

Table 3 Vibrational frequencies (10^{12} c/s)

Symmetry direction			Longitudinal frequencies				Transverse frequencies				
			Optical mode		Acoustic mode		Optical mode		Acoustic mode		
<i>q</i>	<i>q</i>	<i>q</i>									
0.2	0	0	4.4625	(4.50)	0.6786	(0.69)	2.4207	(2.44)	0.4122	(0.40)	
0.4	0	0	4.3862	(4.26)	1.2432	(1.22)	2.4625	(2.47)	0.5972	(0.58)	
0.6	0	0	3.8126	(3.69)	1.6208	(1.56)	2.4954	(2.49)	0.7308	(0.76)	
0.8	0	0	3.2050	(3.02)	1.6021	(1.59)	2.4987	(2.50)	0.7708	(0.76)	
1	0	0	4.0285		1.4327	(1.45)	2.5032	(2.50)	0.8382	(0.82)	
0.2	0.2	0	4.1876	(4.01)	0.7892	(0.81)	T ₁ 2.3302	(2.38)	0.5369	(0.52)	
							T ₂ 2.4602	(2.44)	0.2689	(0.40)	
0.4	0.4	0	3.8702	(3.89)	1.4362	(1.41)	T ₁ 2.4295	(2.44)	0.8289	(0.83)	
							T ₂ 2.5434	(2.52)	0.6342	(0.70)	
0.6	0.6	0	3.5206	(3.74)	1.5021	(1.54)	T ₁ 2.4596	(2.45)	0.8259	(0.94)	
							T ₂ 2.5687	(2.53)	1.3021	(1.19)	
0.1	0.1	0.1	4.3858	(4.54)	0.5416	(0.54)	2.4205	(2.38)	0.3252	(0.32)	
0.2	0.2	0.2	4.4062	(4.41)	0.9082	(0.91)	2.4354	(2.43)	0.5304	(0.52)	
0.3	0.3	0.3	4.3708	(4.36)	1.3455	(1.33)	2.4385	(2.43)	0.7908	(0.76)	
0.4	0.4	0.4	4.3438	(4.30)	1.6302	(1.59)	2.5002	(2.46)	0.8994	(0.87)	
0.5	0.5	0.5	4.2802	(4.24)	1.6442	(1.59)	2.5488	(2.53)	0.8740	(0.85)	

Values in parentheses are experimental values¹¹.

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REVISED VAN DER WAALS RADIUS FOR HYDROGEN

R. SRINIVASAN, MEENA HARIHARAN and J. VIJAYALAKSHMI

Department of Crystallography and Biophysics, University of Madras, Madras 600 025, India.

THE availability of a large amount of crystallographic structural data through the Cambridge structural data base has been used for a variety of purposes. In particular, since the data base also covers structures analysed by neutron diffraction, the precise location of hydrogens in such studies has led to interesting analyses, such as C-H...O, C-H...N type of hydrogen bonds¹ and revision of C-H bond lengths, precise molecular geometry and related features². More recently, Nyburg and Faerman³ reported the effective non-bonding (van der Waals) shapes of non-metallic elements such as N, O, F, S, Cl, Se, Br and I atoms.

The value currently in use⁴ for the van der Waals radius of hydrogen is 1.2 Å and even in the discussion of the C-H...X type of hydrogen bonds, this value is being used in the literature¹.

A survey of non-bonded H...H contact distances from organic structures was carried out using the

Cambridge structural data files up to May 1986 updates. A preliminary survey involving both X-ray and neutron diffraction data indicated that there were more than 300 distances with d less than 2.4 Å. It was therefore felt adequate to examine those with d less than 2.2 Å. This screening led to 46 compounds with neutron diffraction data alone having 55 contacts with $d < 2.2$ Å. Some of the structures were discarded with the following criteria (a) those with R -factor $> 12\%$, (b) those involving disorder and (c) those with more than two heavy atoms in the case of coordination compounds.

This reduced the set to 31 structures with 41 distances less than 2.2 Å. These are given in table 1. It may be noticed that the values are as low as 2 Å (table 1). It is clear that in this case that the hydrogens are attached to oxygen atoms and obviously the hydrogens are likely to carry effective charge on them.

To arrive at the minimum contact distance for neutral hydrogen (i.e. with nil charge) we may ignore all cases excepting when both X and Y are carbon atoms in table 1. Even here, we notice that the values range from 2.05 Å onwards. Some of these occur with X and Y as part of the ring systems. The choice can be narrowed down still further by demanding that both carbons should belong to methyl groups or atleast linear aliphatic chain. There are four such distances with values 2.18, 2.15, 2.19 and 2.12 Å. It would seem prudent to take the average of these which works out to 2.16 Å as the most optimum distance d for H...H contact. The effective charge on these groups is assumed to be zero. This establishes conclusively that the van der Waals radius 1.2 Å for hydrogen normally used in literature is on the high side and a value of 1.08 Å which is about 10% less than the conventional value is to be preferred.

