TABLE 11

Raman frequencies (cm^{-1}) for KCN polymorphs [146]

Pressure (kbar)	0.001	6.58	16.5	20.1	27.6	0.001	0.001	21.7
Temp. (K)	293					87	60	383
Phase	I	I	I	I & IV	IV	V	VI	III
ν_{CN}	2078.2 [a]	2083.5	2090	2090 2088 (sh)	2090	2080.0 [a]	2081.1 [a]	2090

[a] ± 0.2 cm^{-1}; all others ± 0.5 cm^{-1}.

TABLE 12

ν_{CN}	$d\nu/dp$ (cm^{-1} $kbar^{-1}$) [146]
KCN I	0.50 (20°C)
KCN I	0.574 (110°C)
KCN III	0.45 (110°C)
KCN IV	0.32 (20°C)
NaCN II	0.57

results are consistent with a unit cell of high occupancy and low symmetry.

$AgNO_3$ has also been investigated at high pressure [148]. Adams and Sharma [148] have studied phases I, II, III and metastable phase V. In the latter phase doublets occur in ν_4, ν_1 and ($\nu_1 + \nu_4$) regions, and with the shape of the ν_3 envelope are all indicative of a low site symmetry and relatively high unit cell occupancy.

The first solid studied in the DAC was calcite, $CaCO_3$ [149]. The results showed that ν_1, normally IR inactive, appeared in the spectrum with pressure; ν_2 shifted from 882 to 865 cm^{-1} and splitting of ν_4 occurred. Other studies were made with calcite up to 61 kbar. The authors pointed out that the spectra at higher pressures resembled that of a calcium carbonate polymorph, vaterite, with a hexagonal unit cell containing 2 or more molecules per unit cell. Fong and Nicol [150] have studied $CaCO_3$ to 40 kbar, and have interpreted their data in terms of two phases of calcite, II and III, occurring at 14 kbar and 18 kbar. Recent Raman spectra have verified that the high pressure phases are not aragonite [151]. Only superficial studies have been made with aragonite and $MgCO_3$ under pressure [48].

(4) $NaNO_2$ and KNO_2

Infrared spectra of KNO_2 and $NaNO_2$ and Raman spectra of the polymorphs of KNO_2 have been studied at high pressures [152,153]. $NaNO_2$ (C_{2v}^{20}, $z = 1$) undergoes a phase transition at 39°C and 10 kbar and KNO_2 undergoes a transition at 6.3 kbar. In the IR studies it was determined that the symmetric modes lose intensity with pressure and all bands undergo blue shifts. The Raman studies have led to conclusions concerning the nature of the polymorphs and the order-disorder in these phases.

(5) Dihydrogen phosphates

The paraelectric crystals of KH_2PO_4 and RbH_2PO_4 were studied by IR at pressures to 60 kbar [154]. For both compounds the protons were found to be dynamically disordered between the two possible O·H···O sites connecting the PO_4^{3-} groups. A new phase was found at 10 kbar in which the hydrogens became ordered while the PO_4^{3-} tetrahedra became disordered. In pressure