

8. Watts, J. D. and Dupuis, M., *J. Comp. Chem.*, 1988, 9, 158.
9. Covick, L. A. and Sando, K. M., *J. Comp. Chem.*, 1990, 11, 151.
10. 3L Parallel FORTRAN user guide, INMOS, 1989.
11. Duke, A. J., *Chem. Phys. Lett.*, 1972, 13, 76.
12. Raffanetti, R. C., *Chem. Phys. Lett.*, 1973, 20, 335.

ACKNOWLEDGEMENTS. We thank C-DAC, Pune, for provid-

ing their parallel computation facility and for funding this venture. We used the 'MOLECULE' code (a Stockholm Institute of Physics program system) for the basic routines required in two-electron integral calculation.

Received 18 February 1991, revised accepted 18 June 1991

Fast solid-state reactions between bifluorides and vanadates at ambient temperature

B. N. Wani, S. J. Patwe and U. R. K. Rao

Applied Chemistry Division, Bhabha Atomic Research Centre, Bombay 400 085, India

We have examined solid-state reactions occurring at room temperature at a fast rate across an interface between NH_4 /alkali metal bifluorides and NH_4 /alkali metal vanadates resulting in the formation of oxyfluoro-compounds in various reaction configurations from the point of view of delineating the mechanism of the reaction, nature of the products formed, and kinetics of the reaction. The reaction, initiated by moisture, always progresses from the bifluoride into the vanadate by transport of the bifluoride across an ever-growing layer of the product, and the product invariably contains the new compound with a stoichiometry of 1:2 in vanadate to bifluoride. We have also determined relative reaction rates.

MANY solid-state reactions, such as those used in the formation of ferrites, alloys, etc., have measurable reaction rates at temperatures much higher than the ambient temperature. This is because such reactions are diffusion-controlled and the diffusion rates are negligibly small at ordinary temperatures. Reactions between solids are complex and reactivity depends on several factors. For instance, the rate of reaction between two single crystals¹ of MgO and TiO_2 at 1550°C depends on the faces of the two crystals that are in physical contact with each other. KHF_2 is known to exist in two polymorphic phases, one tetragonal at $T < 198^\circ\text{C}$ and the other cubic at $T > 198^\circ\text{C}$. Recently, in some other context, we found that the tetragonal form of KHF_2 does not react with Nb_2O_5 even after three hours of heating at 180°C , whereas the cubic form reacts readily at 210°C . Hellstern and Schultz² found that Fe and Zr react to form alloys at room temperature by ball milling, but the products were amorphous. Goyal *et al.*³ reported that orthorhombic-V modification of Na_2SO_4 trans-

forms into another, orthorhombic-III, modification of Na_2SO_4 by grinding at room temperature. During the last decade several examples⁴⁻⁹ have been found by our group and by others¹⁰, in which two (or three) solids, when mixed at room temperature and on application of mechanical force such as grinding with a pestle in an agate mortar, form a new compound in a single phase. Such reactions take place in the solid state readily at ambient temperature without necessity of heating and with such ease as though they are taking place in solution. The product is crystalline. The structure of the product is totally different from that of either reactant. Recently we showed¹¹ that two crystalline solids, one a bifluoride and the other a vanadate, even without grinding, interact at room temperature by merely keeping in contact with each other at an interface and form a third crystalline solid at the interface. The structure of the product is totally different from that of either of the reactants. A preliminary report of this was made in ref. 11. It is difficult to rationalize this observation. The formation of the product involves change of symmetry, translation of atoms, breaking of bonds and making of new linkages, all taking place with almost no additional energy externally supplied above the thermal energy $k_B T$. Here we describe experiments aimed at identification of the reaction products and determination of the kinetics of these reactions. Experiments have also shown that the synthesis proceeds through catalytic initiation by traces of moisture.

Methods

The chemicals used were NH_4HF_2 (Riedel), NaHF_2 (IR grade), KHF_2 (BDH, AR grade), NH_4VO_3 (AR

grade) and NaVO_3 (GR). KVO_3 was prepared by heating in air a mixture of K_2CO_3 and V_2O_5 at 600 C for a few hours.

In order to study the nature and kinetics of the reaction between a given bifluoride and a vanadate, different reaction configurations were employed. Various combinations of rods, pellets and powders were used in this study. The rods pellets were obtained by cold pressing the powders directly from the reagent bottles (without grading into any particular particle sizes) in a die plunger system at 4000 kg cm^{-2} .

The configurations used were of two types. In the first, shown in Figure 1,a, the bifluoride rod (6 mm dia

and about 8 mm high) was plugged into a loosely packed powder of the vanadate and left standing. The top view of this arrangement before and after the commencement of the reaction is shown in Figure 1,b & c. As the reaction progresses, a coloured ring of the product concentric with the bifluoride rod spreads on to the vanadate powder and the ring diameter increases with time.