Table 1 List of compounds with H...H contact distance (d) less than 2.2 Å. The symbols X and Y refer to the attached groups in X-H....H-Y

Compound	Reference	X,Y	Remarks	d (Å)
(1,10-phenanthroline)-tetra-deuteroborotriphenyl phosphine copper(I)	<i>Inorg. Chim. Acta.</i> , 1984, 83 , 177.	C,C	Both carbons on aromatic ring	2.05
4,4'-Bis (dimethyl amino) diphenyl ammonium iodide	<i>Acta Crystallogr.</i> , 1984, C40 , 1055.	N,C	Imino nitrogen and carbon	2.14
		N,C	On aromatic ring	2.14
β -L-arabinose	<i>Acta Crystallogr.</i> , 1977, B33 , 3033.	C,C	Both carbons on aliphatic rings	2.16
2,2'-(ethylene diamino)bis (2-methyl-3-butanone oximato)nickel (II) perchlorate	<i>Acta Crystallogr.</i> , 1978, B34 , 436.	C,C	Both methyl carbons of aliphatic chain	2.18
(Tetrahydroborato-H,H')-(terpyridine)-cobalt	<i>Inorg. Chem.</i> , 1982, 21 , 192.	C,C	Both carbons on aromatic rings	2.20
Aqua-manganese(II) acetate hexahydrate	<i>Acta Crystallogr.</i> , 1977, B33 , 1357.	C,C	Both carbons on methyl groups	2.15
Ammonium oxo-bis (oxalato)-diaquo-niobium (v) trihydrate	<i>J. Less-Common Met.</i> , 1977, 51 , 259.	O,O	Both oxygens belong to water	2.18
Cyclodecane 1,6 trans diol	<i>Acta Crystallogr.</i> , 1973, B29 , 2278.	C,C	Both carbons on cyclo ¹⁰ decane ring	2.13
Aqua (L-glutamato) cadmium (II) hydrate	<i>Acta Crystallogr.</i> , 1977, B33 , 801.	O,O	Both oxygens belong to water	2.16
Copper (II) formate tetrahydrate	<i>Ferroelectrics</i> , 1972, 4 , 147.	O,O	Both oxygens belong to water	2.19
		O,O	Both oxygens belong to water	2.07
		O,O	Both oxygens belong to water	2.01
		O,O	Both oxygens belong to water	2.00
L-cysteic acid monohydrate	<i>Acta Crystallogr.</i> , 1973, B29 , 1167.	O,O	One oxygen on hydroxyl group and the other on water	2.12

Contd. . . .

(Table 1 contd.)

Ferrocene	<i>Acta Crystallogr.</i> , 1979, B35, 1074.	C,C Both carbons on cyclopentadienyl ring	2.18
β -D-Fructopyranose	<i>Acta Crystallogr.</i> , 1977, B33, 3510.	O,O Both oxygens on hydroxyl groups	2.13 2.18
Glycyl-glycine hydrochloride monohydrate	<i>Acta Crystallogr.</i> , 1972, B28, 2083.	O,O One oxygen on hydroxyl group and the other on water.	2.20
Glycolic acid	<i>Acta Crystallogr.</i> , 1971, B27, 333.	O,O Both oxygens belong to hydroxyl groups	2.11 2.20
Bis (Mu-2-hydroxo)-aqua-bis (2,2'-bipyridine)-sulfanato dicopper (II) tetrahydrate	<i>J. Chem. Soc., Dalton</i> , 1983, 703.	O,O Both oxygens belong to water	2.13
Potassium D-gluconate monohydrate	<i>Acta Crystallogr.</i> , 1974, B30, 1421.	C,C Both carbons on aliphatic chains	2.19
L-ascorbic acid	<i>Acta Crystallogr.</i> , 1968, B24, 1431.	O,O Both oxygens on hydroxyl groups	2.17
L-threonine	<i>Pramana, (J. Phys.)</i> , 1973, 1, 247.	C,O Both on aliphatic chain	2.17
β -L-lyxopyranose	<i>Acta Crystallogr.</i> , 1978, B34, 3809.	O,O Both on hydroxyl groups	2.19
Methyl- β -D-ribose pyranoside	<i>Acta Crystallogr.</i> , 1978, B34, 188.	O,O Both on hydroxyl groups	2.19
Methyl- α -D-galactopyranoside-monohydrate	<i>Acta Crystallogr.</i> , 1979, B35, 902.	O,O Both on hydroxyl groups O,O One on hydroxyl group and the other on water	2.18 2.19
Methyl- α -D-glucose pyranoside	<i>Acta Crystallogr.</i> , 1977, B33, 728.	C,C Both on aliphatic ring	2.20
Oxalic acid dihydrate	<i>Acta Crystallogr.</i> , 1969, B25, 2437.	O,O One oxygen belongs to carboxyl group and the other to water	2.06
Pyrene	<i>Acta Crystallogr.</i> , 1972, B28, 2977.	C,C Both on aromatic rings	2.07
Sucrose	<i>Acta Crystallogr.</i> , 1973, B29, 790.	O,O Both on hydroxyl groups O,O Both on hydroxyl groups	2.17 2.19
Bis(cyclopentadienyl) trihydrido tantalum	<i>J. Am. Chem. Soc.</i> , 1977, 99, 1775.	C,C Both carbons on cyclopentadienyl rings	2.12
Dialuric acid monohydrate	<i>Acta Crystallogr.</i> , 1969, B25, 1970.	O,O One of water and the other of hydroxyl group	2.19
Potassium hydrogen bis(acetylsalicylate)	<i>J. Mol. Struct.</i> , 1968, 1, 283.	C,C Both of aliphatic ring	2.17
Potassium hydrogen mesotartrate	<i>J. Chem. Soc., Perkin</i> 1975, 2, 1549.	C,O Both on aliphatic chain	2.07
(3,3'-Dimethyl-3,3'-(2-Nitropropanediylidene diamino)-bis (2-butanone-oximato)-N,N',N'',N''')-nickel (II)	<i>Acta Crystallogr.</i> , 1981, B37, 347.	C,C Both carbons on methyl groups	2.12

