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## **Inclusion Complexes of a New Host, 4,5-Bis(4-methoxyphenyl)-2-(4-nitrophenyl)-1*H*-imidazole, with Various Guests**

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The title host compound forms crystalline inclusion complexes, the colour of which depend on the guest. It forms a complex with 2-phenylethanol (**6**), which when heated changes colour and emits the characteristic fragrance of the latter. The complex formed with trichloroacetic acid shows solid-state fluorescence.

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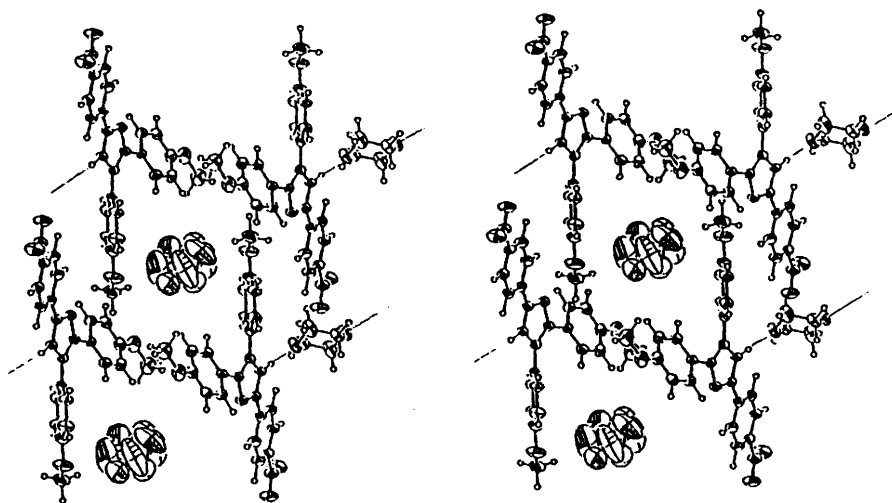
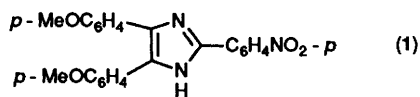
We have found recently that 4,5-bis(4-methoxyphenyl)-2-(4-nitrophenyl)-1*H*-imidazole (**1**) reacts with a wide variety of

organic compounds to give inclusion complexes the colour of which depend on the guest (see Table).

**Table.** Host-guest molar ratios and colorations of imidazole inclusion complexes.

Compd. no.	Guest	Molar ratio host:guest	Crystal form	Colour	Colour analysis*			Crystallization solvent
					Hue $\lambda_d$ (nm)	Chroma Pe (%)	Lightness Y (%)	
(1)	—	1:0	Prisms	Orange-yellow	588	84.0	33.7	MeCN
(2)	Dioxane	1:1	Needles	Red	605	70.3	21.8	Dioxane
(3)	0.5H <sub>2</sub> O	2:1	Needles	Purple-black	601	24.1	2.5	C <sub>6</sub> H <sub>6</sub> -H <sub>2</sub> O
(4)	0.5EtOH, 0.5H <sub>2</sub> O	2:1:1	Needles	Black	610	66.0	3.0	EtOH-H <sub>2</sub> O
(5)	—	1:0	Needles	Vermillion	610	68.4	10.0	C <sub>6</sub> H <sub>6</sub>
(6)	PhCH <sub>2</sub> CH <sub>2</sub> OH	1:2	Needles	Yellow	579	82.1	54.0	PhCH <sub>2</sub> CH <sub>2</sub> OH
(7)	4 <i>H</i> -Pyridone	1:1	Leaflets	Yellow	589	78.7	53.5	CHCl <sub>3</sub>
(8)	HCO <sub>2</sub> H	1:1	Needles	Orange-yellow	588	84.0	37.1	HCO <sub>2</sub> H
(9)	2HCO <sub>2</sub> H	1:2	Columns	Orange	591	82.5	27.4	HCO <sub>2</sub> H
(10)	EtCO <sub>2</sub> H	1:1	Leaflets	Red	601	64.2	15.1	EtCO <sub>2</sub> H
(11)	ClCH <sub>2</sub> CO <sub>2</sub> H	1:1	Prisms	Yellow	592	84.3	28.0	EtOH
(12)	CCl <sub>3</sub> CO <sub>2</sub> H	1:1	Needles	Yellow	580	75.4	52.8	EtOH
(13)	PhCO <sub>2</sub> H	1:1	Columns	Orange	588	84.9	38.2	EtOH
(14)	<i>p</i> -MeOC <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> H	1:1	Prisms	Orange	593	84.7	25.4	EtOH
(15)	<i>p</i> -ClC <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> H	1:1	Columns	Red	597	73.6	12.7	EtOH
(16)	<i>p</i> -NO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> H	1:1	Prisms	Prisms	592	78.7	16.2	EtOH

\* Colour analyses were performed according to the X<sub>10</sub>Y<sub>10</sub>Z<sub>10</sub> standard colorimetric system which has been recommended by the CIE (Commission International de l'Eclairage, 1964) for colour representation. Hue, chroma and lightness are specified therein.