In the second arrangement, shown in Figure 1,d, first a 6-mm-dia and 10-mm-high bifluoride pellet was introduced into the annular space of a 12-mm-dia die and then the vanadate powder was poured around and above the bifluoride pellet but not below it. By pressing this powder, a composite pellet of vanadate encompassing the bifluoride was obtained. In this composite pellet, the top surfaces of the outer and inner pellets are flush with each other. The top view of this pellet, before and after the reaction sets in, is shown in Figure 1,e & f. Here also, as time advances, formation and growth of a coloured ring of the product, concentric with the inner pellet, are noticed. The rate of increase in the thickness of the coloured band with time is monitored by means of a travelling microscope.

The pairs of reactants studied in configuration II are given in Table 1, along with the products formed at the interface.

Knowing the dimensions and weights of the materials in the inner as well as in the composite pellet, the green densities of the two reactants in the composite pellet were estimated. The estimated densities in a typical composite pellet are 1.40 g cm^{-3} for NH_4HF_2 and 1.50 g cm^{-3} for the NH_4VO_3 , and, taking the theoretical densities to be 1.50 g cm^{-3} and 2.32 g cm^{-3} for the two solids, the packing efficiencies are 93% and 65% in NH_4HF_2 and NH_4VO_3 respectively.

The coloured product formed in all cases of pairs of reactants in configurations I and II were carefully scooped out and their powder X-ray diffraction (XRD) patterns recorded on a Philips automatic powder diffractometer, model PW 1820, using nickel-filtered CuK_α radiation. For a given pair of reactants, the XRD patterns of materials scooped from both the configurations are identical.

