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Evaluating the host potential of 9,9'-bifluorenyl-9,9'-diol for anisole and the three methylanisole isomers, and its behaviour in mixed guest solutions

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Abstract

In the present investigation, 9,9'-bifluorenyl-9,9'-diol (**H**) was assessed for its host potential for anisole (ANI) and the three methylanisole isomers (2MA, 3MA and 4MA), through crystallization experiments, and it was thus demonstrated that **H** has the ability to enclathrate each of these four guest solvents. Additionally, the selectivity behaviour of **H** was evaluated when presented with mixtures of these anisoles, and the results suggested that each of the methylated anisoles was preferred in one or another instance, dependent upon the other guest solvent/s present, while, more notably, ANI remained consistently disfavoured. However, the observed host selectivity was not appropriate to suggest that **H** may serve as a host candidate for the separation of ANI/MA solutions through host–guest chemistry protocols. Single crystal X-ray diffractometric analyses on each of the complexes produced in this work showed that, with the exception of **H**·0.75(4MA₂), extreme guest disorder and/or severe twinning of the crystals existed, and Platon's SQUEEZE routine was required in most instances. As such, these experiments did not provide explanations for the selectivity behaviour of the host compound in the mixed guest solutions through a consideration of the host–guest interactions present in each complex. However, from the successful obtention of the crystal structure of **H**·0.75(4MA₂), it was observed that the guest species was retained in the crystals of the complex by means of both (host)O–H···O(guest) and (host/guest)C–H···C–C(guest/host) close contacts. Thermal analysis demonstrated that, while the ANI, 2MA and 3MA inclusion complexes were unstable at ambient conditions, the two 4MA-containing inclusion compounds possessed stability, and comparably so, since similar guest release onset temperatures for their guest release events were observed (*T*_{on}, 65.9 and 68.8 °C). These observations provide some explanation for the preference of **H** for 4MA in a number of the guest competition experiments, more especially those that were equimolar and binary in nature.

Keywords

Host–Guest; Fluorenyl; Inclusion; Anisoles; Single Crystal X-ray Diffraction; Thermal Analysis

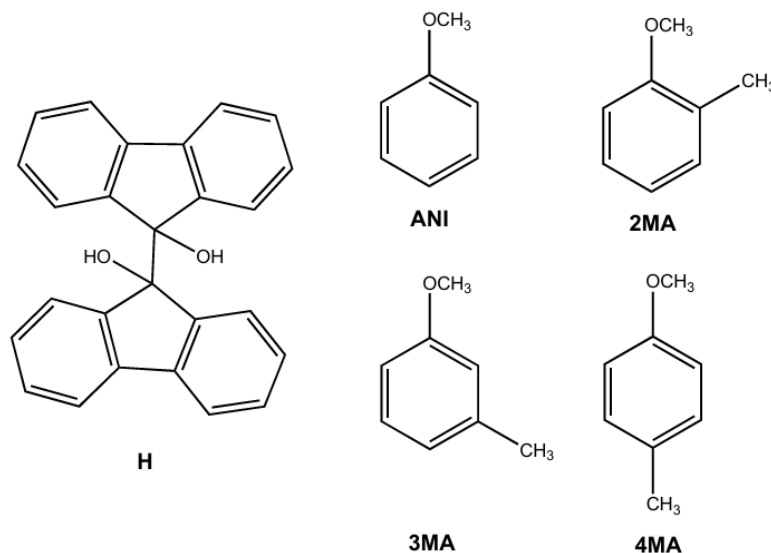
1. Introduction

Anisole (ANI) and its methylanisole isomers (2MA, 3MA and 4MA) (Scheme 1) are important aromatic compounds in several different industries, including the pharmaceutical, chemical, biochemical and agrochemical fields of science, amongst several others. As examples, ANI serves as a male attractant pheromone for the *Holotrichia reynaudi* scarab beetle species, which is an agricultural pest native to India.¹ This compound is also an intermediate towards perfumes and active pharmaceutical ingredients (APIs) including analgesics, anti-inflammatories and anesthetics.² The three positional isomers of ANI, that is 2MA, 3MA and 4MA, are also starting materials towards APIs, agrochemicals, dyes and food additives, and find applications as important intermediates toward the synthesis of methoxybenzaldehydes and methoxybenzoic acids.^{3,4} Additionally, these compounds are oftentimes employed as green solvents in synthetic procedures owing to their reduced toxicity and low environmental impact.⁵

In order to prepare ANI and its MA isomers, the corresponding phenol/cresol may be *O*-methylated using dimethyl carbonate as the alkylating agent with potassium carbonate as the base.⁶ Other alkylation agents such as methanol are also appropriate and these methods generally employ zeolites or alumina as catalysts.^{4,7,8} Further strategies towards these anisoles involve the *C*-methylation of ANI.⁹ While these syntheses appear to be straightforward, this is certainly not the case, and subsequent product streams are seldom pure and usually comprise a mixture of all four of these anisoles.^{10–13} As a result, separation strategies, more especially for mixtures of the positional isomers, are subsequently necessary in order to isolate each one with adequate purity for further ensuing applications.¹⁴ A report by Sholl and Lively¹⁵ has unequivocally demonstrated that these separations, when employing fractional distillation techniques, are not sustainable owing to their high energy demand and consequential extreme fossil fuel depletion propensities. While it is relatively facile to isolate unsubstituted ANI in this particular fashion (its boiling point is 154 °C), the MAs boil within a narrow boiling range (170–172, 175–176 and 174 °C for 2MA, 3MA and 4MA, respectively), and so alternative greener separatory methods are imperative.

Current separation protocols for these anisoles that do not involve distillations include ubiquitous chromatographic applications, but supramolecular chemistry has also been suggested as a highly attractive alternative.^{16–20} As examples of the latter strategy, compounds (–)-(2*R*,3*R*)-2,3-dimethoxy-1,1,4,4-tetraphenylbutane-1,4-diol, *trans*-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylic acid, dimethyl *trans*-9,10-dihydro-9,10-ethanoanthracene-11,12-dicarboxylate, *N,N'*-bis(5-phenyl-5-dibenzo[*a,d*]cycloheptenyl)ethylenediamine and di-(9-(*p*-trifluoromethylphenyl)xanthen-9-yl) peroxide have been demonstrated to possess exceptional host selectivity when crystallized from ANI/MA mixtures. In fact, with the exception of *N,N'*-bis(5-phenyl-5-dibenzo[*a,d*]cycloheptenyl)ethylenediamine, overwhelming selectivity coefficients were calculated during crystallization experiments from many of these mixed guest solutions, suggesting that this significantly greener separatory methodology is feasible on an industrial scale. Moreover, since the complexes formed in this manner are in the solid phase, their isolation from the solution by means of a simple vacuum filtration effectively separates the preferred guest solvent from the others and, as these complexes are glued together through weak and reversible noncovalent interactions (such as $\pi\cdots\pi$, X–H $\cdots\pi$, hydrogen bonding, both classical and nonclassical in nature, and van der Waal's interactions),^{21,22} the guest may readily be recovered from the cavities of its complex through extremely mild heat.

The present investigation focussed on whether the title compound 9,9'-bifluorenyl-9,9'-diol (**H**, Scheme 1) has the ability to form complexes with each of the four anisoles, a consideration that has not been explored to date. All successfully-formed inclusion compounds produced in this work were, moreover, analysed by means of both single crystal X-ray diffraction (SCXRD) and thermal experiments. For completeness, also assessed was the selectivity of **H** when presented with mixed guest solutions, with the view to determining whether it may be an applicable separatory agent for ANI/MA solutions, through host–guest chemistry, owing to the challenges associated with fractional distillations for these separations. This objective was deemed a feasible one since **H** has recently been reported to be a remarkably selective host compound for the purification and/or separation of mixed pyridines.²³ We now report on all of the results so obtained.



Scheme 1 Molecular structures of the host compound 9,9'-bifluorenyl-9,9'-diol (**H**) and the proposed guest solvents anisole (**ANI**) and 2-, 3- and 4-methylanisole (**2MA**, **3MA** and **4MA**).

2. Experimental

2.1 General

All reagents required for the synthesis of **H** as well as the potential guest solvents **ANI** and the MAs were sourced from Merck (South Africa) and were used as received.

^1H -NMR spectra were recorded using a Bruker Ultrashield Plus 400 MHz spectrometer with CDCl_3 as the deuterated solvent, and the spectral data were analysed using Topspin 4.4.1 software.