**Figure.** Stereoscopic view of (2).

**Formation and properties of the inclusion complexes.** Compound (1) has at least three polymorphic forms; (i) orange-yellow prisms A, (ii) dark red fine needles B, and (iii) vermilion fine needles C. Polymorph B, formed at 100 °C by heating an acetate dihydrate of (1),<sup>1</sup> readily forms inclusion compounds with many organic compounds in the solid state. The inclusion complexes were prepared as follows. For a solid guest com-

pound, an equimolar mixture of the latter and polymorph B was ground in a mortar; the complex so obtained was then recrystallized in an appropriate solvent. For a liquid guest compound in which (1) was soluble, the complex was allowed to crystallize out. Complex formation was confirmed by elemental analysis, IR, TLC, and DSC (differential scanning calorimetry) measurements.

The figure shows a stereoscopic drawing of the X-ray crystal structure of complex (2) along the *c* axis.<sup>†</sup> The dioxane guest molecule exists in two states: in the first, the NH of the imidazole ring is hydrogen bonded and in the second, the molecule, in a disordered state, lies in a cavity encircled by four methoxyphenyl groups. The dioxane molecule plays an important role in the crystal packing of (2).

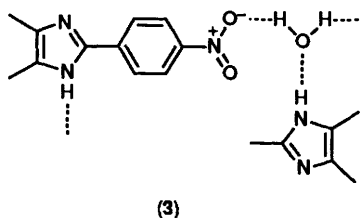
**Complex Formation.**—With 2-phenylethanol. A complex (6) of polymorph B with 2-phenylethanol is thermochromic and, further, when heated emits the fragrance characteristic of 2-phenylethanol. Thus at temperatures > 50 °C it is orange-yellow with a weak fragrance and at > 93 °C (6) it is deep red and the fragrance is stronger. If the heating is done in sealed glass tubes, the colour reverts to the original on cooling. Both

<sup>†</sup> Crystal data. C<sub>23</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub>·C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>, *M*, 489.53, triclinic, *P* $\bar{1}$ , *Z* = 2, *a* = 17.689(3) Å, *b* = 18.681(4) Å, *c* = 6.346(2) Å,  $\alpha$  = 97.93(3)°,  $\beta$  = 90.59(4)°,  $\gamma$  = 142.79(1)°, *V* = 1 230.5(7) Å<sup>3</sup>, *D<sub>m</sub>* = 1.323(1), *D<sub>x</sub>* = 1.321 g cm<sup>-3</sup>, *R* = 0.078 for 3 150 observed reflections, room temperature. Full listings of the X-ray crystallographic results for this study are available, on request, from the Cambridge Crystallographic Data Centre (see 'Instructions for Authors (1990)', *J. Chem. Soc., Perkin Trans. 1*, 1990, Issue 1).

IR spectra and a DSC diagram showed that the hydrogen-bonded phenylethanol leaves above 50 °C and the other, more tightly bound, 2-phenylethanol leaves at 93 °C.

*With 4H-pyridone.* A complex of polymorph B with 4H-pyridone (7) is also thermochromic in the range 120–226 °C. Thus at *ca.* 120 °C it changes from yellow to orange, the latter colour deepening with further heating until at 226 °C it is red; it melts at 227 °C. This reaction was irreversible.

*With water.* Addition of a little water to a warmed benzene solution of the polymorph B gave purple–black fine needles of (3) which showed sharp and strong  $\nu(\text{NH})$  absorption; the splitting into two of the  $\nu_s(\text{NO}_2)$  band suggests the presence of two types of hydrogen bonding as shown in (A).<sup>2</sup> Similarly, a warmed (*ca.* 40 °C) aqueous ethanolic solution of polymorph B gave black fine needles of (4), the IR spectrum which was very similar to that of (3) except for the presence of ethanol



absorption. Both complexes showed broad absorption in the region 370–650 nm.

*With CCl<sub>3</sub>CO<sub>2</sub>H.* The complex formed between polymorph B with trichloroacetic acid exhibited a five-fold enhanced solid-state fluorescence (emission maximum at 548 nm) over that showed by the former.

### Acknowledgements

This work was supported by a grant-in-aid for Scientific Research on Priority Areas from the Ministry of Education, Science and Culture, Japan (No. 0507-01628501). Y. S. acknowledges for helpful advice of Professor Fumio Toda, Ehime University.

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*Paper 0/02268C*  
Received 22nd May 1990  
Accepted 9th July 1990