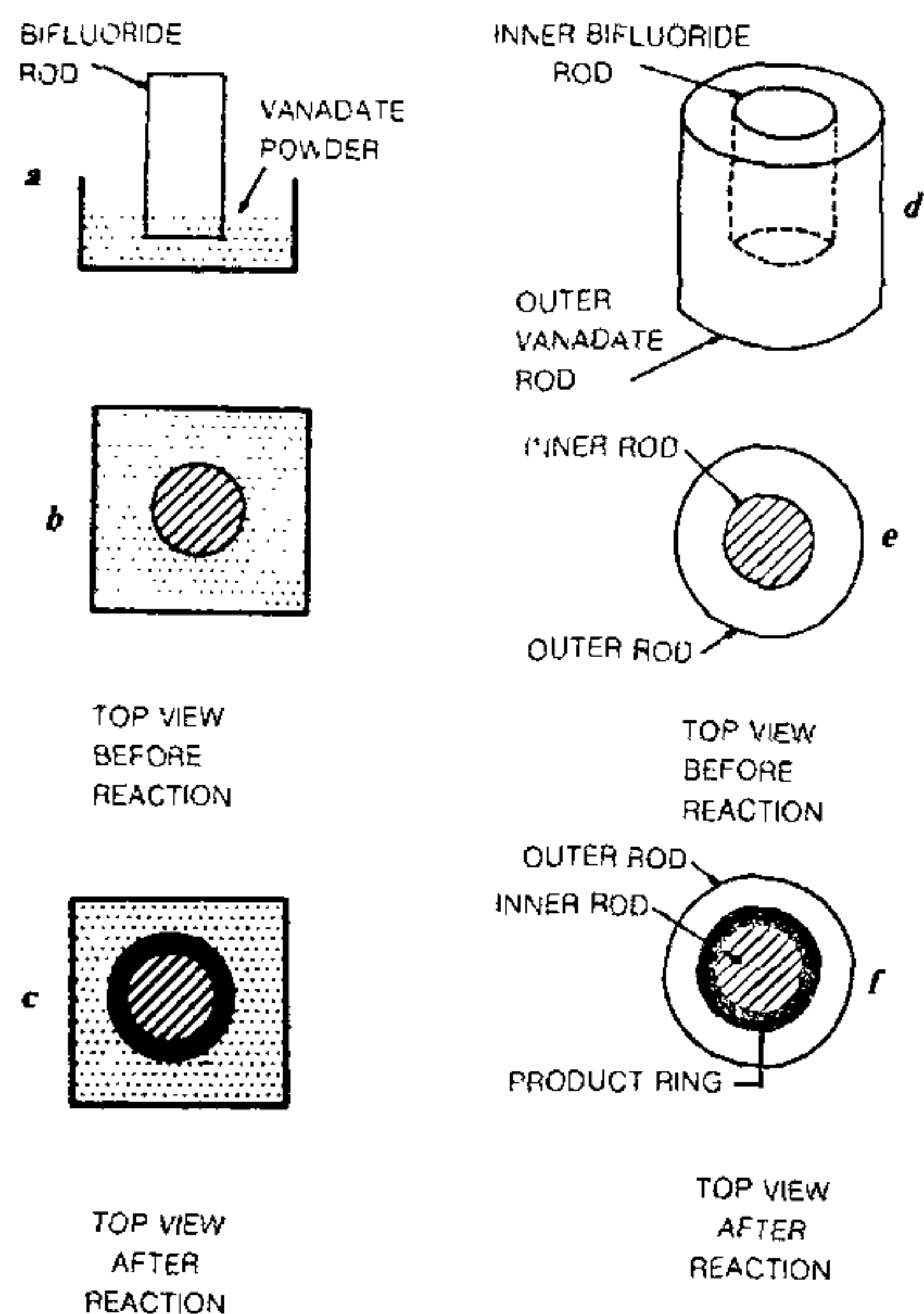


Figure 1. Reaction configurations (configuration I shown in a, configuration II shown in d,) employed for solid-state reaction between bifluorides and vanadates.

Table 1. Reactants and products of solid-state reaction in configuration II

Inner rod	Powder/ outer rod	Product at interface	Technique	(ref)	System
NH_4HF_2	NH_4VO_3	$[\text{NH}_4]_3 \text{VO}_2\text{F}_4$	Solution	(12)	Orthorhombic
NaHF_2	NH_4VO_3	$[\text{NH}_4] \text{Na}_3 \text{VO}_2\text{F}_4$	Grinding	(*)	Tetragonal
KHF_2	NH_4VO_3	$[\text{NH}_4] \text{K}_2 \text{VO}_2\text{F}_4$	Grinding	(*)	Orthorhombic
NH_4HF_2	NaVO_3	$[\text{NH}_4]_2 \text{NaVO}_2\text{F}_4$	Grinding	(4)	Cubic
NaHF_2	NaVO_3	$\text{Na}_3 \text{VO}_2\text{F}_4$	Solution	(12)	Orthorhombic
KHF_2	NaVO_3	$\text{NaK}_2 \text{VO}_2\text{F}_4$	High temp.	(13,*)	Cubic
NH_4HF_2	KVO_3	$[\text{NH}_4]_2 \text{KVO}_2\text{F}_4$	Grinding	(*)	Orthorhombic
KHF_2	KVO_3	Not identified			

*Present work

Initiation of the reaction

In view of the hygroscopic nature of ammonium bifluoride, it is quite natural to expect that moisture may play a role in initiating the reaction between the two reactants. The following experiments were conducted to ascertain the role of moisture: (i) The two reactants, NH_4HF_2 and NH_4VO_3 , were separately dried under different conditions, and then mixed in 1:2 ratio. Drying over silica gel or P_2O_5 and mixing the reactants together under a nitrogen blanket brought about the reaction immediately with the formation¹² of $[\text{NH}_4]_3\text{VO}_2\text{F}_4$. (ii) When the two reactants were dried by individually pumping them under a running vacuum of 10^{-3} torr (0.13 pascal), and mixed under vacuum and agitated together, there was no reaction even after half an hour of mixing. The reaction was initiated instantaneously when the vacuum was released to traces of moisture for about 30 sec; the mixture turned yellow and the reaction proceeded to completion, as confirmed by powder XRD. These experiments have demonstrated that moisture is essential for initiating the reaction.

It was shown by the following experiment that, once the reaction is initiated, external moisture is not required for further progress of the reaction. A pellet-inside-pellet configuration of the $\text{NH}_4\text{HF}_2/\text{NH}_4\text{VO}_3$ pair, immediately after preparing in air, was sealed in a nitrogen-filled tube. At the end of the reaction, after all the inner bifluoride rod was consumed, the sample was weighed. It did not show any increase in weight from the starting pellet-inside-pellet weight.

Identification of the products

The XRD patterns of the coloured products formed at the interface for all the pairs of reactants in Table 1 were compared with those of the products reported in the literature and prepared by other routes such as solution crystallization¹², grinding⁴ and high-temperature synthesis¹³. In other cases, marked by an asterisk (Table 1) where such information is not available in the literature, the products were prepared by grinding the reactants and the XRD patterns obtained for comparison. In all the cases the patterns, either taken from the literature or generated by us, agreed with those of the scooped-out materials. The XRD patterns of the coloured products from configuration II obtained in the case of NaVO_3 with three different bifluorides are given in Figure 2, a-c. The fit of various interplanar spacings with these patterns is given in Tables 2-5.

