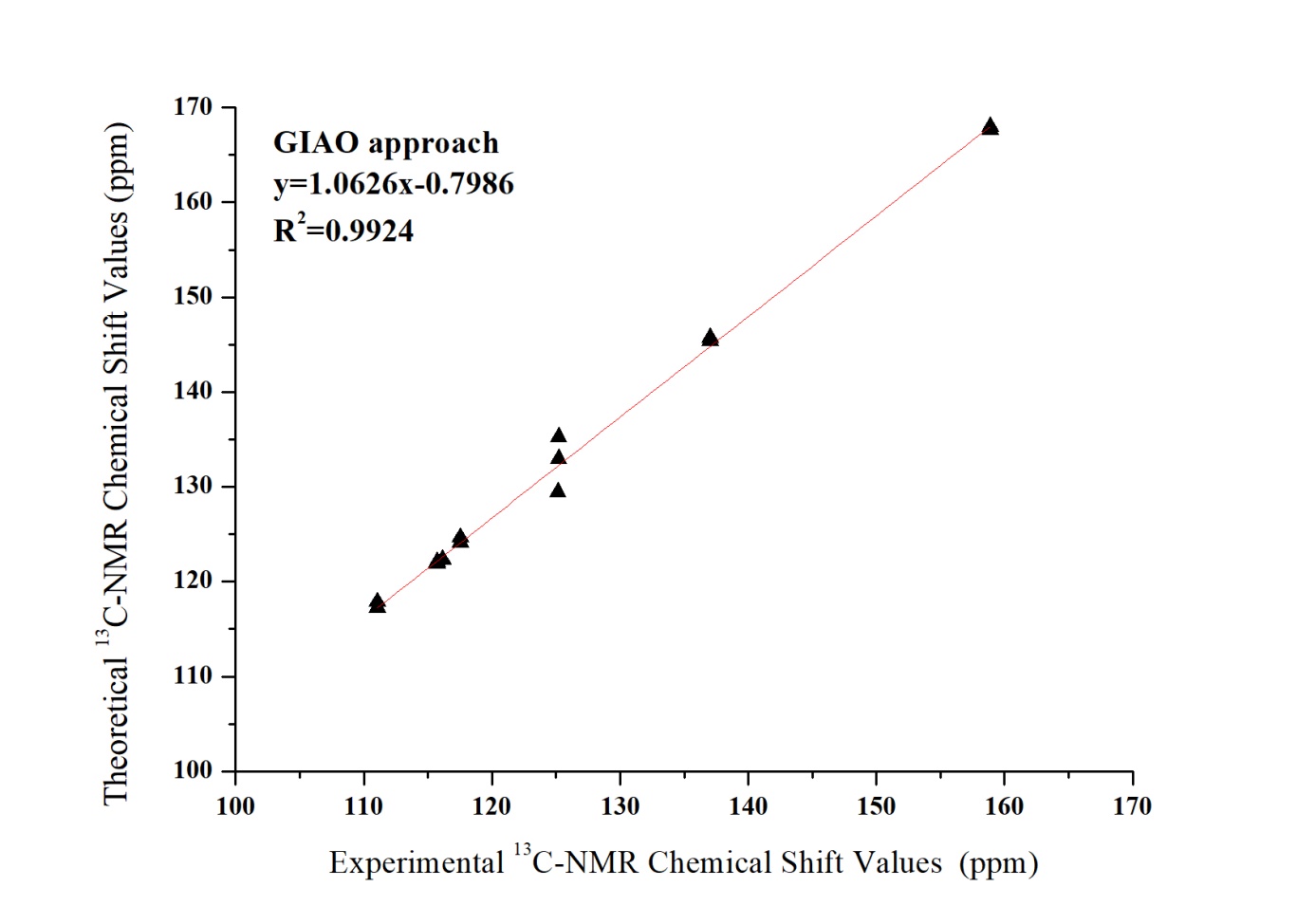
**S.3** Correlation graph for the bond angles of the 