This downward revision is naturally relevant to the discussion of hydrogen bond in the literature involving the C-H group⁵. In particular, these have figured in the discussion of biomolecular structures, including amino acids^{1,6} and nucleic acids⁷ and others⁵.

A glance at table 1 indicates that among other distances listed, there are a number of cases with X, Y both as oxygens. In particular there are about five cases of d ranging from 2 to 2.13 Å with an average of 2.07 Å when both X and Y are water oxygens. This is clearly attributable to the fact that there is

effective charge of 0.3e on water protons.

A more detailed analysis on the effect of the charge on the hydrogen radius is in progress and the details will be reported later.

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SERUM ELECTROLYTES LEVELS IN RELATION TO THE PROGRESSION OF DIFFERENT TRANSPLANTED TUMOURS IN MICE MODEL SYSTEM

ARCHANA SENGUPTA, RANJIT MALLICK, SANTI RANJAN DUTTA and RATHIN SARKAR

Department of Experimental Carcinology, Chittaranjan National Cancer Research Centre, Calcutta 700 026, India.

ELECTROLYTES play an important role in cell division, cellular proliferative process as well as in other biological and biochemical functions¹⁻³. The extra- and intracellular concentrations of electrolytes and their transport as well as intracellular sequestration system appeared to have immense role in the above process. Alteration of intracellular concentrations of sodium and potassium of different tumour cells has been documented⁴. However, there is hardly any report regarding the levels of serum electrolytes in relation to the progression of tumour. It is therefore, of considerable interest to examine the serum electrolytes in animal model system using different types of transplanted tumours with a view to understanding the relationship between the levels of serum electrolytes and the

progression of different transplanted tumour systems following transplantation.

Normal Swiss mice of different tumour models were used for the study. The tumour involved Dalton's lymphoma (Lymphoma) Sarcoma-180 (S-180) and Ehrlich's carcinoma. The mice were 7-8 weeks of age with body weight ranging from 16 to 25 g (mean weight 20 ± 3.9 g).

Originally, lymphoma was found as a spontaneous thymal tumour of DBA mice and later this tumour line was maintained in the ascites form by serial *in vivo* transfer of tumour cells (1:1) in adult Swiss mice for a long time. S-180 and Ehrlich's carcinoma were also maintained in ascites form by serial *in vivo* transfer of tumour cells in adult Swiss mice.

Different batches of animals were used for the present experiments and the mice were given transplantation i.p. with 1×10^6 S-180, Ehrlich's carcinoma and lymphoma cells per mouse. Blood was collected from tumour-bearing mice by direct cardiac puncture on 5th, 10th and 20th day following transplantation of tumour cells under ether anaesthesia. Serum was separated by centrifuging the blood at 500 g for 15-20 min. Blood was collected from normal Swiss mice following the same procedure on 5th, 10th and 20th day and served as controls. Serum levels of sodium and potassium were performed with flame photometer using commercial standards⁵. For statistical analysis, student's *t* test was done.

Levels of serum electrolytes in relation to the progression of different transplanted tumours exhibited interesting pictures (tables 1 and 2). However, progression of tumour was evaluated on the basis of tumour cell count during the days of tumour progression (table 3). It is evident from table 1 that

Table 1 Serum sodium level (mmol/l) in mice-bearing sarcoma-180 Ehrlich's carcinoma and lymphoma in relation to different days of tumour progression following transplantation of tumour cells

Days of tumour progression	Sarcoma	Carcinoma	Lymphoma	Control
5th	145.2 ± 6.17	120.12 ± 4.9	112.04 ± 6.29	142 ± 3.2
10th	143.12 ± 6.86	116.16 ± 3.47	107.08 ± 5.45	143.0 ± 3.2
20th	143.32 ± 7.91	110.04 ± 4.0	101.2 ± 4.2	143.12 ± 4.39

The number of animals used is 25 and the values are mean \pm SD.