The **H**·0.778(**ANI**), **H**·0.778(**2MA**), **H**·0.667(**3MA**), **H**·0.667(**4MA**₁) and **H**·0.75(**4MA**₂) complexes afforded crystals of appropriate quality for a structural investigation through SCXRD analysis. (Note that two separate experiments furnished two different complexes with **4MA**, labelled as **4MA**₁ and **4MA**₂.) Two instruments were applicable. The first was a Bruker Kappa Apex II diffractometer with graphite-monochromated Mo $\text{K}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). APEXII software facilitated data acquisition and analysis, with program SAINT used for cell refinement and data reduction. Numerical absorption corrections were applied using the SADABS software.²⁴ The crystal structures were solved with SHELXT-2018/2,²⁵ and least-squares refinement was carried out using SHELXT-2018/3,²⁶ with SHELXE²⁷ serving as the graphical user interface (GUI). The second instrument was a Bruker D8 Quest diffractometer, equipped with a Photon II CPAD detector and $\text{I}\mu\text{S}$ 3.0 Mo source ($\text{K}\alpha$, $\lambda = 0.71073 \text{ \AA}$). APEX4 software enabled diffraction data acquisition, SAINT aided with cell refinement and data reduction, and SADABS assisted with numerical absorption corrections.²⁸ The structures were solved through the dual-space method implemented in SHELXT-2018/2,²⁵ followed by least-squares refinement using SHELXL-2019/3.²⁶ Structural visualization was facilitated by the SHELXL²⁷ GUI, and molecular diagrams were prepared using ORTEP-3 for Windows (version 2023.1).²⁹ All non-hydrogen atoms were refined anisotropically. Carbon-bound hydrogen atoms were positioned using standard geometric constraints (C–H bond lengths: $0.95 \text{ \AA}$ for aromatic carbons, $1.00 \text{ \AA}$ for methine, and $0.99 \text{ \AA}$ for methylene) and refined by employing the riding model approximation, with $U_{\text{iso}}(\text{H})$ fixed at $1.2U_{\text{eq}}(\text{C})$. Hydrogen atoms of the methyl groups were allowed rotational freedom about the C–C bond to best match the experimental electron density (HFIX 137 in program SHELXL²⁶), with $U_{\text{iso}}(\text{H})$ parameters fixed at $1.5U_{\text{eq}}(\text{C})$ and C–H bond lengths restrained to $0.98 \text{ \AA}$. Refinement of the hydroxyl hydrogen atoms was carried out with rotational freedom about the C–O bond to achieve optimal agreement with the experimental electron density (HFIX 147 in SHELXL²⁷), with $U_{\text{iso}}(\text{H})$ fixed at $1.5U_{\text{eq}}(\text{O})$ and O–H bond lengths restrained to $0.84 \text{ \AA}$. The crystal structures of the novel complexes **H**·0.778(**ANI**), **H**·0.778(**2MA**), **H**·0.667(**3MA**), **H**·0.667(**4MA**₁) and **H**·0.75(**4MA**₂) were deposited at the Cambridge Crystallographic Data Centre (CCDC), and their CCDC accession numbers are 2474917, 2474918, 2474921, 2474919 and 2474920, respectively.

Gas chromatography (GC) was employed for the quantification of the ANI/MA guest compounds in any mixed guest complexes prepared in this study. All analyses were performed on an Agilent Technologies 7890A gas chromatograph paired with an Agilent 5975C VL mass spectrometer (GC-MS), which was equipped with an Agilent J&W GC Cyclosil-B column. The temperature program initiated with a 1 min hold time at 50 °C, followed by a ramp of 10 °C·min⁻¹ to attain a final temperature of 110 °C, which was held for an additional 4 min. The total run time was 12 min, with a split ratio of 1:80 and a flow rate of 1.5 mL·min⁻¹. Dichloromethane served as the dissolution solvent for all these experiments.

Thermal analysis was used to evaluate the relative thermal stabilities of the single-solvent complexes. These experiments were carried out by means of a Perkin Elmer STA6000 Simultaneous Thermal Analyser, and the resultant data were processed via Perkin Elmer Pyris 13 Thermal Analysis software. Prior to these analyses, the crystalline complexes were isolated from solution by vacuum filtration, washed with petroleum ether (bp 40–60 °C) under suction, patted dry in folded filter paper, and subsequently transferred to ceramic pans for analysis. An empty pan served as the reference. High purity nitrogen was employed as the purge gas, and all samples were heated from approximately 50 °C to 250 °C at a heating rate of 10 °C·min⁻¹.

2.2 Synthesis of 9,9'-bifluorenyl-9,9'-diol (**H**)

The host compound was synthesised in accordance with a previously reported procedure.³⁰

2.3 Single-solvent host crystallization experiments

These crystallization experiments were performed in order to determine whether **H** possessed host ability for each of ANI and its MA derivatives. As such, the solid host compound (0.05 g, 0.14 mmol) was dissolved in an excess of each liquid guest solvent (5–10 mmol) and the mixture gently heated to facilitate complete host dissolution. The resulting solutions in the glass vials were left open at ambient temperature and pressure, enabling slow evaporation of some of the guest solvent. This gradual increase in solution saturation promoted nucleation and subsequent crystal growth. The crystals were collected by vacuum filtration, washed with petroleum ether (bp 40–60 °C) to remove residual surface-bound guest solvent, and then dissolved in CDCl₃ for ¹H-NMR spectroscopic analysis. The host-to-guest (H:G) ratios of the resulting complexes were determined by integrating distinct proton signals associated with both host and guest compounds.

2.4 Equimolar guest competition experiments

These experiments were conducted to evaluate the preferential binding behaviour of **H** when presented with equimolar binary, ternary and quaternary guest solutions. In each case, **H** (0.05 g, 0.14 mmol) was dissolved in these solutions in which the combined guest amount was 5 mmol, whilst considering all possible guest combinations. The solutions were sealed in their glass vials and stored at 4 °C to promote crystallization under controlled conditions. Once crystals formed, these were treated as in the single-solvent crystallization experiments. Overall H:G ratios were determined through ¹H-NMR spectroscopy, while guest-to-guest (G:G) ratios were quantified using GC analyses. Each experiment was performed in duplicate to ensure reproducibility, with percentage estimated standard deviations (% e.s.d.s) reported accordingly.

2.5 Binary guest competition experiments with varied guest concentrations

To systematically evaluate the selectivity behaviour of **H** in binary guest systems in which guest concentrations varied, a series of host crystallization experiments were carried out using mixtures of guest A (G_A) and guest B (G_B) at defined molar ratios (20:80, 40:60, 60:40 and 80:20; 5 mmol combined amount). The host compound (0.05 g, 0.14 mmol) was dissolved in each guest mixture, and the resulting solutions were sealed in glass vials and stored at 4 °C to induce crystallization. Upon crystal formation, these were isolated and processed following the same protocol applied in the equimolar competition experiments. The relative guest compositions within

the resulting mixed guest complexes were quantified by GC analyses. Selectivity profiles were constructed in accordance with the selectivity model developed by Pivovar *et al.*, in which the molar fraction of guest A (Z_A) or guest B (Z_B) present in the crystalline phase was plotted against its corresponding molar fraction in the original solution (X_A or X_B).³¹ The selectivity coefficient (K), which provides a quantitative measure of the host preference for a particular guest species, was calculated using $K_{A:B} = Z_A/Z_B \times X_B/X_A$, where $X_A + X_B = 1$.³¹ A theoretical reference line corresponding to $K_{A:B} = 1$ was incorporated into the selectivity plots to denote a non-selective host. Experimental K values were compared relative to this baseline to reveal any host selectivity. According to the criterion reported by Nassimbeni and coworkers, a selectivity coefficient equal to or greater than 10 is indicative of a highly efficient host compound and signifies strong potential for practical separations.³² (Notably, the results from the equimolar binary crystallization experiments (Table 2) were also incorporated into these plots for comparative purposes.)

2.6 Software

All crystallographic analyses were carried out by means of program Mercury.³³ This software facilitated the generation of structural visualisations, including unit cell frameworks, host–guest packing arrangements, and void space diagrams. For the latter figures, the guest molecules were omitted from the packing models, and the resulting void spaces that thus formed were quantitatively analysed using a spherical probe with a radius of 1.2 Å.

3. Results and discussion

3.1 Single-solvent host crystallization experiments

After crystallization of **H** from each of ANI and the three MAs and analysis of the ensuing solids through ¹H-NMR spectroscopy, Table 1 was populated with the so-obtained H:G ratios. (All relevant ¹H-NMR spectra are provided in the Supplementary Information (SI), Figures S1a–e.)

Table 1 H:G ratios^a of complexes formed when **H** was crystallized from each of ANI and the MAs.

Guest solvent	H:G ratio
ANI	2:1
2MA	1:1
3MA	1:1
4MA	3:2, 1:1 ^b

^aDetermined using ¹H-NMR spectroscopy with CDCl₃ as the deuterated solvent.

^bTwo separate experiments furnished complexes with different H:G ratios.

Therefore, **H** possessed the ability to enclathrate each of the four anisoles (Table 1). 2MA and 3MA were complexed with 1:1 H:G ratios, while ANI formed a 2:1 inclusion compound with the host species. In the case of 4MA, the first complex that formed had a H:G ratio of 3:2. However, when the crystal was analysed by SCXRD (see later), it was extremely weakly diffracting and twinning was, furthermore, suspected. As such, the crystallization experiment was repeated, this time slowing it down by adding more guest solvent in this particular instance. As a result of the different experimental conditions between the two crystallizations, it was not surprising that the H:G ratio of the new complex had changed (it was now 1:1, as shown by ¹H-NMR spectroscopy). Satisfyingly, this new sample was readily analysed by SCXRD (see later).

3.2 Equimolar guest competition experiments

The guest and overall H:G ratios observed in the host crystallization experiments from the equimolar mixed guest solutions are provided in Table 2, together with the % e.s.d.s since these experiments were carried out in duplicate to ascertain their repeatability. (Figures S2–S12 in the SI are the applicable GC traces after GC analysis to obtain the guest ratios and the ¹H-NMR spectra required to calculate the overall H:G ratios.) The favoured guest species in each experiment is highlighted by means of bold red text.