4,4'-oxydiphthalonitrile

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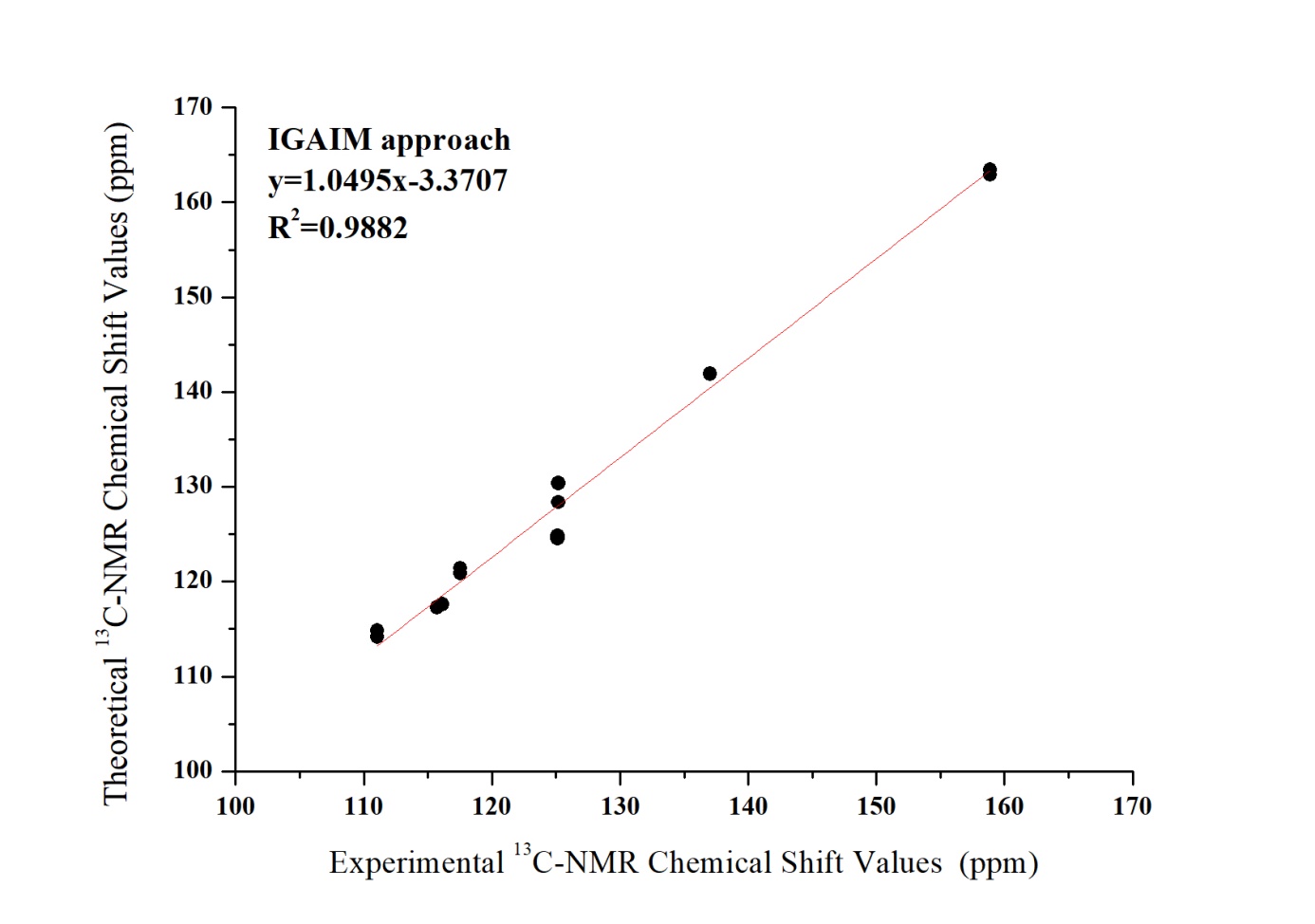