Identification of diffusing species

It may be noted that, in the arrangement shown in

Table 2. A fit of the powder XRD pattern of $[\text{NH}_4]_3\text{Na}_2\text{VO}_2\text{F}_4$

d_{obs} (Å)	d_{cal} (Å)	hkl	Relative intensity
5.830	5.827	101	100
4.150	4.155	201	32
3.170	3.181	112	17
2.910	2.915	202	26
2.630	2.635	321	23
1.980	1.982	331	9

System Tetragonal
 $a_0 = 10.224 \pm 0.016$ Å, $c_0 = 7.069 \pm 0.011$ Å

Table 3. A fit of the XRD pattern of $\text{K}_2\text{NaVO}_2\text{F}_4$

d_{obs} (Å)	d_{cal} (Å)	hkl	Relative intensity
4.779	4.777	111	26
4.138	4.140	002	8
2.921	2.924	220	100
2.388	2.388	222	40
2.067	2.067	400	75
1.690	1.689	224	20
1.593	1.593	115	5
1.463	1.463	404	19

System cubic
 $a_0 = 8.276 \pm 0.002$ Å

Table 4. A fit of the powder XRD pattern of $[\text{NH}_4]_2\text{K}_2\text{VO}_2\text{F}_4$

d_{obs} (Å)	d_{cal} (Å)	hkl	Relative intensity
6.172	6.176	021	22
5.680	5.684	111	18
5.011	5.015	220	15
4.152	4.151	311	41
3.520	3.526	420	20
3.143	3.140	421	100
3.095	3.099	212	68
2.979	2.972	430	22
2.818	2.819	041	46
2.714	2.718	340	22
2.389	2.389	512	27
2.254	2.252	432	36
2.201	2.203	602	36
2.166	2.166	721	35
2.090	2.090	223	64
1.927	1.926	423	25
1.901	1.903	722	15
1.833	1.834	143	15
1.755	1.755	170	15
1.689	1.689	362	23
1.661	1.661	024	28
1.578	1.578	851	15
1.542	1.542	504	15
1.433	1.433	770	30
1.414	1.414	1112	12

System orthorhombic
 $a_0 = 17.1802 \pm 0.006$ Å,
 $b_0 = 12.351 \pm 0.004$ Å,
 $c_0 = 6.898 \pm 0.002$ Å

Figure 1a, if the vanadate is taken in the form of a rod and the bifluoride in the form of loosely packed powder, the progress of the reaction is seen by the

Table 5. A fit of the powder XRD pattern of $[\text{NH}_4]_2\text{KVO}_2\text{F}_4$

d_{obs} (Å)	d_{cal} (Å)	hkl	Relative intensity
5.096	5.094	120	100
4.495	4.494	012	37
4.396	4.393	211	50
4.171	4.154	112	14
3.453	3.460	310	10
3.143	3.139	230	80
3.121	3.117	103	54
2.831	2.833	023	12
2.557	2.555	411	15
2.309	2.306	050	18
2.246	2.247	024	23
2.141	2.138	510	10
2.085	2.085	052	10
2.004	2.006	243	10
1.731	1.731	451	8
1.701	1.700	315	10
1.575	1.576	270	15

System: orthorhombic
 $a_0 = 10.887 \pm 0.005$ Å,
 $b_0 = 11.527 \pm 0.005$ Å,
 $c_0 = 9.762 \pm 0.006$ Å

growth of yellow band of product around the girth of the rod upward against gravity. When the bifluoride is in the form of the central rod and vanadate is the surrounding powder, the bifluoride is found to move into the vanadate and form the coloured product in an increasing circle (Figure 1,c) around the rod, as discussed earlier. The same is true of all other pairs.

Thus it is clear that the reaction proceeds in all cases in one direction only, i.e. from bifluoride to vanadate. This leads one to think that the HF part of the bifluoride may be responsible for the initiation of the reaction at the interface of the two solids and the subsequent progress towards the vanadate phase. If HF were solely responsible for the reaction, the product of reaction in pairs 1, 2 and 3 (see Table 1) should have been identical. Similarly the product in pairs 4, 5 and 6 should have been the same. On the contrary the products are different in all the cases although they contain the same anionic species, viz. $\text{VO}_2\text{F}_4^{3-}$; the cation is that of the corresponding bifluoride used for the reaction. This is demonstrated in Figure 2, a-c, in which the XRD patterns of the coloured products obtained from pellet-inside-pellet configuration of pairs 4, 5 and 6 are shown. The more interesting result is that, although no stoichiometry is maintained in the pellet-inside-pellet configuration for all the reactant pairs given in Table 1, the coloured product compound always had the same (2:1) stoichiometry of bifluoride to vanadate. This confirms that during the reaction the bifluoride along with its associated cation moves into the vanadate and forms the coloured compound.