Table 2 Guest and overall H:G ratios of the mixed complexes formed when **H** was crystallized from the equimolar mixed guest solutions.^a

ANI	2MA	3MA	4MA	Guest ratios (% e.s.d.s)	Overall H:G ratio
X	X			39.6: 60.4 (1.6)	2:1
X		X		44.5: 55.5 (0.5)	3:1
X			X	31.4: 68.6 (10.0)	2:1
	X	X		41.0: 59.0 (7.7)	1:1
	X		X	29.7: 70.3 (1.0)	2:1
		X	X	43.1: 56.9 (2.9)	2:1
X	X	X		29.0: 49.0 :22.0 (0.3)(0.7)(1.1)	2:1
X	X		X	24.5: 45.5 :30.0 (2.2)(1.4)(0.8)	1:1
X		X	X	14.1:19.5: 66.4 (1.1)(3.1)(4.2)	1:1
	X	X	X	27.4:31.4: 41.2 (1.4)(1.7)(0.4)	3:1
X	X	X	X	17.4: 31.5 :20.3:30.8 (1.4)(0.5)(0.3)(0.5)	2:1

^aGuest and overall H:G ratios were obtained using GC and ¹H-NMR spectroscopy, respectively.

From Table 2, **H**, in the binary guest solvent experiments, marginally preferred 4MA. The ANI/4MA, 2MA/4MA and 3MA/4MA experiments furnished mixed guest complexes with 68.6, 70.3 and 56.9% 4MA. In the absence of 4MA, 3MA was then favoured, with 3MA accounting for 55.5 and 59.0% of the guest composition in the crystals obtained from the ANI/3MA and 2MA/3MA experiments, respectively. Preferential inclusion of 2MA was observed in the ANI/2MA complex (when 4MA and 3MA were absent), and the resultant crystals then contained 60.4% 2MA.

The ternary guest competition experiments revealed that 2MA was preferred in the ANI/2MA/3MA and ANI/2MA/4MA experiments, which produced crystals with 49.0 and 45.5% 2MA, respectively. Similarly, 4MA was the predominant guest in the complexes isolated from the ANI/3MA/4MA and 2MA/3MA/4MA mixtures, with the resulting crystals comprising 66.4 and 41.2% 4MA.

In the quaternary mixture, **H** showed a preference for 2MA (31.5%), once more, followed closely by 4MA (30.8%). Most notable is that ANI was never a favoured guest in any of these experiments, while each of the MAs was preferred which depended upon the number and nature of the other guest species present in the solution.

Finally, the overall H:G ratios varied widely, and this observation correlates with the differing ratios observed in the single-solvent host crystallization experiments (Table 1).

3.3 Binary guest competition experiments with varied guest concentrations

The GC traces obtained after analysing the various mixed guest complexes may be observed in the SI, Figures S13–S18. Selectivity profiles were constructed upon host crystallization from the binary guest solutions where the guest ratios were varied (Figures S19a–f in the SI); the 50:50 G_A:G_B data points from Table 2 have been inserted into these plots for the sake of completeness. Additionally, the K values for each data point in these profiles have been summarised in the SI, Table S1.

In the 2MA/ANI, 3MA/ANI, 3MA/2MA, 4MA/2MA and 4MA/3MA mixtures (Figures S19a, S19b, S19d, S19e and S19f in the SI), no significant host selectivity was observed, and the data points were positioned close to the line representing no selectivity (where K = 1). Consequently, K values were low (Table S1), ranging between 1.1 and 1.5 (2MA/ANI), 1.2 and 3.0 (3MA/ANI), 1.2 and 1.9 (3MA/2MA), 1.2 and 5.9 (4MA/2MA), and 0.9 and 3.3 (4MA/3MA). Notably, the host preference in these experiments was not consistently for one guest only, the selectivity behaviour changing as the guest concentrations changed. On the other hand, in the 4MA/ANI experiments (Figure S19c of the SI), **H** exhibited a clear and consistent preference for 4MA, particularly in solutions containing 40, 60 and 80% 4MA. In these instances, the crystals contained 72.3, 92.7 and 95.4% 4MA,

respectively. However, the K values remained low (≤ 8.5). (Note that the 50:50 data point here appears to be an outlier and does not fit the profile; this is unsurprising given the high % e.s.d. (10.0) for this experiment (Table 2)).

3.4 Single crystal X-ray diffractometry

Table 3 contains the crystallographic data relevant to obtaining the crystal structures of the successfully formed complexes produced in this investigation, while their corresponding ORTEP representations are provided in Figures S20a–e of the SI.

Solving a number of these crystal structures was not trivial owing to either twinned crystals and/or severe guest disorder. The ANI- and 2MA-containing complexes crystallised in a large trigonal space group exhibiting large channel voids. The guest electron density was extensively disordered over a large volume and around symmetry elements ensuring it to be extremely challenging to fit the molecule models to the electron density. More especially in the case of the inclusion compound with 2MA, the crystal was very weakly diffracting and, as a result, the data quality was poor. Therefore, it was difficult to determine the H:G ratio by this technique. When the guest electron densities for both these structures were removed by Platon's SQUEEZE routine,³⁴ one obtained a structure with one host molecule in the asymmetrical unit cell with $Z = 18$, indicating that there were 18 host molecules in the unit cell. This SQUEEZE routine suggested that there were 811 and 892 guest electrons in the voids per cell for the two complexes, respectively, and thus 14.0 and 13.5 guest molecules per unit cell were calculated. Therefore, the H:G ratios were 18:14 (9:7) for both. In each instance, the $wR2$ values of the squeezed structures were significantly improved compared with the original structures indicating that the initial high $wR2$ values were solely due to poor guest modelling owing to the extreme disorder. (ANI: $wR2$: 0.3050 $\rightarrow$ 0.1490; 2MA: $wR2$: 0.3999 $\rightarrow$ 0.1731, see Table S2 in the SI).

The complex with 3MA was initially solved in a large triclinic unit cell (7008.5 Å³) with six host and four guest molecules in the asymmetric unit cell; one guest molecule was disordered around an inversion point. Residual electron density around the guests indicated more complex disorder that could not be modelled. The H:G ratio from this structure was determined to be 12:7. Subsequent refinement caused Platon to suggest a new unit cell with half the c length and volume. The reciprocal lattice for this new cell advocated twinning, but applying twinning routines were not successful. Here, the H:G ratio was determined to be 1:0.522 but residual electron density demonstrated additional guest disorder orientations. Upon squeezing the data, $wR2$ decreased from 0.2300 to 0.1856. The number of electrons in the void was then calculated to be 250, and thus the final H:G was 6:4 (3:2).

The crystals for the first sample containing 4MA (labelled as 4MA₁) were thin needles that were very weakly diffracting requiring long exposure times. Additionally, the data suggested the crystal was twinned, but applying the twinning routines was unsuccessful. There were three host and two guest molecules in the asymmetric unit cell. One of the guest molecules was disordered over two orientations but residual electron density, once more, suggested additional disorder orientations. Platon's SQUEEZE routine calculated 291 guest electrons in the voids per cell with $Z = 6$, and thus there were 4.4 guests per cell. Rounding this to 4 indicated a 6:4 (3:2) H:G ratio. The $wR2$ value, however, did not improve significantly (0.3659 $\rightarrow$ 0.3313) after this procedure, possibly indicating that the crystal was twinned. Interestingly, these data suggest a common host packing compared with the complex with 3MA.

Owing to the difficulties in solving the previous 4MA-containing structure (4MA₁), a second sample (4MA₂) was analysed in a similar fashion. These crystals were grown significantly slower than those with 4MA₁ and resulted in a different crystal structure, with two host species and one guest molecule in the unit cell; the guest was disordered over an inversion point and the final H:G ratio was 4:3. The relatively low $wR2$ of 0.1075 indicated that there were no real challenges whilst solving this structure. The SQUEEZE routine calculated 201 guest

electrons in the void per cell, thus resulting in 3.0 guest species. With $Z = 4$, the H:G ratio was thus 4:3, as indicated earlier.

The unit cell parameters of the complexes with ANI and 2MA were comparable, as were these data for the 3MA and 4MA₁ complexes (Table 3). Accordingly, their powder XRD patterns were calculated using program Mercury, after guest deletion, and these are presented in Figures S21a and b, and Figures S22a and b, in the SI, respectively. The striking resemblance between each pair of patterns suggests that the host molecules in these pairs adopted an isostructural packing arrangement.

Interestingly, the H:G ratios as obtained from ¹H-NMR analysis differed significantly from those of the crystals selected for crystal structure analysis, with the exception of the **H**·0.667(4MA₁) complex, which concurred exactly. A plausible reason for these apparent anomalies may be as a result of the instability, at ambient conditions, of the ANI-, 2MA- and 3MA-containing inclusion compounds, as ascertained through thermoanalytical experiments (see later).