**S.4** Correlation graphic for experimental and theoretical wavenumbers of the 4,4'-oxydiphthalonitrile.



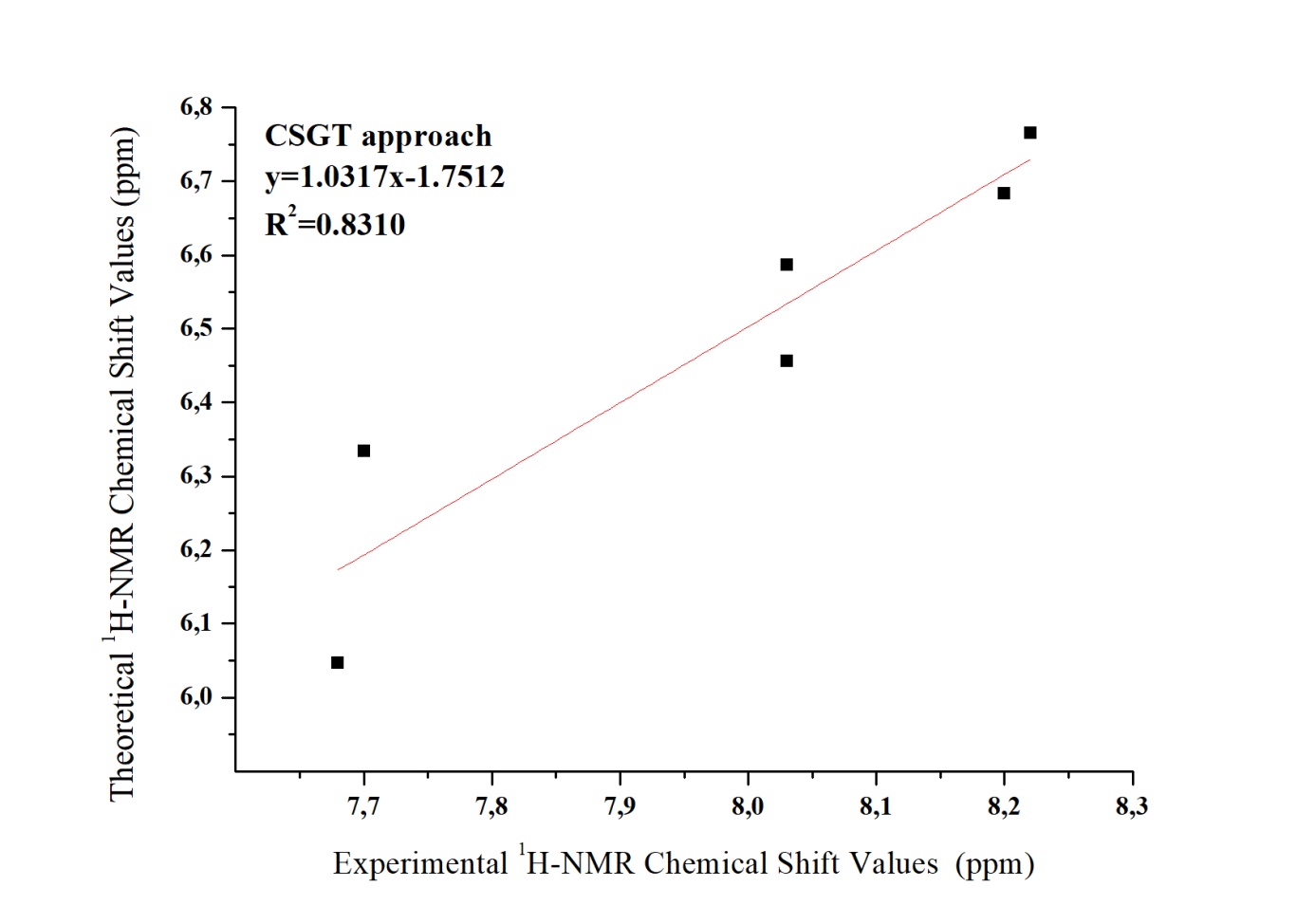
**S.5** Correlation graphic for experimental and theoretical 13C-NMR chemical shift values respect to CSGT approach of the 4,4'-oxydiphthalonitrile.