Progress of reaction

The progress of the reaction between the bifluoride and

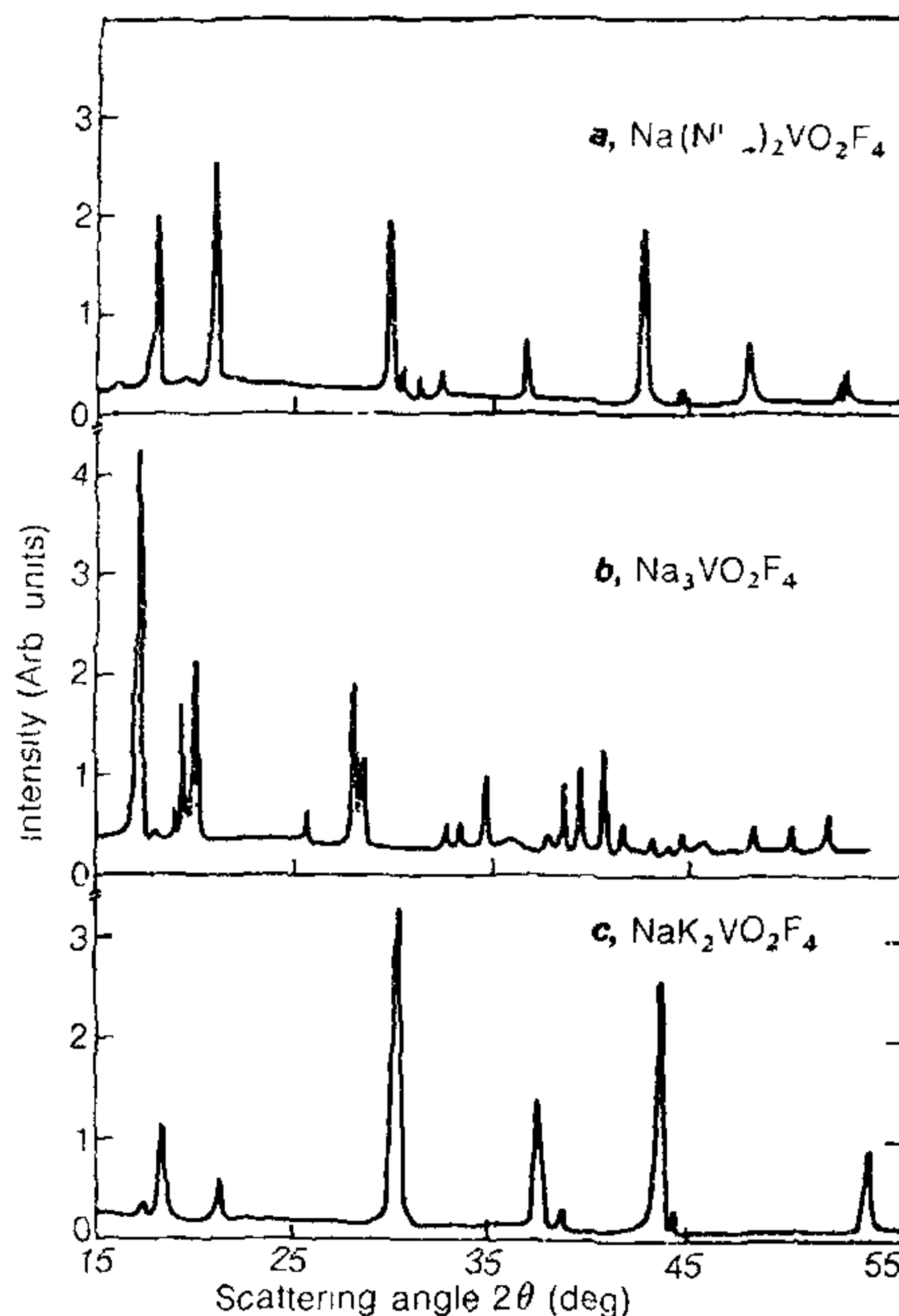


Figure 2. XRD patterns of the coloured product scooped out from the interface of three pairs of reactants. a, NH_4HF_2 and NaVO_3 ; b, NaHF_2 and NaVO_3 ; and c, KHF_2 and NaVO_3 , showing that all three products are different; if only free HF were diffusing in all the three cases, the product would have been identical in all cases.

the vanadate in the solid state is followed in the configuration II by monitoring the rate of increase in the thickness of the coloured ring with time using a travelling microscope. The thickness at given time points was measured along different diameters of the ring. As many as fifteen independent measurements were made at each time point, and their mean and standard deviations as a function of time were plotted. The scatter in the mean values is large. This is understandable since, firstly, the particles in either reactant are not of uniform size (not graded) and the progress of reaction in a given direction critically depends on the size of the particles and hence the observed scatter in the thickness of the coloured product. Secondly, the pellet is made by cold-pressing and the green density will always be much lower than the theoretical one owing to voids distributed at random in the pellet which impede the reaction.