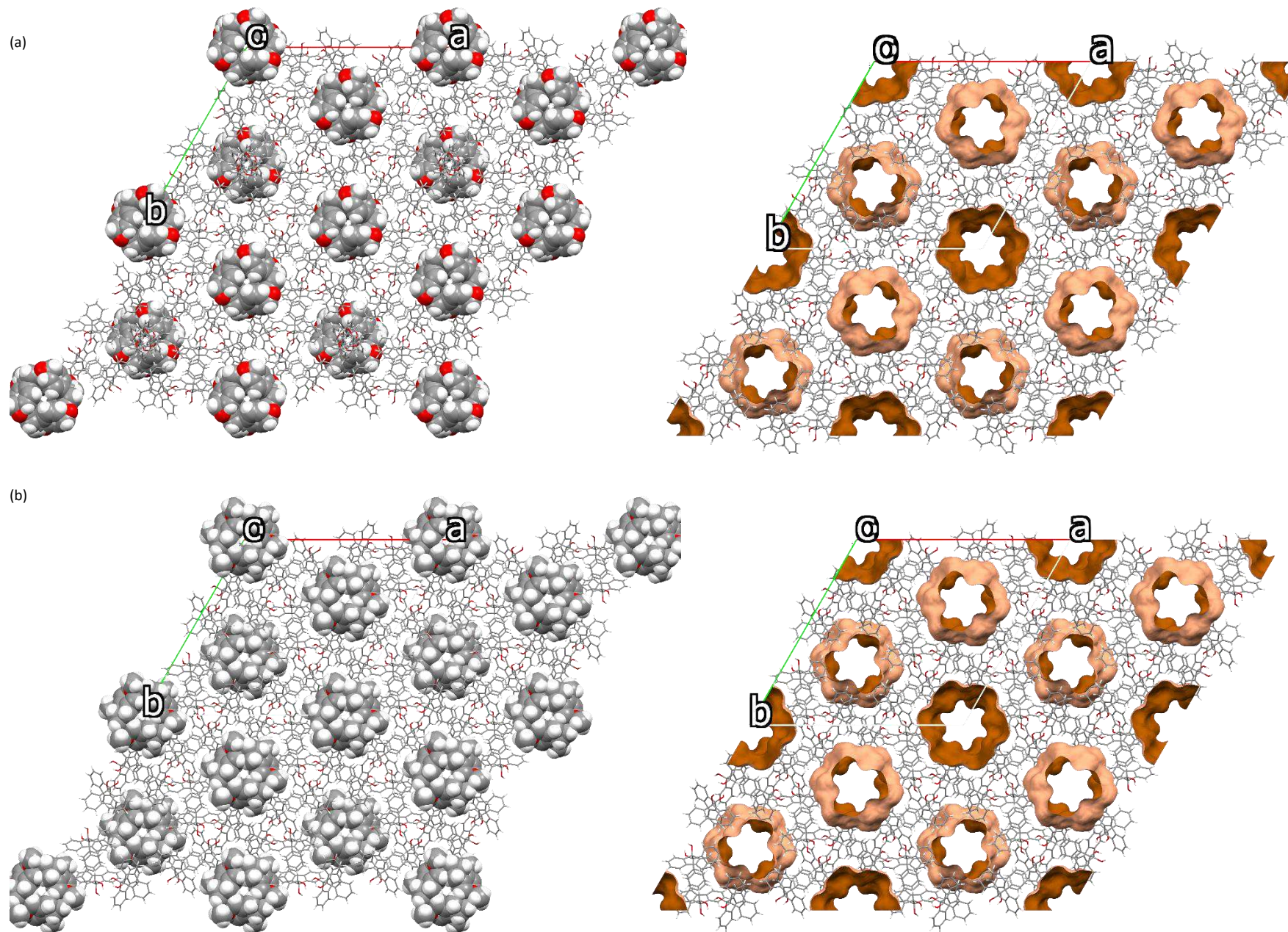
Table 3 Crystallographic data for the complexes of **H** with ANI, 2MA, 3MA, 4MA₁ and 4MA₂.

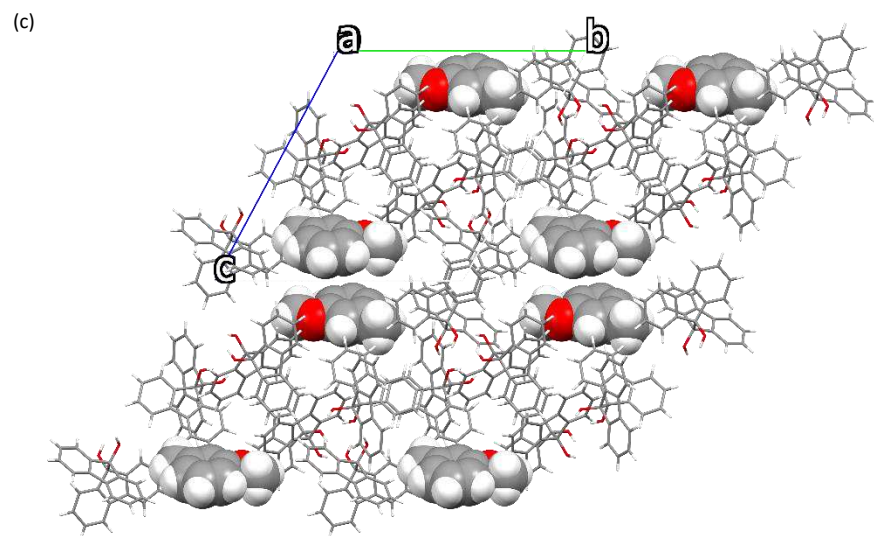
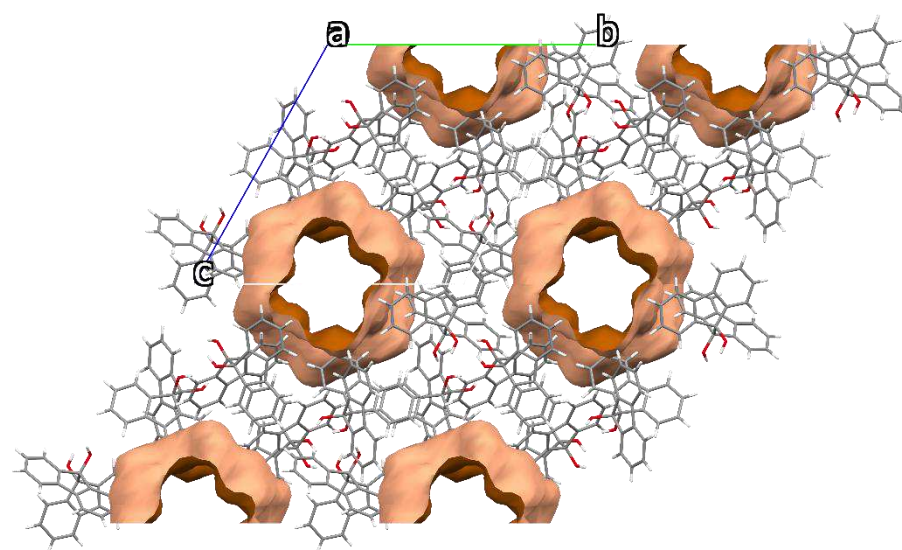
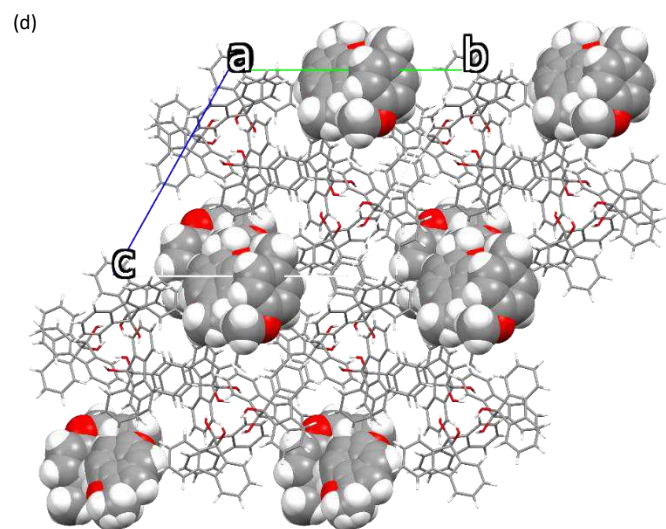
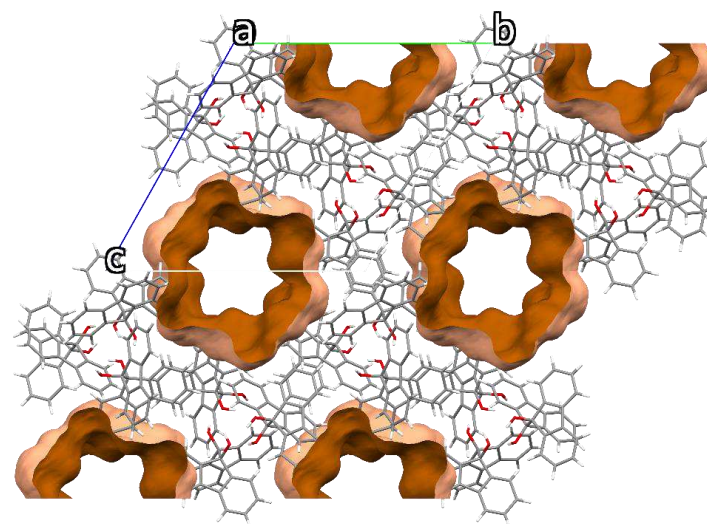
	H -0.778(ANI)	H -0.778(2MA)	H -0.667(3MA)	H -0.667(4MA ₁)	H -0.75(4MA ₂)
Chemical formula ^a	C ₂₆ H ₁₈ O ₂ ·0.727(C ₇ H ₈ O)	C ₂₆ H ₁₈ O ₂ ·0.727(C ₈ H ₁₀ O)	C ₂₆ H ₁₈ O ₂ ·0.667(C ₈ H ₁₀ O)	C ₂₆ H ₁₈ O ₂ ·0.667(C ₈ H ₁₀ O)	C ₂₆ H ₁₈ O ₂ ·0.75(C ₈ H ₁₀ O)
Formula weight	441.05	806.25	426.02	1331.53	1816.09
Crystal system	trigonal	trigonal	triclinic	triclinic	triclinic
Space group	<i>R</i> -3	<i>R</i> -3	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1
μ (Mo-Kα)/mm ⁻¹	0.078	0.070	0.077	0.079	0.078
a/Å	31.8624(9)	32.0983(7)	12.1377(8)	12.2150(9)	10.2266(4)
b/Å	31.8624(9)	32.0983(7)	18.4488(11)	18.3885(12)	12.6915(5)
c/Å	12.1461(6)	12.1248(4)	18.7002(13)	18.5519(14)	19.3221(8)
α/°	90	90	115.101(2)	115.854(2)	84.9386(16)
β/°	90	90	101.188(2)	101.141(3)	83.8825(15)
γ/°	120	120	102.425(2)	100.542(2)	77.5793(14)
V/Å ³	10678.9(8)	10818.6(6)	3505.2(4)	3506.8(4)	2429.68(17)
Z	18	9	6	2	1
F(000)	4179	3816	1346	1404	958
Temp./K	200	200	200	200	200
Restraints	123	5	240	367	102
Nref	5239	4409	14267	12412	9910
Npar	295	277	900	974	664
R	0.0997	0.1447	0.0880	0.1501	0.0485
wR2 ^b	0.3050	0.3999	0.2300	0.3659	0.1075
S	1.11	1.67	1.13	1.24	1.13
θ _{min} –max/°	1.8, 27.1	1.8, 25.4	2.2, 26.4	2.3, 25.5	2.0, 26.4
Tot. data	97634	84400	146183	125414	199246
Unique data	5239	4409	14267	12412	9910
Observed data [<i>I</i> > 2.0 σ(<i>I</i>)]	4523	3175	11725	10444	7230
R _{int}	0.046	0.151	0.053	0.094	0.063
Completeness	0.999	0.998	0.998	0.960	0.999
Min. resd. dens./e·Å ⁻³	–0.43	–0.83	–0.93	–0.57	–0.32
Max. resd. dens./e·Å ⁻³	0.70	1.23	0.75	0.79	0.23
Density/g·cm ⁻³	1.234	1.114	1.211	1.261	1.241

