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Visualizing changes of molecular conformation in solid-state by a common structural determination technique: single crystal X-ray diffraction

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Single crystal X-ray diffraction

The identical crystal was applied to carry out single crystal X-ray diffractions on Bruker D8 Venture diffractometer equipped with CMOS detector using graphite-monochromated Mo-Ka radiation (0.71073 Å) at different temperature from 150 to 298 K with an interval of 15 K. All the data were reduced by the SAINT[1], then corrected by SADABS[2] routines under APEX3[3] software package. The structures at different temperature were solved by dual space method using SHELXT[4] subprogram and refined by SHELXL[5] subprogram with full-matrix least squares on F^2 under Olex2[6] software package. All non-hydrogen atoms were refined anisotropically, and all the hydrogen atoms were resided their positions by geometrical calculation and refined isotropically using a riding model.

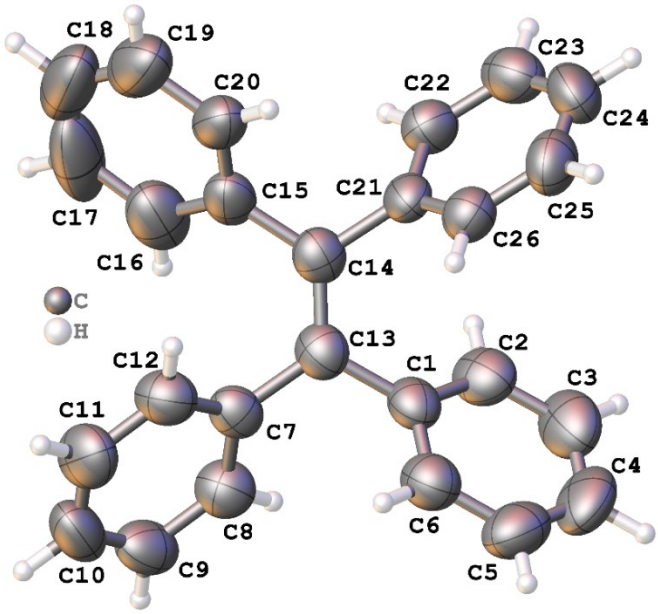

Figure S1. The asymmetric unit of TEP at 150 K with 90 % probability level, the H atoms are not labelled for clarity.

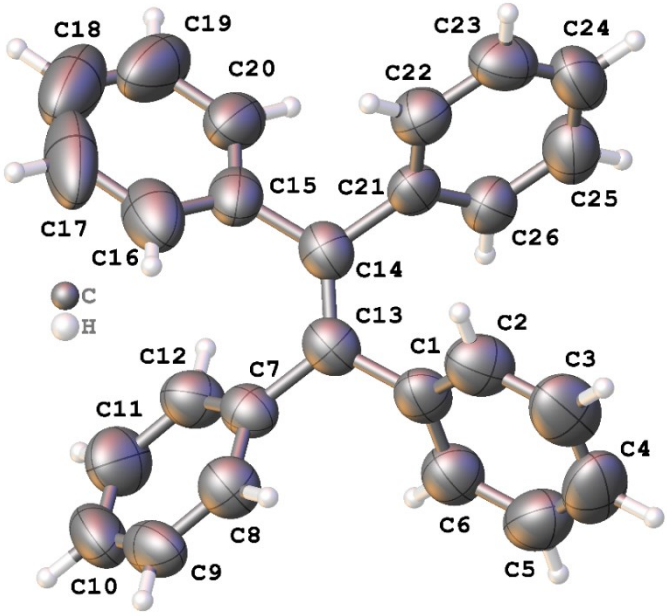

Figure S2. The asymmetric unit of TEP at 165 K with 90 % probability level, the H atoms are not labelled for clarity.