Figure 3 shows a plot of the rate of growth of the thickness of the coloured ring, i.e. $W(t)/t$, versus time for

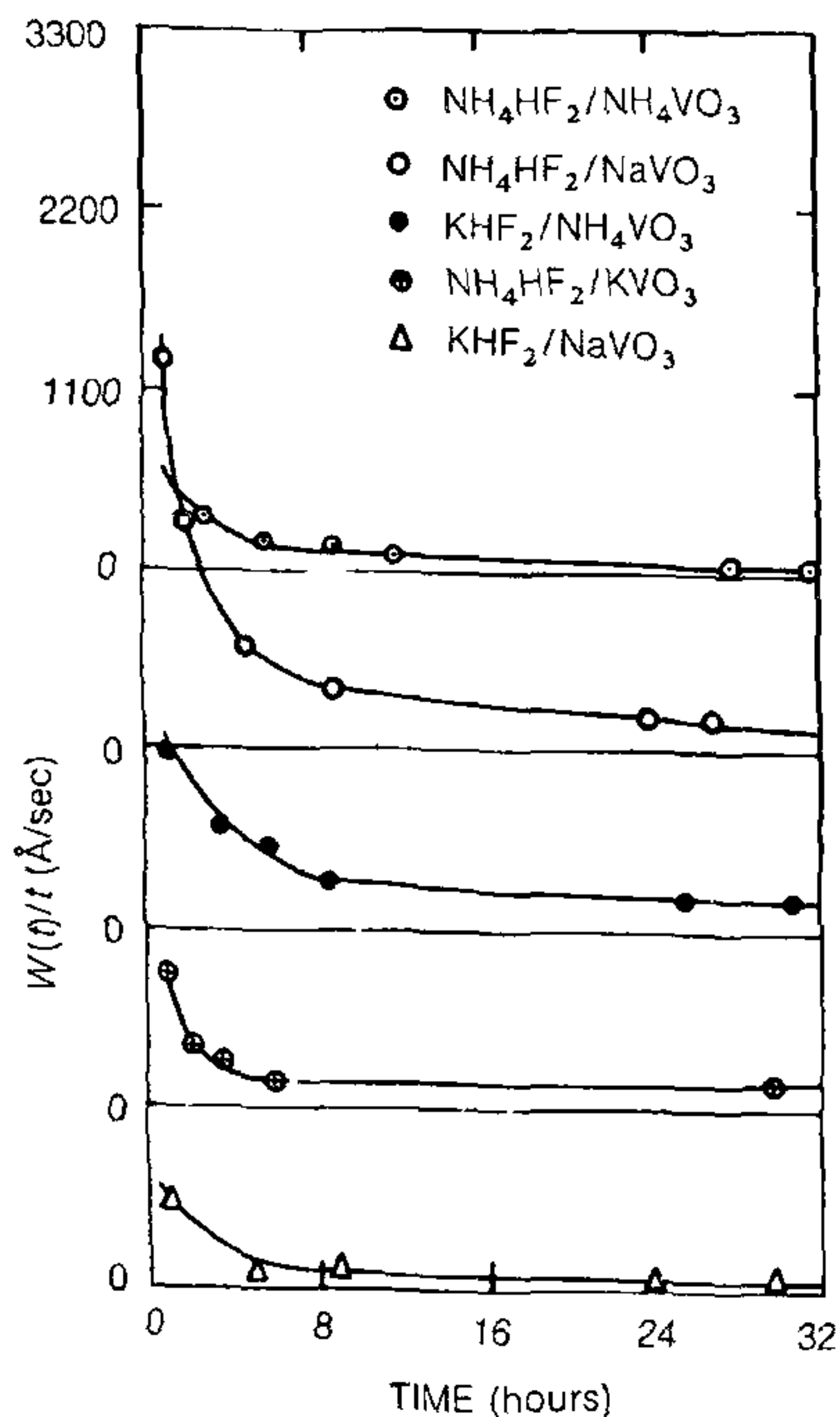


Figure 3. Plot of rate of increase in the thickness of the product $W(t)/t$ vs time for different pairs of reactants

the different pairs given in Table 1. For the pair $\text{NH}_4\text{HF}_2/\text{NH}_4\text{VO}_3$, initially the rate of growth of ring thickness is approximately $360 \pm 90 \text{ \AA}$ per sec. The rate falls with time and appears to level off at about $50 \pm 15 \text{ \AA}$ per sec after approximately 30 h. This fall in the rate is understandable since, once the product is formed at the interface between the two solids, further reaction is possible only if the ammonium bifluoride can cross the barrier of the product layer into the ammonium vanadate phase. The width of the coloured product layer is continuously increasing and hence the observed decrease in reaction rate with time.