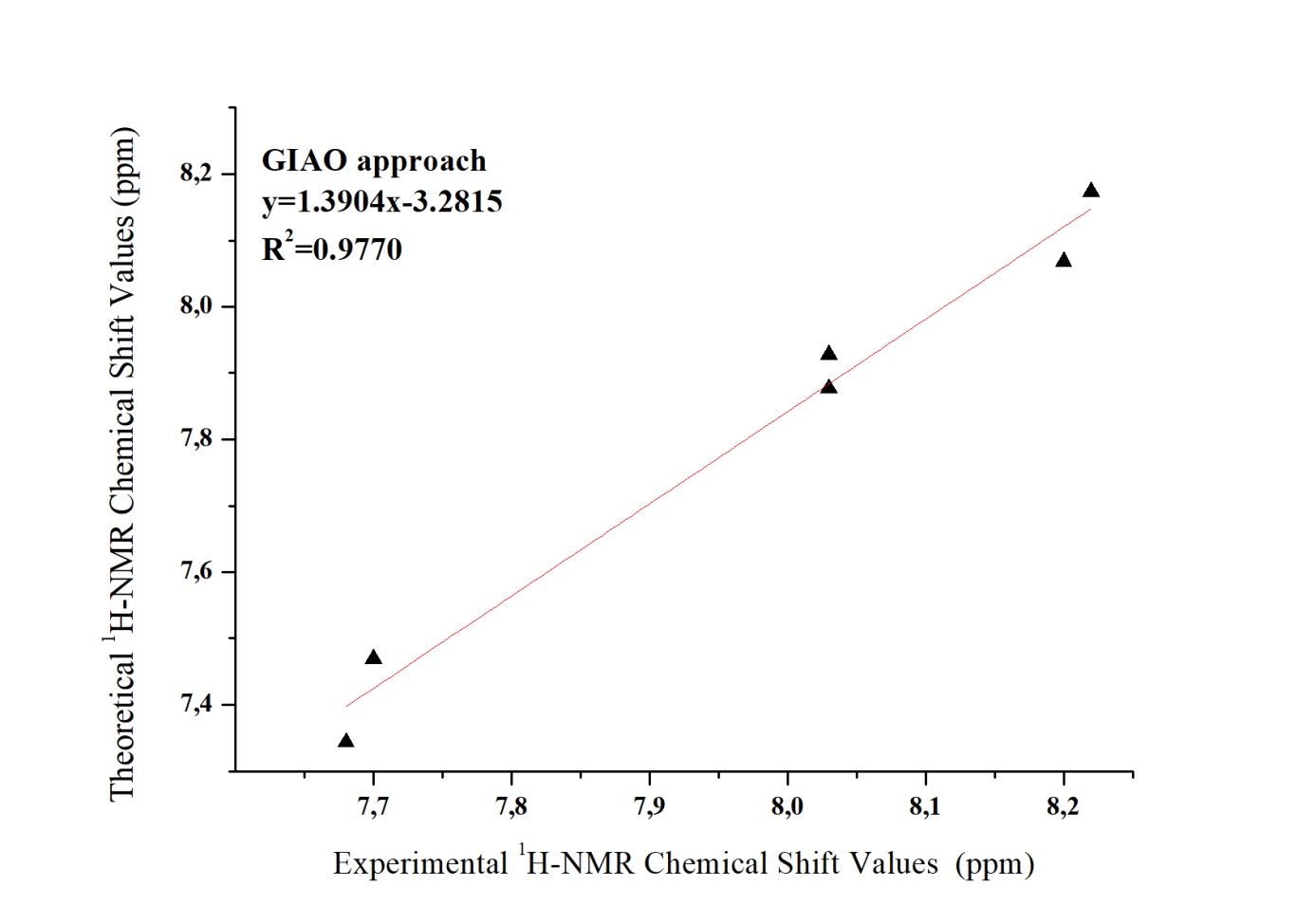
**S.6** Correlation graphic for experimental and theoretical 13C-NMR chemical shift values respect to GIAO approach of the 4,4'-oxydiphthalonitrile.