^aThe H:G ratios here were those obtained after the SQUEEZE procedure.^bThese wR2 values were those obtained prior to the SQUEEZE procedure. Table S2 in the SI provides the wR2 values after the SQUEEZE procedure.

Figures 1a–e illustrate the unit cells and corresponding host–guest packing arrangements (left), with the guest molecules rendered in spacefill representation and the host framework in capped-stick format. The adjacent images (right) display the associated void diagrams. In all instances, the guest molecules were accommodated in wide-open, continuous and unidirectional channels within the crystals of the complexes. Notably, the isostructural nature of the host packing in the ANI and 2MA, and 3MA and 4MA₁, complexes is further evident upon comparison of Figures 1a and b, and 1c and d.

Owing to the severe guest disorder in these complexes (with the exception of $\text{H}\cdot 0.75(4\text{MA}_2)$), it was deemed inappropriate to analyse the host...guest interactions present, as these data are not reliable given the difficulty that was experienced during the solving of these crystal structures. Therefore, the reasons for the host affinity behaviour in mixed anisoles could not be ascertained through SCXRD experiments.





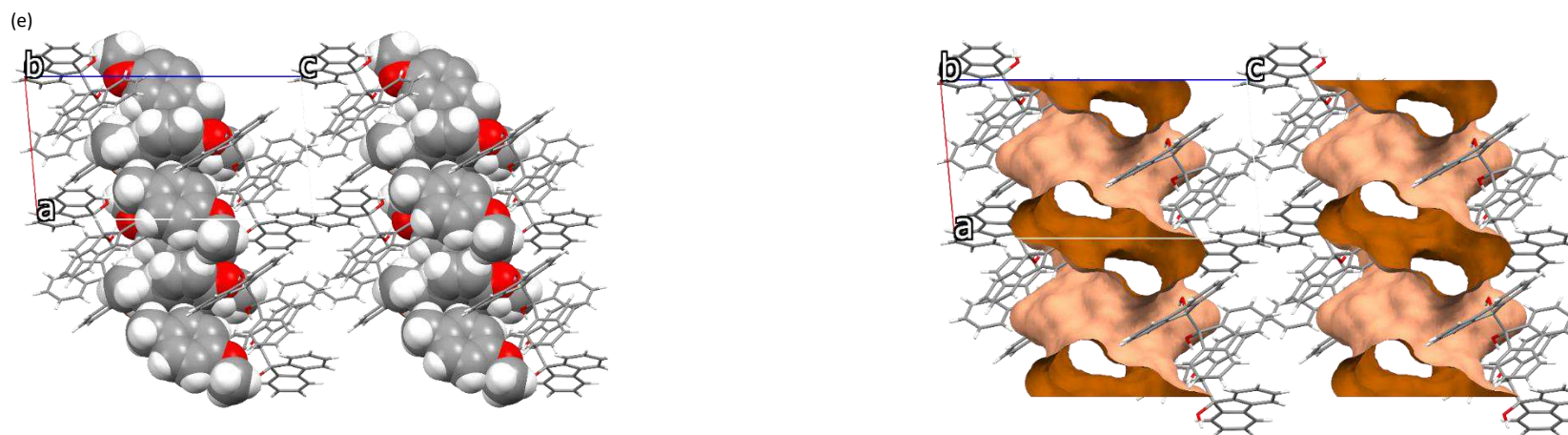


Figure 1 Unit cells with host-guest packing (left) and respective void diagrams (right) for the complexes (a) $\text{H} \cdot 0.778(\text{ANI})$, (b) $\text{H} \cdot 0.778(2\text{MA})$, (c) $\text{H} \cdot 0.667(3\text{MA})$, (d) $\text{H} \cdot 0.667(4\text{MA}_1)$ and (e) $\text{H} \cdot 0.75(4\text{MA}_2)$.

Given the reliability of the data obtained for the **H**·0.75(4MA₂) complex, its structural parameters are briefly discussed here, with particular focus on the noncovalent interactions responsible for guest retention. This complex experienced neither intermolecular nor intramolecular $\pi\cdots\pi$ interactions of relevance. Additionally, while the host and guest molecules did not engage in C–H $\cdots\pi$ interactions, three of these contacts were observed within host molecules, as presented in Table 4 and shown in Figure 2 (H $\cdots\pi$ 2.77–2.89 Å, C $\cdots\pi$ 3.386(2)–3.460(2) Å and 117–127°).

Table 4 Parameters of the intramolecular (host)C–H $\cdots\pi$ (host) interactions in the **H**·0.75(4MA₂) complex.

Interaction	H $\cdots\pi$ /Å	C $\cdots\pi$ /Å	C–H $\cdots\pi$ /°
(host1)C–H $\cdots\pi$ (host1)	2.77	3.422(2)	127
(host2)C–H $\cdots\pi$ (host2)	2.89	3.460(2)	120
	2.84	3.386(2)	117

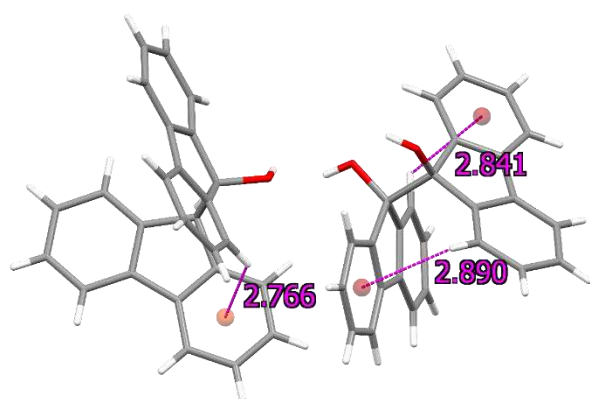


Figure 2 Intramolecular (host)C–H $\cdots\pi$ (host) interactions identified in the **H**·0.75(4MA₂) complex.

Displayed as a stereoview in Figure 3 are the hydrogen bonding interactions in **H**·0.75(4MA₂), between the guest and host molecules and, also, those inter- and intramolecular in nature involving host molecules only. Table 5 provides the pertinent interaction parameters; A denotes the acceptor and D the donor atoms. The two classical (host)O–H $\cdots$ O(guest) hydrogen bonds that were identified involved both host molecules in the unit cell (host1 and host2) and each disordered guest component. Here, the H $\cdots$ O distances measured 2.05 and 2.35 Å and O $\cdots$ O 2.854(2) and 3.125(4) Å; the bond angles were 159 and 154°. The inter- and intramolecular classical (host)O–H $\cdots$ O(host) interactions, as well as one intramolecular non-classical (host)C–H $\cdots$ O(host) close contact, measured 1.84–2.57 Å (H $\cdots$ O), 2.601(2)–2.670(2) Å (O $\cdots$ O) and 3.021(3) Å (C $\cdots$ O), as applicable, with accompanying bond angles of 110–161°.