Similar measurements were made on the other pairs of reactants included in Table 1. The trend in all the cases (Figure 3) is the same and similar to that observed for $\text{NH}_4\text{HF}_2/\text{NH}_4\text{VO}_3$. The reaction between KHF_2 and KVO_3 at room temperature was too slow to be followed by this method.

It is interesting at this stage to refer to the ideas of Tammann and Mansuri¹⁴ regarding reactivity between two solids. According to these authors, perceptible reaction between two solids occurring by defect

migrations can be observed only at temperatures above the Tammann temperature which is equal to $0.52 T_m$, where T_m is the melting point in kelvin of any reactant. At and above this temperature, the defects become mobile. In all the bifluorides studied here, the ambient temperature is above their Tammann temperature.

Other related studies

It may be added here that we have performed similar studies on a large number of pairs of reactants, with binary oxides in place of vanadates. They include studies relating to Sb(III), Sb(IV) and Sb(V) oxides; different oxides of iron; Re_2O_3 (Re = rare earth); UO_2 and U_3O_8 ; V(III), V(IV) and V(V) oxides. Similar results obtained in these cases will be published elsewhere. It will suffice to mention two striking results of these studies on binary oxides:

(i) It was shown earlier¹⁵ that, by grinding together V_2O_5 and NH_4HF_2 at room temperature, two possible products are produced depending upon the ratio of the two reactants. If oxide and bifluoride are in 1:2 ratio, the product is $\text{NH}_4\text{VO}_2\text{F}_2$, which is believed to contain polymeric anion¹⁶ with infinite chains of V-O-V and V-F-V. If the ratio is 1:6, the product⁶ is $[\text{NH}_4]_3\text{VOF}_6$ with discrete anions of $[\text{VOF}_6]^{3-}$. In recent experiments in this series, in the pellet-inside-pellet configuration between V_2O_5 and NH_4HF_2 , where no stoichiometry between the two reactants is implied, the product formed at the interface was $[\text{NH}_4]_3\text{VOF}_6$. Thus, of the two possible compounds, $\text{NH}_4\text{VO}_2\text{F}_2$ and $[\text{NH}_4]_3\text{VOF}_6$, the system appears to have selected the latter, probably because structurally this compound is more suitable for transport of the bifluoride across it to the V_2O_5 side.

(ii) In the case of $\text{U}_3\text{O}_8/\text{NH}_4\text{HF}_2$, the initial rate of reaction of 200 \AA sec^{-1} is maintained for nearly 8 h. This is different from the kinetic behaviour exhibited by all other pairs shown in Table 1, where the reaction rate to start with is high, falls off with time, and remains constant afterwards.

Summary

From the foregoing we conclude that the solid-state reaction observed at ambient temperature between a bifluoride and a vanadate is (i) initiated by trace amounts of moisture, (ii) propagated, without necessity of additional moisture, by the unidirectional transport of bifluoride across the ever-growing layer of the product into the vanadate side, (iii) found to result in the formation of a crystalline product with stoichiometry of 1:2 in vanadate and bifluoride and a structure totally different from that of either reactant, and (iv) relatively fast to start with and slows down with time and then levels off.

RESEARCH ARTICLES

Further experiments using other physical techniques for *in situ* study of kinetics are in progress.

1. Ray, R., *J Mater Sci.*, 1970, 5, 1038
2. Hellstern, E. and Schultz, L., *Appl Phys. Lett.*, 1986, 49, 1163.
3. Goyal, Q. R., Deshpande, V. V. and Kar Khanavala, M. D., *Indian J. Chem.*, 1971, 9, 1006
4. Wani, B. N., Rao, U. R. K., Venkateswarlu, K. S. and Gokhale, A. S., *Thermochim. Acta*, 1982, 58, 87.
5. Rao, U. R. K., Wani, B. N. and Venkateswarlu, K. S., *Thermochim. Acta*, 1988, 125, 229.
6. Rao, U. R. K., Venkateswarlu, K. S. and Wani, B. N., *J. Fluorine Chem.*, 1986, 31, 29.
7. Wani, B. N., Patwe, S. J., Rao, U. R. K. and Venkateswarlu, K. S., *J. Fluorine Chem.*, 1989, 44, 177.
8. Patwe, S. J., Wani, B. N., Rao, U. R. K. and Venkateswarlu, K. S., *Can J. Chem.*, 1989, 67, 1815.
9. Wani, B. N. and Rao, U. R. K., *Synth. React. Inorg. Met. Org. Chem.*, 1991, 25, 779
10. Pourroy, G. and Poix, P., *J. Fluorine Chem.*, 1989, 42, 257.

