Dense Carbon Monoxide to 160 GPa: Stepwise Polymerization to Two-Dimensional Layered Solid.\textsuperscript{1} YOUNG JAY RYU, MINSOEB KIM, Washington State University, RANGA DIAS, Lyman Laboratory of Physics, Harvard University, DENNIS KLUG, Steacie Institute for Molecular Science, National Research Council of Canada, CHOONG-SHIK YOO, Washington State University — Carbon monoxide (CO) is one of simple molecular systems like N$_2$, O$_2$ and H$_2$, yet been studied at pressures above 5-10 GPa. It is also the first molecular system found to transform into a nonmolecular polymeric solid in high energy density at 5.5 GPa; yet, little is known about its structure and transformation beyond this pressure. This imposes a serious short fall in understanding high-pressure behaviors of heteronuclear diatomic systems like CO in comparison with those of homonuclear diatomic systems like N$_2$. Here, we present a series of pressure-induced phase transformations in CO to 160 GPa: from a molecular solid to a highly colored, low-density polymeric phase I to translucent, high-density phase II to transparent, and indirect-gap semi-metallic phase III. The properties of these polymorphs are consistent with those expected from recently predicted 1D $P2_1/m$, 3D $P2_12_12_1$, and 2D $Cmcm$ structures, respectively. Thus, the present results suggest a stepwise polymerization of CO triple bonds to ultimately a 2D singly bonded layer structure, as recently found in dense nitrogen (LP-N).

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