Table Error! No text of specified style in document. Hydrogen bonding parameters in the **H**·0.75(4MA₂) complex.

Interaction	H $\cdots$ A/Å	D $\cdots$ A/Å	D–H $\cdots$ A/°
(host1)O–H $\cdots$ O(disordered guest component 1) ^a	2.05	2.854(2)	159
(host1)O–H $\cdots$ O(host1) ^b	2.22	2.628(2)	110
(host1)O–H $\cdots$ O(host2) ^a	1.89	2.670(2)	154
(host2)O–H $\cdots$ O(disordered guest component 2) ^a	2.35	3.125(4)	154
(host2)O–H $\cdots$ O(host1) ^a	1.84	2.651(2)	161
(host2)O–H $\cdots$ O(host2) ^b	2.13	2.601(2)	115
(host1)C–H $\cdots$ O(host1) ^c	2.57	3.021(3)	110

^aClassical intermolecular hydrogen bonding; ^bClassical intramolecular hydrogen bonding; ^cNon-classical intramolecular hydrogen bonding.

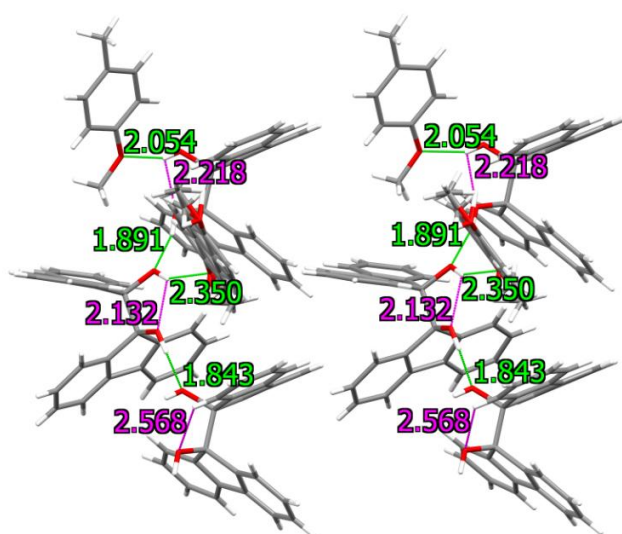
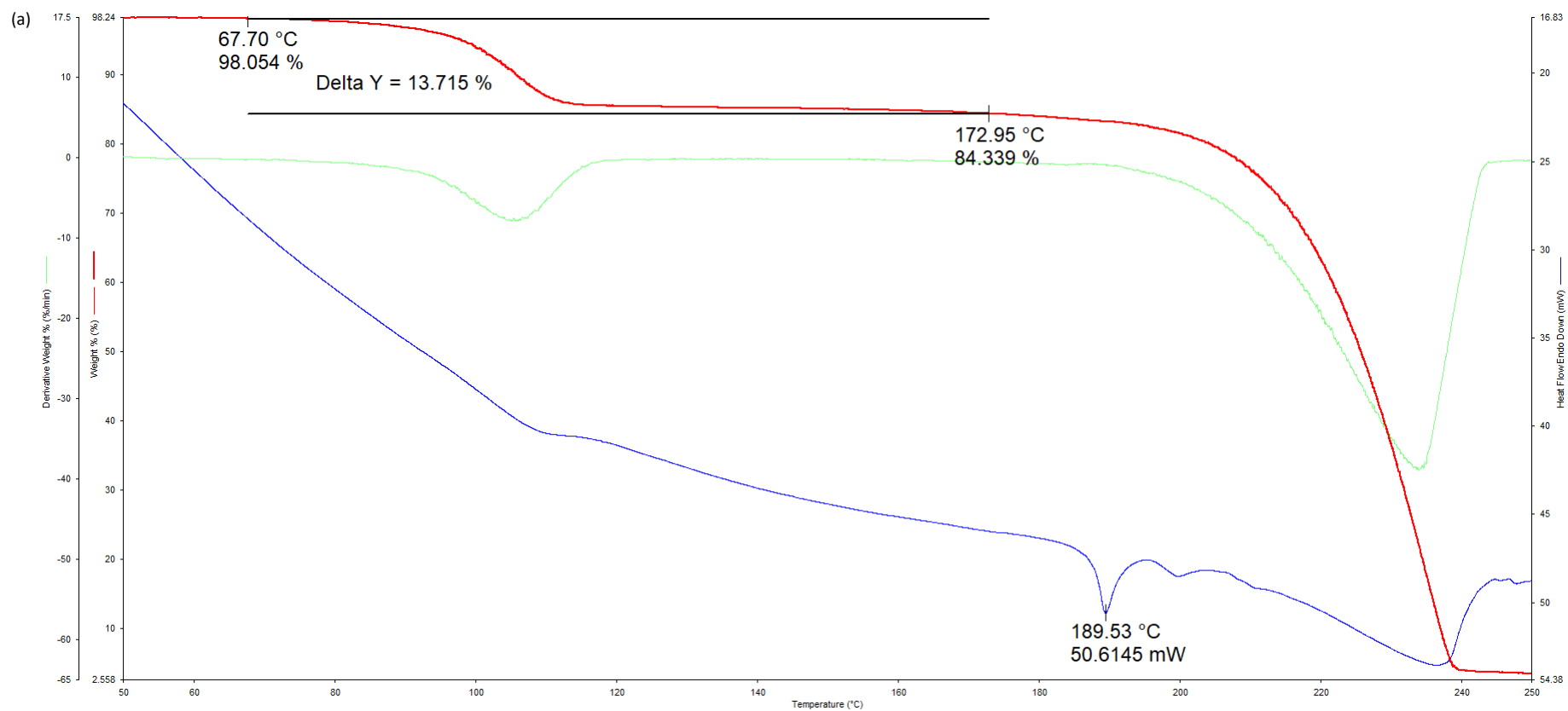


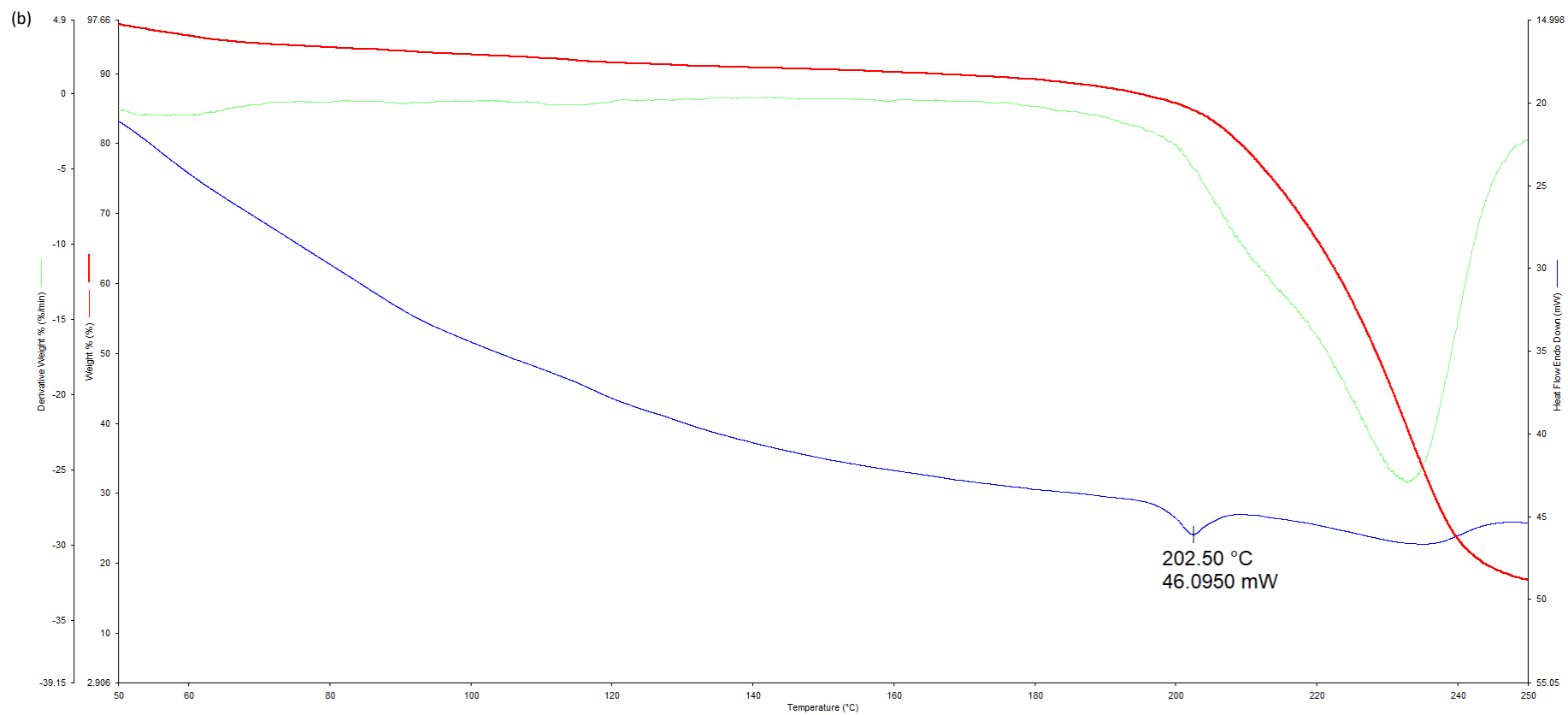
Figure 3 Stereoview of the classical and non-classical hydrogen bonding interactions present in the $\text{H} \cdot 0.75(4\text{MA}_2)$ complex; intermolecular bonds are denoted in green and intramolecular bonds in magenta.