11. Wani, B. N. and Rao, U. R. K., *J. Solid State Chem.*, 1991, 94, 428.
12. Sengupta, A. K. and Bhaumik, B. B., *Z. Anorg. Allg. Chem.*, 1972, 390, 311.
13. Pausewang, G. and Dehnicke, K., *Z. Anorg. Allg. Chem.*, 1969, 369, 265.
14. Tammann, G. and Mansuri, Q. A., *Z. Anorg. Allg. Chem.*, 1923, 126, 119.
15. Rao, U. R. K., Venkateswarlu, K. S. and Wani, B. N., *Thermochim. Acta*, 1984, 81, 23.
16. Sastry, M. D., et al., *Phase Transitions*, 1987, 9, 345.

ACKNOWLEDGEMENT We thank Dr K. R. Rao, Head, Solid State Physics Division, BARC; Prof. S. Ramaseshan, and Prof. E. S. Rajagopal, Indian Institute of Science, Bangalore, for their painstaking review and critical comments on the paper. We are grateful to Dr R. M. Iyer, Director, Chemical and Isotope Group, and Dr P. N. Moorthy, Head, Applied Chemistry Division, BARC, for their interest in this work.

Received 8 April 1991; revised accepted 22 August 1991

RESEARCH COMMUNICATIONS

Crystal structure of the mesogenic compound *trans*-4-propylcyclohexyl-4-(*trans*-4-propylcyclohexyl) benzoate

C. I. Venkatramana Shastry, A. M. Babu, M. A. Sridhar, S. B. Bellad, A. Indira and J. Shashidhara Prasad

Department of Studies in Physics, University of Mysore, Manasagangotri, Mysore 570006, India

It is of interest to study the effects of structural changes due to additional atoms on the physical properties of compounds of a homologous series. We have earlier reported¹ the structure of the nematogenic compound *trans*-4-propylcyclohexyl-4-(*trans*-4-ethylcyclohexyl) benzoate (TPEB). In this paper we report the crystal structure of the next higher member of a homologous series, *trans*-4-propylcyclohexyl-4-(*trans*-4-propylcyclohexyl) benzoate (TPPB).

Good single crystals of TPPB were obtained by slow-evaporation technique using acetone as solvent. X-ray diffraction intensity data were collected on an Enraf Nonius diffractometer using Mo K_α radiation. A ω -2 θ scanning mode was employed, and Lorentz and polarization corrections were applied.

The structure was solved by direct methods using MULTAN80 (ref. 2) with $E > 1.537$. The phase set with best combined figure of merit was used for computing the E map. This map gave only a partial structure showing the benzene ring and C=O. Karle recycling of this fragment failed to develop the structure any further. Hence this fragment was assumed to be correctly oriented but wrongly positioned. Repositioning was

carried out, whereupon the full molecule was generated. Full-matrix and block-diagonal least-squares refinement was carried out using the LSTSQ-NRCVAX (ref. 3) program. Refinement with isotropic thermal parameters converged R to 0.3264, and refinement with anisotropic thermal parameters reduced it to 0.240. The hydrogen atoms were generated manually, but were not included in the refinement. The last least-squares cycle was calculated with 65 atoms, 235 parameters and 1360 out of 1363 reflections. Unit weights were used. The final residuals are $R_f = 0.240$ and $R_w = 0.238$ (where $R_f = \Sigma(F_o - F_c)/\Sigma F_o$, $R_w = [\Sigma(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$), and the maximum shift/sigma ratio 0.070. The maximum and minimum electron-density peaks in the final difference map were +1.07 and -0.85 e Å⁻³ respectively. The computational work was carried out on a Wipro PC-AT 386/387 using the NRCVAX structure determination package³. The high residuals are due to the nonavailability of sufficient number of reflections with $I > 2\sigma(I)$ as the data set was poor.

Figure 1 shows the numbering scheme of the molecule projected on the best plane. Atomic coordinates and thermal parameter data have been submitted as supplementary material to the journal. Tables 1 and 2 give the bond lengths and angles and torsion angles for non-hydrogen atoms. The bond distances and angles are in good agreement with the standard values and those of TPEB. The equation for the best plane of the molecule is $4.58(3)X + 8.67(6)Y + 4.18(12)Z = 2.546(21)$. The equations for the best planes of the two cyclohexane cores and the benzene ring are $0.73(9)X - 8.73(8)Y + 9.71(11)Z = 4.07(14)$, $-2.33(8)X -$