substance: Nb_2O_5
property: crystal structure, lattice parameters, density of H-Nb_2O_5

crystal structure: monoclinic, space group C_2^1 – P2 [64G], C_{2h}^1 – P2/m [76K], Z = 14.

This is the stable form at high temperatures (T > 1100°C). The idealized structure is shown in Fig. 1, The major difference from the preceding structure is the presence of tetrahedrally coordinated Nb. These tetrahedral sites lie in tunnels and 1/2 of the available sites are occupied in H-Nb_2O_5. Detailed unit cell projection: Fig. 2.

lattice parameters

a	21.16 Å	RT		64G
b	3.822 Å			
c	19.35 Å			
β	119.8°			
a	21.153 Å			76K
b	3.8233 Å			
c	19.356 Å			
β	119.80°			
a	21.1848 $\cdot(1+0.56328\cdot10^{-5}T)$ Å	T = 273...1273 K	from thermal expansion (T in K)	72M, 73D
b	3.8236 Å (not dependent on T)			
c	19.3680 $\cdot(1+0.58856\cdot10^{-5}T)$ Å			
β	119.63 $\cdot(1+0.26456\cdot10^{-5}T)^o$			
V	$1363.4\cdot(1+0.880152\cdot10^{-5}T)$ Å^3			

density

d_{calc}	4.55 g cm^{-3}	64G

interatomic distances
(in Å) [76K]

Nb atom	Surrounding oxygens and distances to them				Mean Nb – O distance
Nb(1)	O(19^{iv})	1.838(5)	O(19^{ii})	1.838(5)	1.826
	O(21)	1.813(4)	O(21^{viii})	1.813(4)	
Nb(2)	O(2)	1.9116(2)	O(2^{ii})	1.9116(2)	1.968
	O(9)	2.005(5)	O(9^{v})	2.005(5)	
	O(11)	1.986(5)	O(11^{v})	1.986(5)	
Nb(3)	O(5)	1.775(4)	O(7)	1.973(5)	2.006
	O(18^{iv})	2.327(3)	O(19^{iv})	1.989(6)	
	O(34^{iii})	1.986(1)	O(34iv)	1.986(1)	
Nb(4)	O(3)	2.267(4)	O(5)	2.112(4)	2.006
	O(6)	1.872(4)	O(8)	1.801(5)	
	O(24)	1.991(1)	O(24^{ii})	1.991(1)	
Nb(5)	O(4)	2.269(4)	O(6)	1.954(4)	1.999
	O(9)	1.807(5)	O(15^{v})	2.001(3)	
	O(25)	1.982(1)	O(25^{ii})	1.982(1)	

Nb(6)	O(7)	1.866(5)	O(10)	1.753(4)	2.051
	O(12)	2.194(4)	O(16^{iv})	2.479(3)	
	O(26)	2.007(1)	O(26^{ii})	2.007(1)	
Nb(7)	O(8)	2.023(5)	O(10)	2.226(4)	1.987
	O(11)	1.824(5)	O(13)	1.991(5)	
	O(27)	1.930(1)	O(27^{ii})	1.930(1)	
Nb(8)	O(12)	1.865(4)	O(12^{iv})	2.340(3)	2.034
	O(14)	1.769(4)	O(16)	2.258(4)	
	O(28)	1.986(1)	O(28^{ii})	1.986(1)	
Nb(9)	O(13)	1.808(5)	O(14)	2.154(4)	2.003
	O(15)	1.830(4)	O(17)	2.243(4)	
	O(29)	1.992(1)	O(29^{ii})	1.992(1)	
Nb(10)	O(3)	1.983(1)	O(3')	1.983(1)	1.992
	O(21)	2.034(5)	O(23)	1.868(4)	
	O(24)	2.242(4)	O(36)	1.843(5)	
Nb(11)	O(4)	1.982(1)	O(4^{i})	1.982(1)	1.997
	O(22)	1.801(5)	O(23)	1.949(4)	
	O(25)	2.269(4)	O(31^{v})	2.000(5)	
Nb (12)	O(16)	2.013(1)	O(16^{i})	2.013(1)	2.018
	O(26^{iv})	2.276(4)	O(28)	2.230(4)	
	O(30)	1.774(4)	O(32)	1.801(4)	
Nb(13)	O(17)	1.987(1)	O(17^{i})	1.987(1)	1.999
	O(29)	2.225(4)	O(30)	2.130(4)	
	O(31)	1.836(4)	O(33)	1.831(5)	
Nb(14)	O(18)	1.974(1)	O(18^{i})	1.974(1)	2.000
	O(32)	2.034(4)	O(34)	2.281(4)	
	O(35)	1.769(4)	O(36^{vi})	1.966(5)	
Nb(15)	O(1^{v})	1.887(1)	O(20)	1.920(1)	1.972
	O(20^{i})	1.920(1)	O(22^{vi})	2.027(5)	
	O(33)	1.974(5)	O(35)	2.103(4)	

Symmetry code

(i)	*x*,	1+*y*,	*z*:	(ii)	*x*,	–1+*y*,	*z*;
(iii)	1–*x*,	–1+*y*,	–*z*;	(iv)	1–*x*,	*y*,	–*z*;
(v)	1–*x*,	*y*,	1–*z*;	(vi)	1+*x*,	*y*,	*z*;
(vii)	–1+*x*,	*y*,	*z*;	(viii)	–*x*,	*y*,	–*z*.

The interconversion of B, T and H-forms has been investigated under pressure in the temperature range RT...1300^{o}C [72T]

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Fig. 1.

H–Nb_2O_5. Idealized structure [70W]. Full circle: are the Nb atoms in tetrahedral sites in the tunnels.

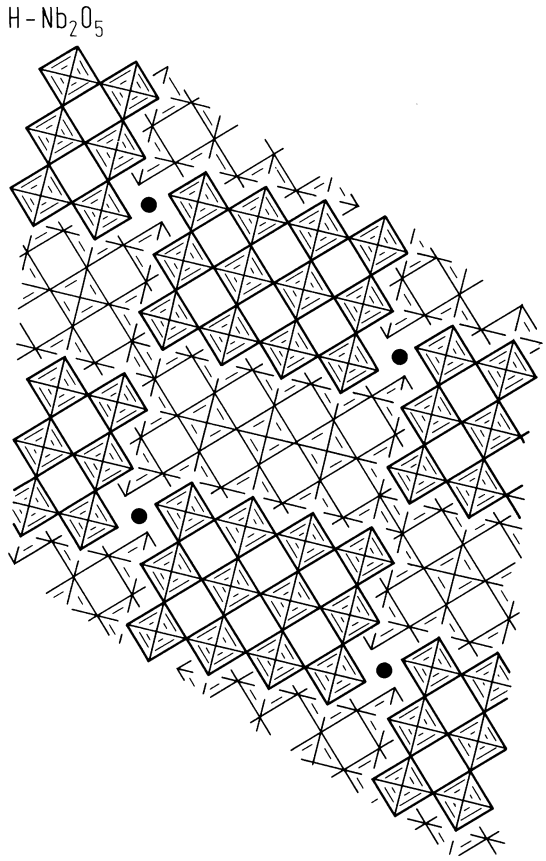

Fig. 2.

H-Nb_2O_5. Details of the projected unit cell [76K].