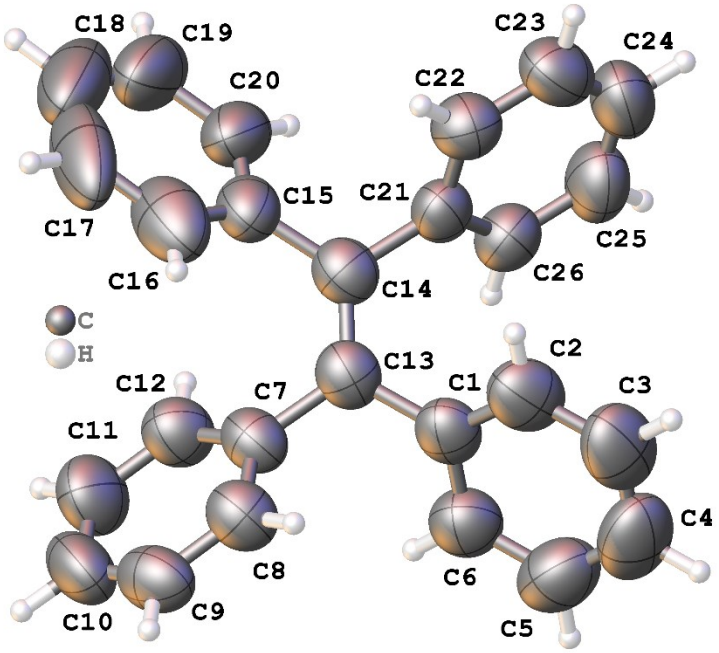

Figure S3. The asymmetric unit of TEP at 180 K with 90 % probability level, the H atoms are not labelled for clarity.

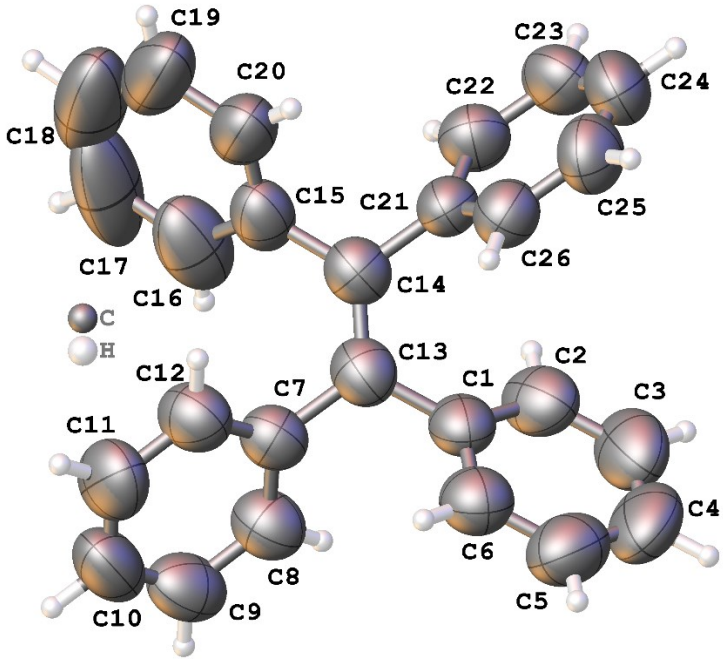

Figure S4. The asymmetric unit of TEP at 195 K with 90 % probability level, the H atoms are not labelled for clarity.

