Polycarbonyl

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Polycarbonyl, (also known as **polymeric-CO**, **p-CO** or **poly-CO**) is a solid metastable and explosive polymer of carbon monoxide.[1] The polymer is produced by exposing carbon monoxide to high pressures. The structure of the solid appears amorphous, but may include a zig zag of equally spaced CO groups.[2]

Contents

Formation[edit]

Poly-CO can be produced at pressures of 5.2 GPa; it is amorphous and yellow to dark red in color.[3] Polymerisation is catalysed by blue light at slightly lower pressures in the δ-phase of solid CO.[4] Another white, crystalline phase can be made at higher temperatures at 6 or 7 GPa.[1]

R. J. Mills discovered this solid, which was first produced in a tungsten carbide anvil in 1947. Originally this was thought to be polymeric carbon suboxide, but the formation does not yield any gas byproduct such as carbon dioxide.[5] The yield of the solid can be up to 95%.[6]

Properties[edit]

The polymer is stable above about 80K. Below this temperature the ε form of solid molecular CO is formed

instead. When the pressure is released the polymer remains stable at atmospheric pressure. The solid dissolves in water, alcohol and acetone.[5] When exposed to the atmosphere it is hygroscopic, becomes gluey, and changes colour, becoming darker.[6] The reaction with water produces carboxylic groups.[7][8]

The solid stores a high energy. It can decompose explosively forming glassy carbon and carbon dioxide.[6] The energy density stored can be up to 8 kJ/g. During the decomposition the temperature can be 2500K.[6] The density is 1.65 gcm^{-3}, however most of the solid produced is porous, so the true density is likely to be higher.[6]

Infrared spectroscopy shows bands at 650, 1210, 1440, 1650 and 1760 cm^{-1}. The 1760 band is likely to be due to the -C-(C=O)-C- structure.[4] The 1600 is due to vibration of a C=C double bond.[6]

The solid is electrically insulating with an electronic gap energy of 1.9 eV.[4]

Nuclear magnetic resonance for the material made from ^{13}CO shows sharp resonance at 223 ppm due to ester or lactone attached carbon, and 151 ppm due to C=C double bonds. There is also broad resonance at 109 and 189 ppm. Over time of a few days, the 223 ppm peak reduces and all the other features increase in strength.[6]

Structure[edit]

Ideas of the structure include a zig zag chain of CO pointing in opposite directions, or five atom rings connected by CO and C-C bonds. The rings are lactones of tetronic acid: -C:-(C=O)-(C-O-)-(C=O)-O-. Interconnections between the rings are zig zags of CO.[4]

Other ideas of the structure of the solid, include graphitic carbon with carbon dioxide under pressure, and a polymer with this C_3O_2 monomer: -(C=O)-O-(C-)=C<. Yet other ideas are that the solid is the same as the polymer of carbon suboxide with oxalic anhydride.[9]

References[edit]

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Other reading[edit]

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- *Sun, Jian; Dennis D. Klug; Chris J. Pickard; Richard J. Needs (2011). "Controlling the Bonding and Band Gaps of Solid Carbon Monoxide with Pressure" (PDF). Physical Review Letters.* ***106*** *(14): 145502. Bibcode:2011PhRvL.106n5502S. doi:10.1103/PhysRevLett.106.145502. ISSN 0031-9007. PMID 21561202.*

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Oxocarbons

Common oxides	• CO • CO 2
Exotic oxides	• CO 3 • CO 4 • CO 5 • CO 6 • C 2O • C 2O 2 • C 2O 3 • C 2O 4 (1,2-Dioxetanedione and 1,3-Dioxetanedione) • C 3O

- C 3O 2
- C 3O 3
- C 3O 6
- C 4O 2
- C 4O 4
- C 4O 6
- C 5O 2
- C 5O 5
- C 6O 6 (Cyclohexanehexone and Ethylenetetracarboxylic dianhydride)
- C 8O 8
- C 9O 9
- C 10O 8
- C 10O 10
- C 12O 6
- C 12O 9
- C 12O 12

Polymers

- Graphite oxide
- C_3O_2
- CO

	• CO_2
Compounds derived from oxides	• Metal carbonyls • Carbonic acid • Bicarbonates • Carbonates • Dicarbonates • Tricarbonates

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