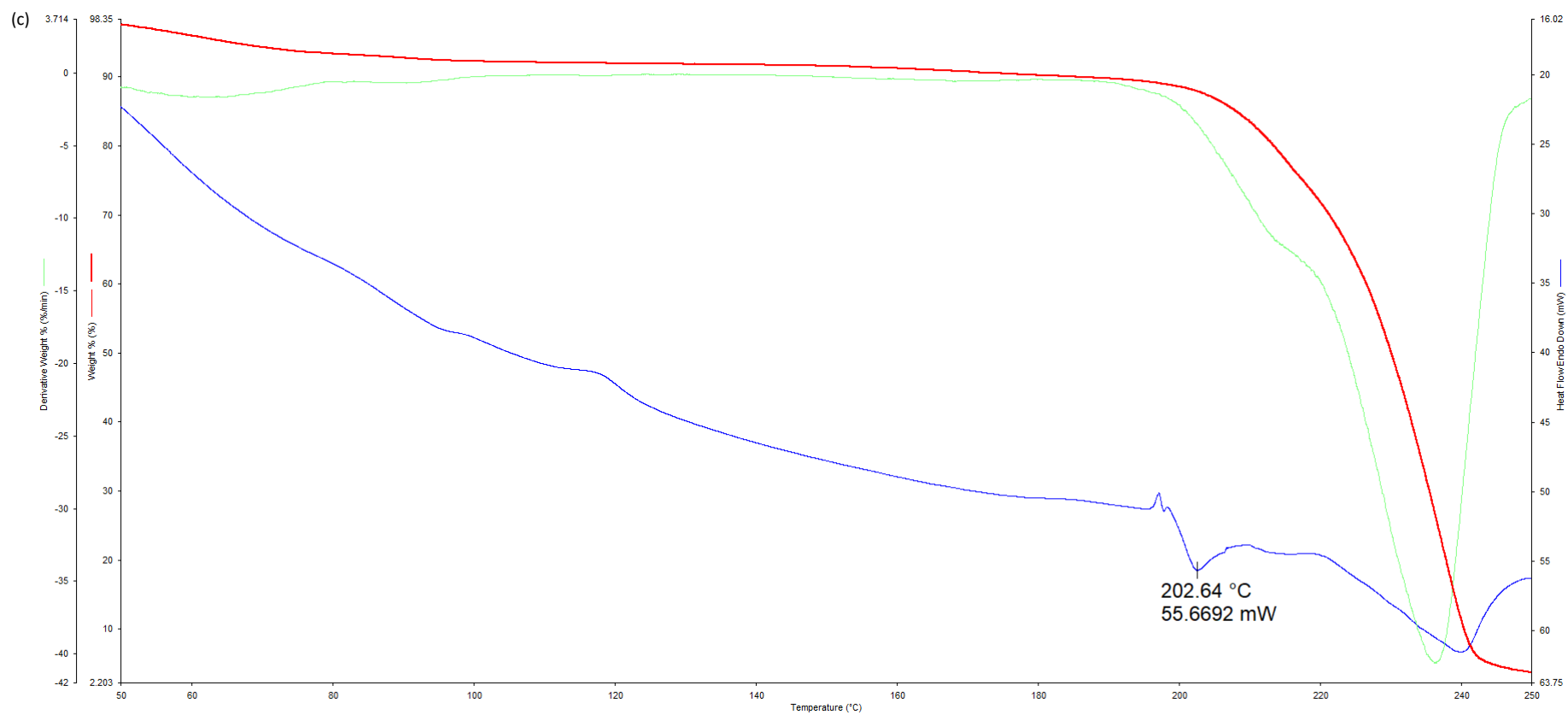
Moreover, **H** participated in (host) $\text{C}-\text{H} \cdots \text{C}-\text{C}(\text{guest})$ and (guest) $\text{C}-\text{H} \cdots \text{C}-\text{C}(\text{host})$ interactions with 4MA_2 , where the $\text{H} \cdots \text{C}$ distances were 2.68–3.07 Å and the bond angles 128–160°.

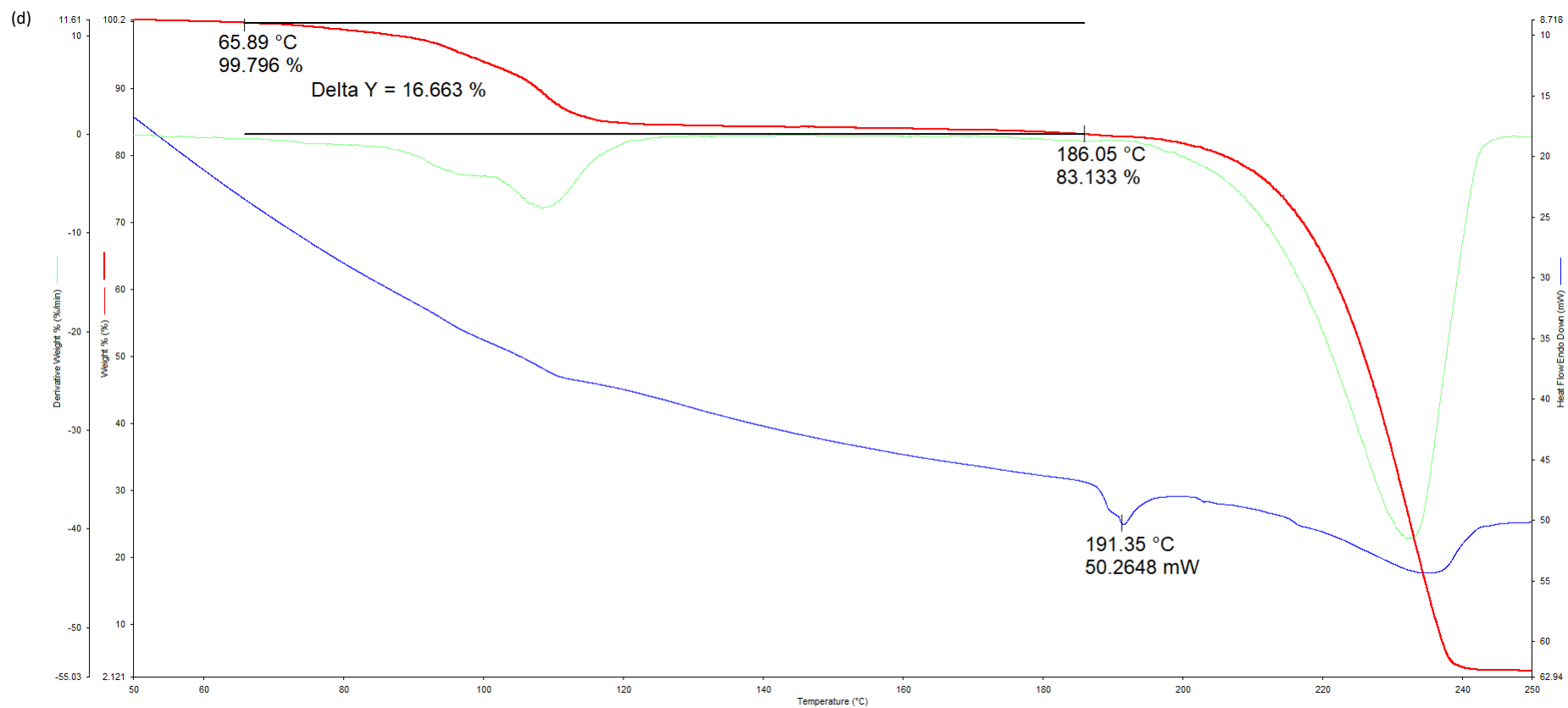
3.6 Thermal analysis

To assess the thermal stabilities of the five complexes formed in this study, thermal analyses were carried out, and the thermogravimetric (TG), its derivative (DTG), and differential scanning calorimetry (DSC) traces so-obtained are provided in Figures 4a–e. Each sample was heated at a rate of $10\text{ }^\circ\text{C} \cdot \text{min}^{-1}$ between approximately 50 and $250\text{ }^\circ\text{C}$. Two key thermal events were identified: these were the onset temperature (T_{on}) of the guest release event, which serves as a measure of the relative thermal stability of the complex, and the peak temperature (T_{p}) of the endotherm associated with the host melt (Table 6).