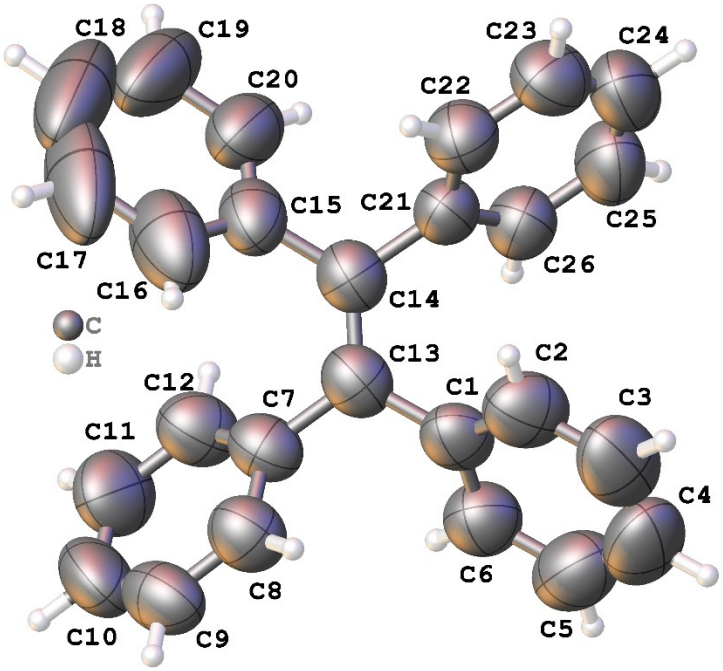

Figure S5. The asymmetric unit of TEP at 210 K with 90 % probability level, the H atoms are not labelled for clarity.

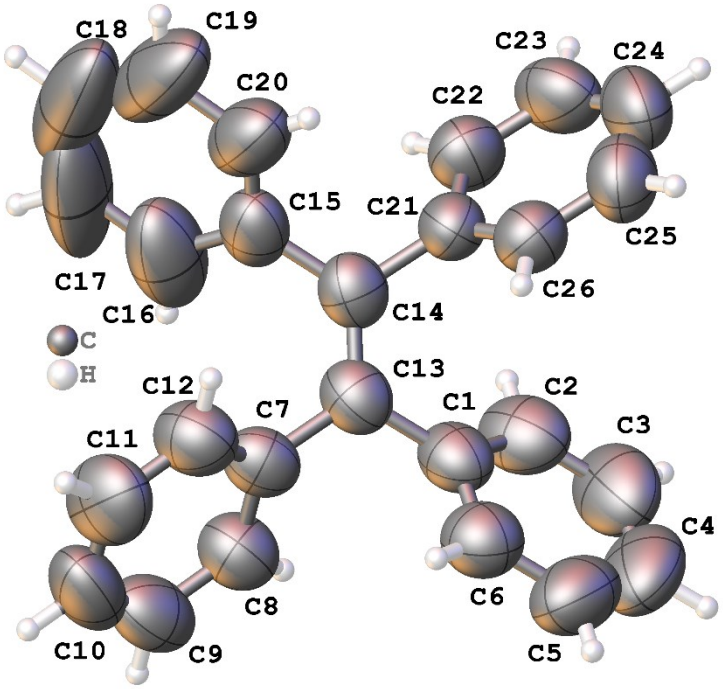

Figure S6. The asymmetric unit of TEP at 225 K with 90 % probability level, the H atoms are not labelled for clarity.

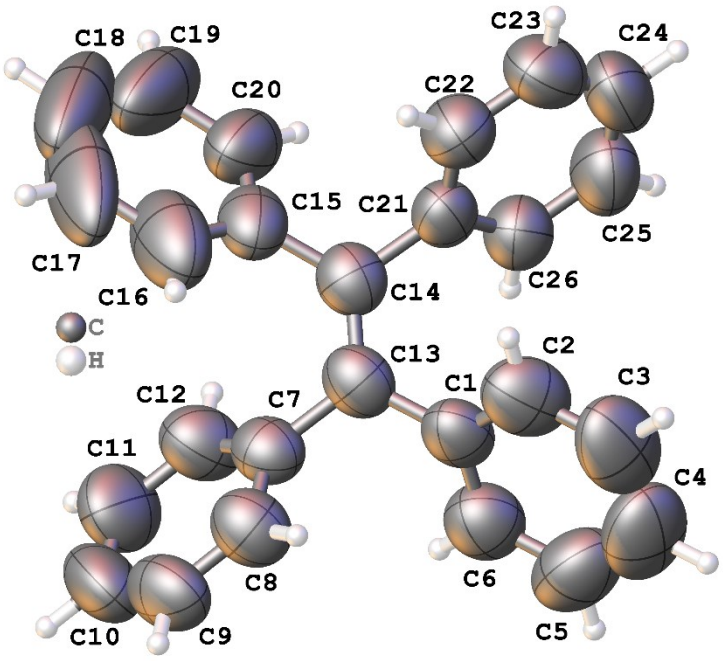

Figure S7. The asymmetric unit of TEP at 240 K with 90 % probability level, the H atoms are not labelled for clarity.

