Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2016

Figures for phonon dispersions and the isosurfaces of electron localization function (ELF):

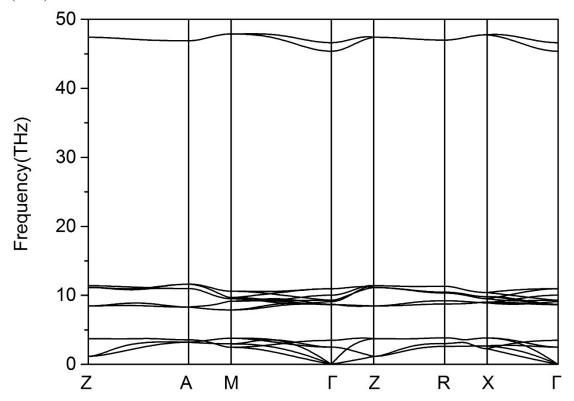


Fig. S1 Phonon dispersions of the I4/mmm structure (α phase) at ambient pressure.

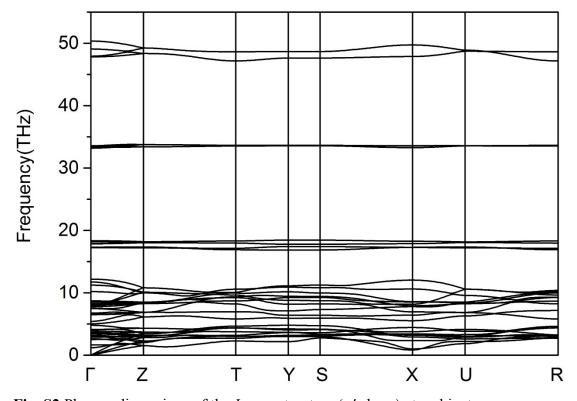


Fig. S2 Phonon dispersions of the *Immm* structure (α' phase) at ambient pressure.

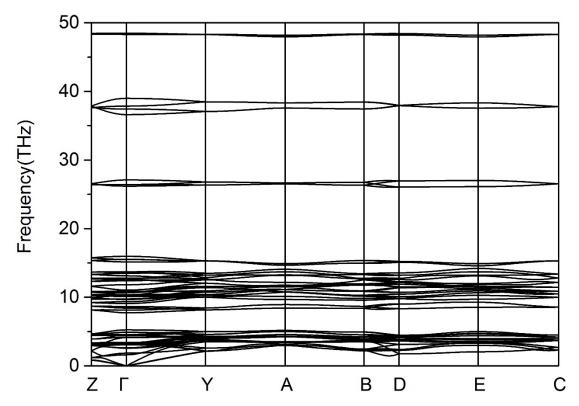


Fig. S3 Phonon dispersions of the C2/c structure at 10.0 GPa.

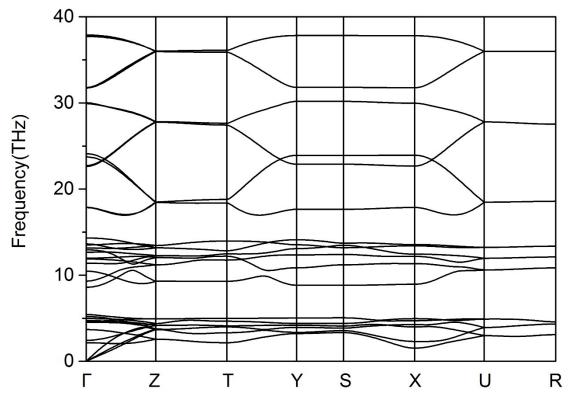


Fig. S4 Phonon dispersions of the *Pnma* structure at 20.0 GPa.

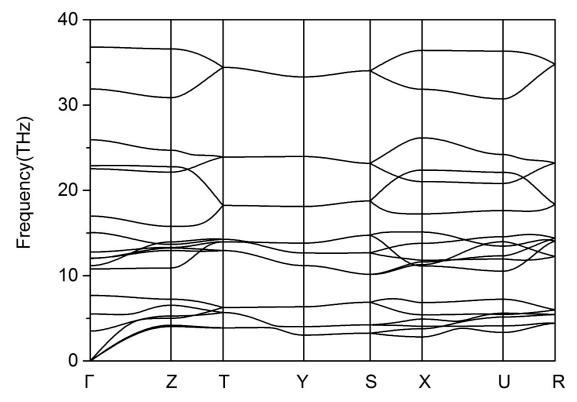


Fig. S5 Phonon dispersions of the *Pmma* structure at 30.0 GPa.

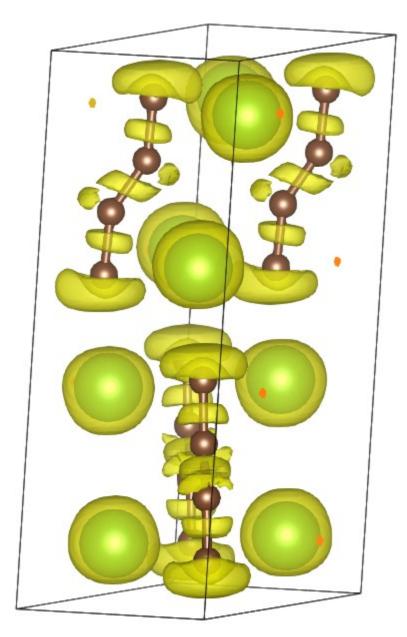


Fig. S6 Isosurfaces of electron localization function (ELF) with the value of 0.78 for the C2/c structure at 10.0 GPa.

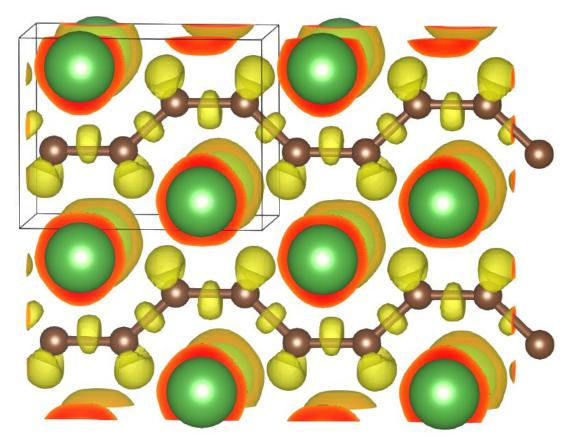


Fig. S7 Isosurfaces of electron localization function (ELF) with the value of 0.78 for the *Pmma* structure at 30.0 GPa.