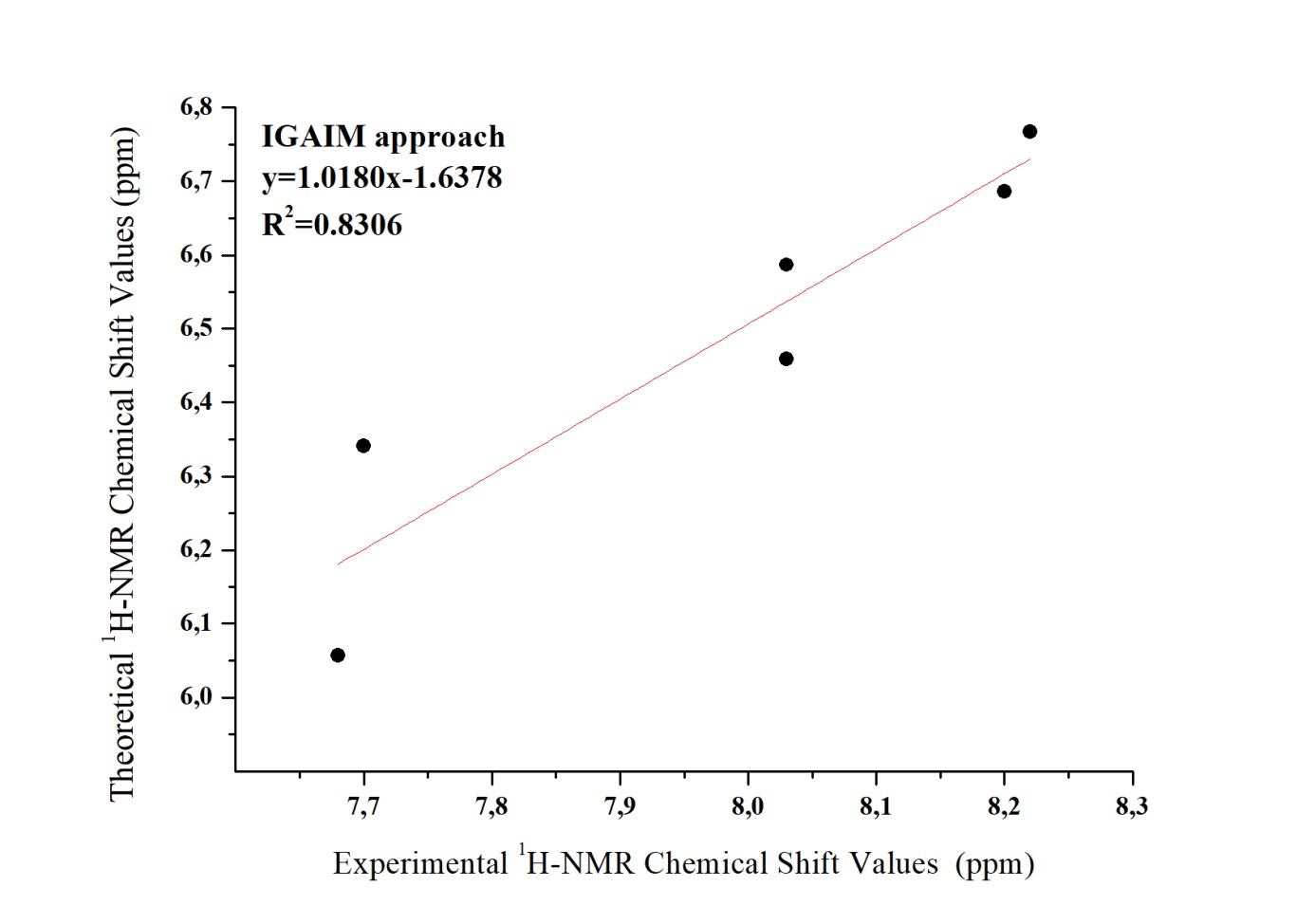
**S.7** Correlation graphic for experimental and theoretical 13C-NMR chemical shift values respect to IGAIM approach of the 4,4'-oxydiphthalonitrile.



**S.8** Correlation graphic for experimental and theoretical 1H-NMR chemical shift values respect to CSGT approach of the 4,4'-oxydiphthalonitrile.



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**S.10** Correlation graphic for experimental and theoretical 1H-NMR chemical shift values respect to IGAIM approach of the 4,4'-oxydiphthalonitrile.

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