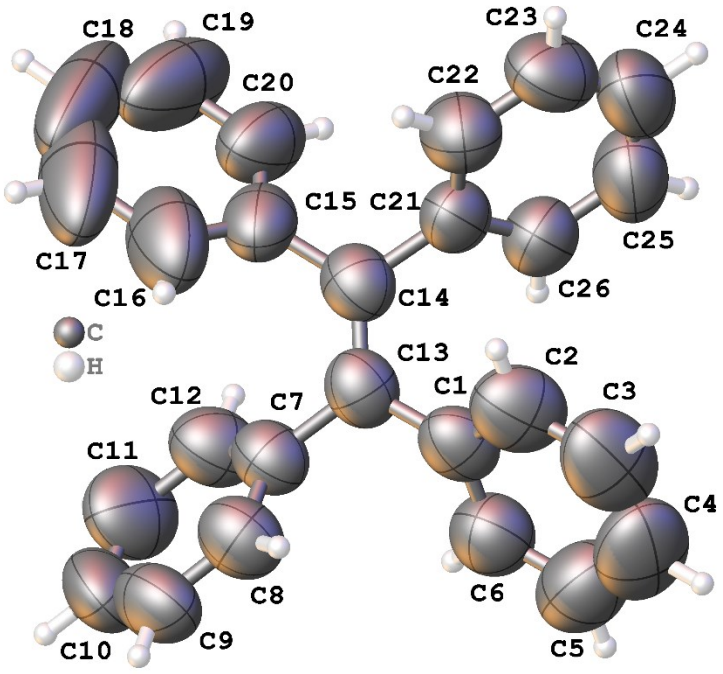

Figure S8. The asymmetric unit of TEP at 255 K with 90 % probability level, the H atoms are not labelled for clarity.

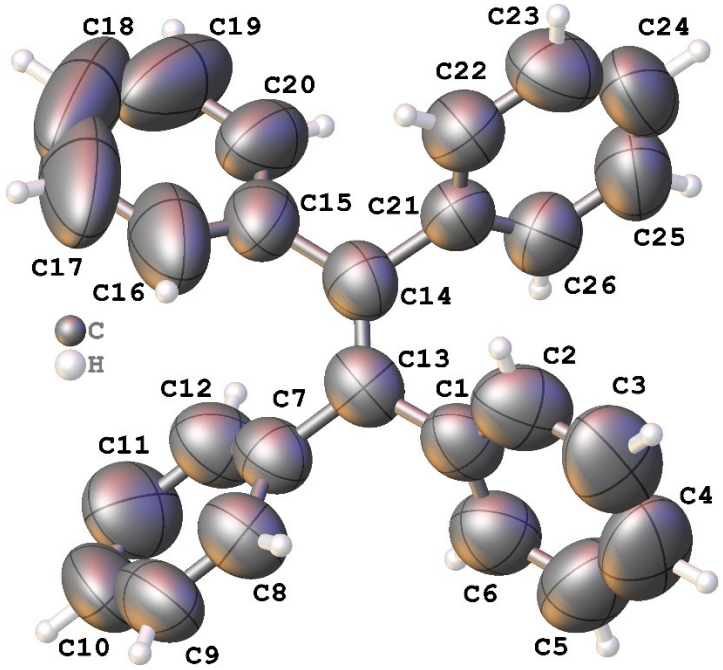

Figure S9. The asymmetric unit of TEP at 270 K with 90 % probability level, the H atoms are not labelled for clarity.

