Improved dielectric properties and grain boundary effect of phenanthrene under high pressure

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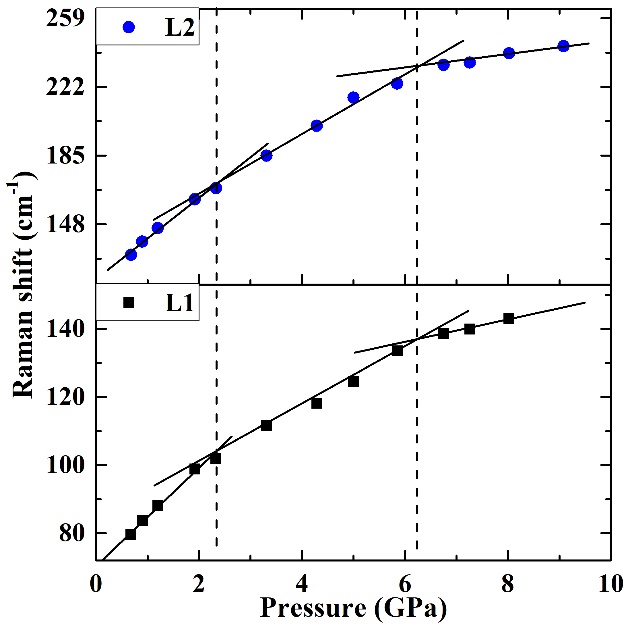
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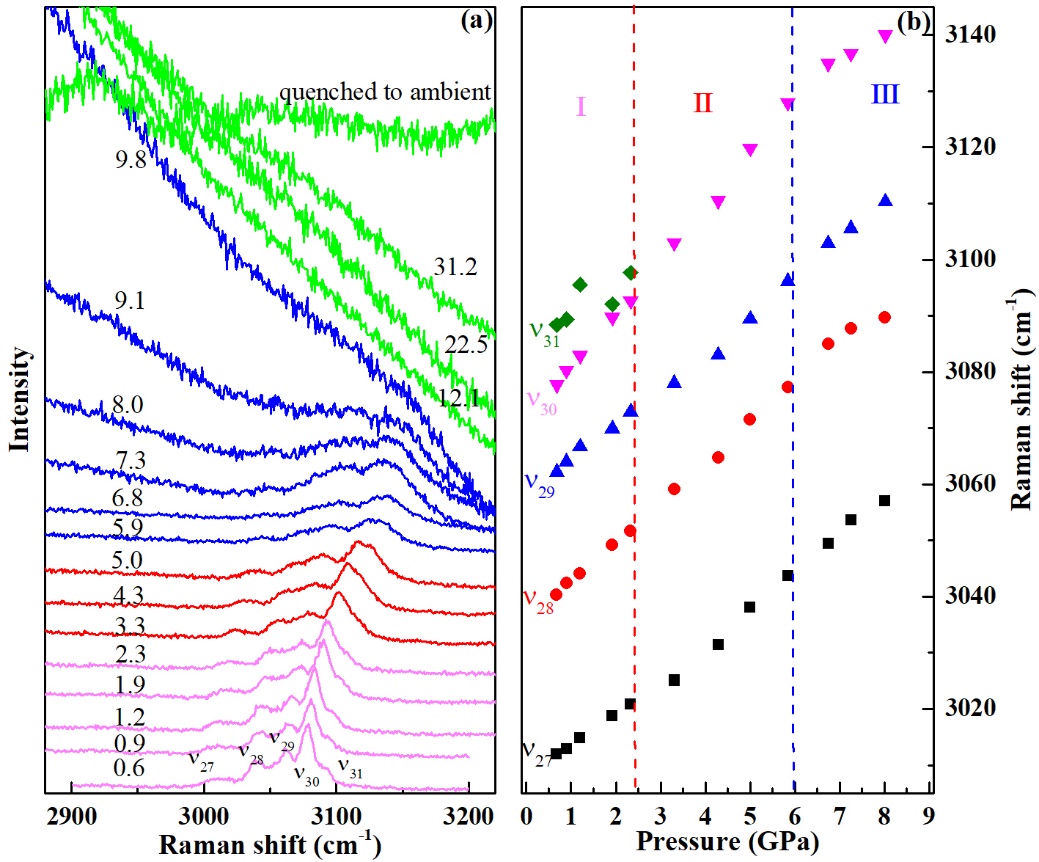
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**Fig. S1** Raman modes of *L*1 and *L*2 as a function of pressure. The solid lines are the linear fit to the data.



**Fig. S2** High pressure Raman spectra of phenanthrene and pressure dependence of the Raman shift in region of 2800-3250 cm-1. Dashed vertical lines represent phase boundaries, and phases are assigned with Roman numbers. (*ν*29, *ν*30) and (*ν*27, *ν*28, *ν*31) correspond to the symmetric and asymmetric stretching vibrations of the C-H bond, respectively.

**Table S1** The pressure dependence of intramolecular and intermolecular bond distances.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Phase | Intramolecular | d*L*Intra/d*P* (Å/GPa) | Intermolecular | d*L*Inter/d*P* (Å/GPa) |
| I | C24-C28 | -0.00087 | C18-H18 | -0.00042 |
| C26-C24 | -0.00150 |
| C16-C26 | -0.00150 |
| C18-C20 | -0.00062 | H18-H8 | -0.02800 |
| C28-C18 | -0.00049 |
| C16-C20 | -0.00100 |
| II | C46-C47 | -0.00160 | C44-C21 | -0.06100 |
| C47-C48 | -0.00210 |
| C45-C46 | -0.00160 | H32-H27 | -0.04100 |
| C44-C45 | -0.00160 |
| C48-C43 | -0.00130 | C44-H32 | -0.00087 |