Foreword

The simple van der Waals solids that crystallize at low temperatures are called cryocrystals in the recent years. They include monatomic cryocrystals of neon, argon, krypton, and xenon, and simple molecular crystals with various types of noncentral intermolecular interaction, such as hydrogen, nitrogen, oxygen, fluorine, carbon monoxide and dioxide, nitrogen monoxide (quadrupole interaction); methane, silane, and their deuterated forms (octupole interaction); ammonia, hydrogen sulfide (dipole interaction, hydrogen bonds), etc. Because of the relative simplicity of these substances, they can easily be considered theoretically and are frequently used as model objects for solving fundamental problems of solid state physics such as lattice dynamics, phase transformations, impurity effects, etc.

Cryocrystals also include a group of substances with special properties – quantum crystals of helium and hydrogen – in which the zero-point energy of their molecules is comparable with the energy of intermolecular interaction. Quantum properties are also exhibited by the rotational subsystem of solid methane. Unique properties are also characteristic of solid oxygen, which combines the properties of a molecular crystal and a magnetic material.

In recent years, cryocrystals find growing practical application in the cryogenic, space, laser, high-pressure technologies, nuclear physics, and other fields of science and technology.

By the time of this writing, a vast body of experimental data on the physical properties of cryocrystals were accumulated, which were published not only in original papers, but also in numerous textbooks and handbooks. The most com-

prehensive report on the properties of monoatomic cryocrystals was given in Klein, M. L., and Venables, J. A., (Eds.), *Rare Gas Solids*, London, Academic, vol. 1 (1976) and vol. 2 (1977); the properties of molecular cryocrystals were considered in most detail in the textbooks of Verkin, B. I., and Prikhot'ko, A. F., (Eds.), *Cryocrystals*, Kiev, Naukova Dumka (1983) and Manzhelii, V. G., and Freiman, Yu. A., (Eds.), *Physics of Cryocrystals*, New York, AIP (1996). Special handbooks were devoted to idividual substances, e.g., Roder, H. M., et al., *Survey of the Properties of the Hydrogen Isotopes below Their Critical Temperatures*, NBS, Technical Note 641, U. S. Government Printing Office, Washington, DC (1973); Eselson, B. N., et al., *Svoistva zhidkogo i tverdogo geliya* (*Properties of Liquid and Solid Helium*), Kiev, Naukova Dumka (1978); Sauers, P. S., *Cryogenics Hydrogen Data Pertinent to Magnetic Fusion Energy*, Lawrence Livermore Laboratory (1979); Eselson, B. N., et al., *Svoistva zhidkogo i tverdogo geliya. Rastvory* ^{3}He–^{4}He (*Properties of Liquid and Solid Helium*: ^{3}He–^{4}He Solutions), Kiev, Naukova Dumka (1982); Verkin, B. I., et al., *Properties of Condensed Phases of Hydrogen and Oxygen*, New York, Hemishere (1990).

With the above in mind, we devoted this hanbook to those cryocrystals that, although they are of a significant research and applied interest, have not yet been described in sufficient detail in modern reference books.

In this handbook, we analyze and systematize the results of studies on the structures, phase diagrams, P–V–T data and thermophysical properties (thermal expansion, heat capacity, thermal conductivity, heats of phase transitions, vapor pressures, compressibilities) of cryocrystals such as nitrogen, carbon monoxide and dioxide, oxygen, fluorine, nitrogen monoxide, hydrogen sulfide, methane, and deuterated methanes. Some principal information on the molecules and properties of substances considered in this handbook are given in Table 1.

When compiling this handbook, we partly took into account materials that were published in the first two monographs mentioned above, but in the major cases we used the data of original works. Quantitative experimental data are mainly represented in the form of tables, and the general dependences of physical properties on thermodynamic parameters are shown in figures. The values that are given in tables represent either generalized experimental data of several investigations or the results of a single most detailed and reliable work. In those cases where the accuracy of measurements is not sufficient or no tabulated data are given in the original work, we only give experimental data in the form of graphs. In those cases where no preference could be given to any of the works available, the tables contain values obtained by different authors. When analyzing the results for some substances (nitrogen, hydrogen sulfide, methane), large attention was paid to isotopic effects, which are of special interest from the physical viewpoint.

Table 1 Principal physical parameters of simle molecules and cryocrystals

Parameter	$^{14}N_2$	$^{15}N_2$	CO	O_2	F_2	N_2O	CO_2	CH_4	CD_4
Molecular weight M, a.m.u.	28.0134	30.03073	28.01055	31.9988	37.9968	44.0128	44.00995	16.04303	20.07491
Molecule symmetry	$D_{\infty h}$	$D_{\infty h}$	$C_{\infty v}$	$D_{\infty h}$	$D_{\infty h}$	$C_{\infty v}$	$D_{\infty h}$	T_d	T_d
Equilibrium bond lenth, Å	1.0977	1.0977	1.1283	1.207	1.4177	N–N 1.1282 N–O 1.1842	1.1599	C–H 1.1014 H–H 1.803	C–D 1.0986 D–D 1.801
Dipole moment D, 10^{-18} esu	–	–	0.112	–	–	0.166	–	–	–
Quadrupole moment Q, 10^{-26} esu	–1.4	–	–2.5	–0.39	–0.88	–3.0	–4.3	–	–
Octupole moment I,10^{-34} esu	–	–	–	–	–	–	–	+4.5	+4.3
Averaged polarizability α, Å	1.767	–	1.977	1.60	–	3.0	2.63	2.60	2.60
Anisotropy of polarizability k	0.1313	–	0.0897	0.2375	–	0.329	0.2664	–	–
Rotational constant B, K	2.8751	2.6840	2.7787	2.081	1.27	0.60592	0.56355	7.56	1.89
Parameters of the 6–12 Lennard–Johnes potential									
ε, K	91.5	91.5	110.0	125.0	116.0	220.0	190.0	148.2	148.2
σ, Å	3.681	3.681	3.590	3.136	3.153	3.879	3.996	3.817	3.817
Nearest-neighbor spacing at $T = 0$ K, r_0, K	3.994	3.990	3.993	3.134	2.979	3.988	3.927	5.858	5.768
Debye temperature at $T = 0$K, Θ_D, K	83.6	81.3	103.3	104.5	110.0	141.0	151.8	141.0	138.0