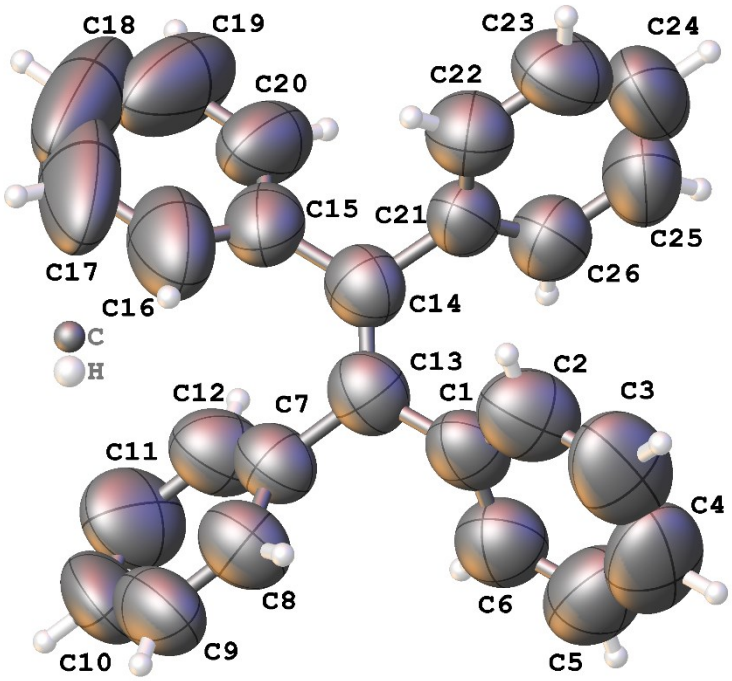

Figure S10. The asymmetric unit of TEP at 285 K with 90 % probability level, the H atoms are not labelled for clarity.

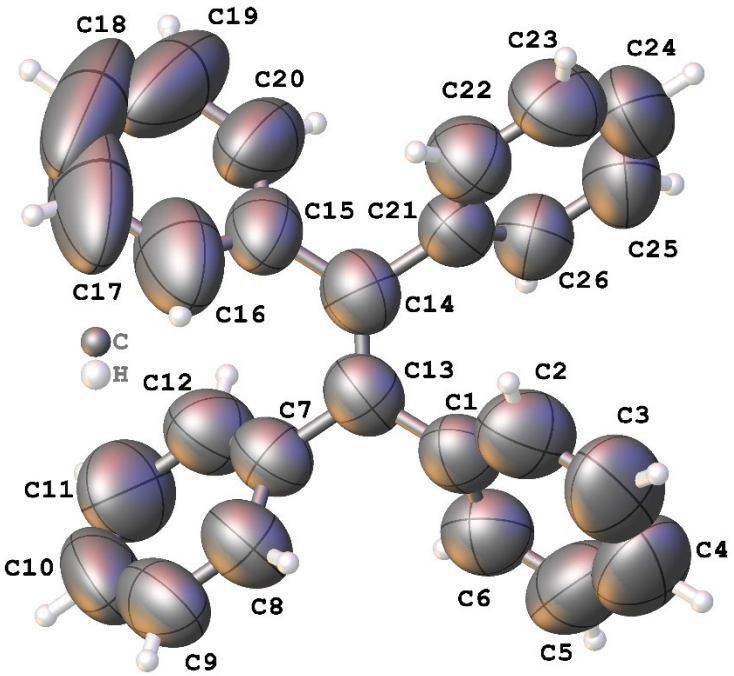

Figure S11. The asymmetric unit of TEP at 298 K with 90 % probability level, the H atoms are not labelled for clarity.

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2. Bruker, *Sadabs*, Bruker AXS Inc., Madison, Wisconsin, USA, 2008/1 edn., 2008.
3. Bruker, *Apex3*, Bruker AXS Inc., Madison, Wisconsin, USA, 2014.3 - 0. edn., 2014.
4. G. M. Sheldrick, Shelxt - Integrated Space-Group and Crystal-Structure Determination, *Acta Crystallogr., Sect. A: Found. Crystallogr.*, 2015, **71**, 3-8.
5. G. M. Sheldrick, Crystal Structure Refinement with Shelxl, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2015, **71**, 3-8.
6. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, Olex2: A Complete Structure Solution, Refinement and Analysis Program, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.