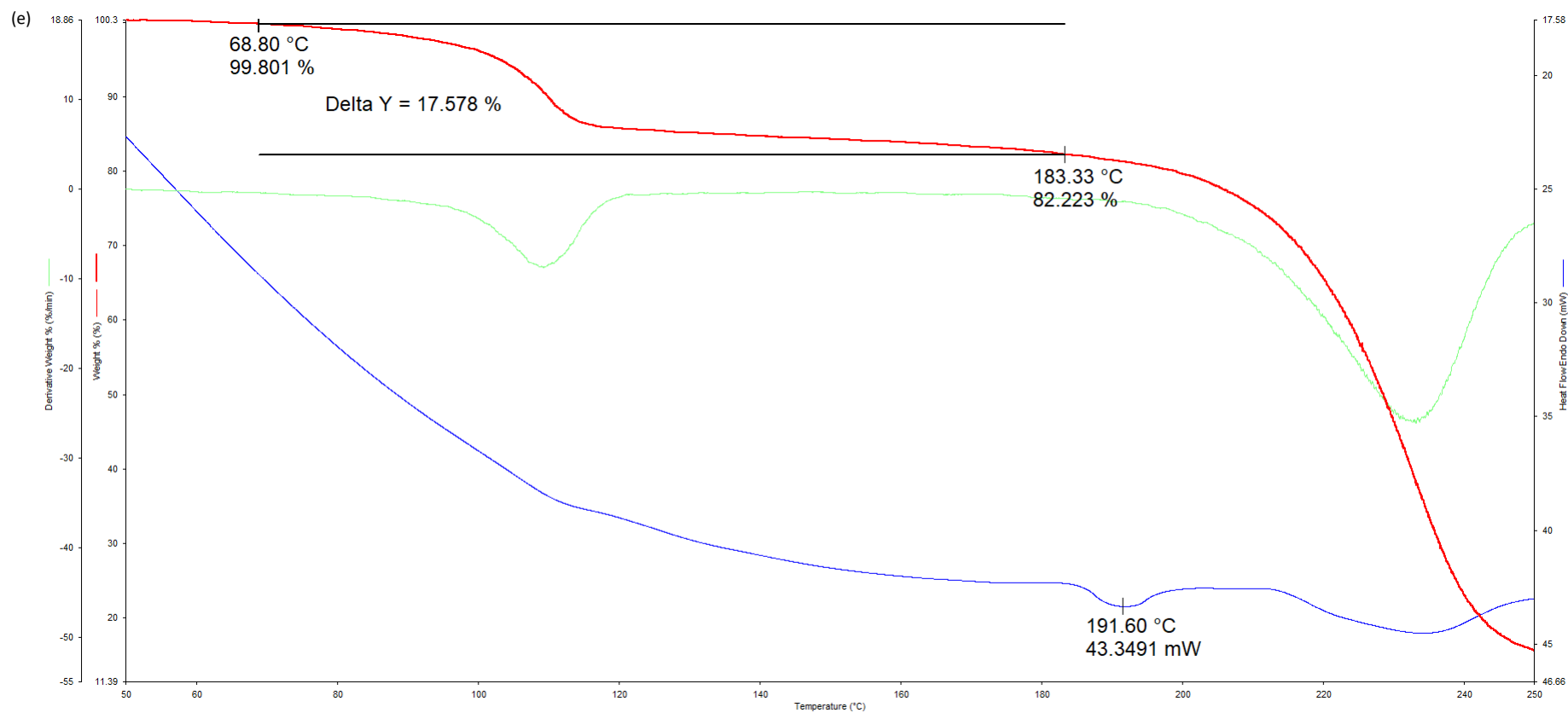


Figure 4 Overlaid TG (red), DTG (green) and DSC (blue; endo down) traces for complexes (a) $\text{H} \cdot 0.778(\text{ANI})$, (b) $\text{H} \cdot 0.778(2\text{MA})$, (c) $\text{H} \cdot 0.667(3\text{MA})$, (d) $\text{H} \cdot 0.667(4\text{MA}_1)$ and (e) $\text{H} \cdot 0.75(4\text{MA}_2)$.

As reported by Weber *et al.*,^{30,35} the pure host melts between 190 and 192 °C, and this agrees largely with the data contained in Table 6, where T_p ranged between 189.5 and 202.6 °C.

Table 6 Thermal data for complexes of **H** formed with the ANI/MA guests.^a

Complex	$T_{on}/^{\circ}\text{C}$	$T_p/^{\circ}\text{C}$	Measured mass loss/%	Expected mass loss/%
H ·0.778(ANI)	^b	189.5	13.7 ^b	18.8
H ·0.778(2MA)	^b	202.5	^b	20.8
H ·0.667(3MA)	^b	202.6	^b	18.4
H ·0.667(4MA ₁)	65.9	191.4	16.7	18.4
H ·0.75(4MA ₂)	68.8	191.6	17.6	20.2

^a T_{on} presents the onset temperature for guest release and T_p is the peak temperature for the host melt.

^bThese complexes were unstable at ambient conditions, and it was thus not possible to determine their T_{on} values.

The **H**·0.778(2MA) and **H**·0.667(3MA) complexes, as observed by the immediate downward trend of the TG in Figures 4b and c, were unstable at ambient conditions. Consequently, T_{on} could not be measured in these two instances and, therefore, nor could the experimental mass losses (Table 6). Furthermore, it is plausible that, given the low measured mass loss for the ANI-containing complex (13.7%) compared with that expected (18.8%), this complex too was unstable at room temperature and pressure (Figure 4a). This observation is not unsurprising since ANI was never preferentially selected by the host species in the mixed guest experiments. Only the two 4MA-containing inclusion compounds were thus noted to be reasonably stable with comparable T_{on} temperatures (65.9 and 68.8 °C).

4. Conclusions

Host compound 9,9'-bifluorenyl-9,9'-diol (**H**) possessed the ability to enclathrate each of ANI and the MAs. Guest competition experiments revealed that **H** has an affinity for the MAs. In the equimolar guest competition experiments, **H** preferentially included 4MA, followed by 3MA and 2MA, while ANI was never selected. Similarly, for the ternary guest competitions, 4MA and 2MA were the predominant guests favoured. During the binary guest experiments in which the amounts of G_A and G_B were varied, low host selectivities were observed. Hence, **H** cannot be utilised as a separatory tool for anisole and methylanisole mixtures through host–guest chemistry strategies. SCXRD analyses were attempted on all complexes but, owing to either crystal twinning and/or extreme guest disorder, the SQUEEZE procedure was required in all but one case (**H**·0.75(4MA₂)), and so these experiments could not be employed in order to obtain reasons for the observed host selectivity behaviour in mixed anisoles. However, the crystal structure for **H**·0.75(4MA₂) posed no challenges, and it was observed that guest retention was as a result of both O–H···O and C–H···C close contacts between the host and guest species. Thermal analyses demonstrated that the ANI, 2MA and 3MA complexes were unstable at ambient conditions and that only the two 4MA-containing inclusion compounds possessed thermal stability (T_{on} 65.9 and 68.8 °C, respectively).

Supplementary information

The crystal structures of complexes (a) **H**·0.778(ANI), (b) **H**·0.778(2MA), (c) **H**·0.667(3MA), (d) **H**·0.667(4MA₁) and (e) **H**·0.75(4MA₂) were deposited at the Cambridge Crystallographic Data Centre (CCDC) and their CCDC numbers are 2474917, 2474918, 2474921, 2474919 and 2474920 respectively. Crystallographic data for these structures are freely accessible at www.ccdc.cam.ac.uk/structures/. The relevant ¹H-NMR spectra for all the single-solvent and equimolar guest experiments, along with the GC traces analysed for binary guest competitions, have been included in the Supporting information (SI). Also, here may be found the selectivity profiles, host selectivities presented in a table, ORTEP diagrams, a table summarising crystal data before and after the SQUEEZE procedure on these complexes and applicable calculated PXRD patterns.

Author contributions

Benita Barton: conceptualization; methodology; funding acquisition; project administration; resources; supervision; visualization; writing original draft. Jaime-lee Groenewaldt: investigation; methodology; validation. Eric C. Hosten: data curation; formal analysis.

Conflict of interest

There are no conflicts of interest to declare.

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References

1. Ward, A.; Moore, C.; Anitha, V.; Wightman, J.; Rogers, D.J. Identification of the sex pheromone of *Holotrichia reynaudi*. *J. Chem. Ecol.* **2002**, *28*, 515–522.
2. Fiege, H.; Voges, H.-W.; Hamamoto, T.; Umemura, S.; Iwata, T.; Miki, H.; Fujita, Y.; Buysch, H.-H.; Garbe, D.; Paulus, W. "Phenol Derivatives" in Ullmann's Encyclopedia of Industrial Chemistry. Weinheim: Wiley-VCH, 2000.
3. EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids). (2013b). Scientific Opinion Flavouring group evaluation 23, revision 4 (FGE.23Rev4): Aliphatic, alicyclic and aromatic ethers including anisole derivatives from chemical groups 15, 16, 22, 26 and 30. *EFSA Journal*, **11**(2), 3092. <https://doi.org/10.2903/j.efsa.2013.3092>
4. Dang, D.; Wang, Z.; Lin, W.; Song, W. Synthesis of anisole by vapor phase methylation of phenol with methanol over catalysts supported on activated alumina. *Chin. J. Catal.* **2016**, *37*, 720–726.
5. Deneme, I.; Yildiz, T.A.; Kayaci, N.; Usta, H. The Hansen solubility approach towards green solvent processing: n-channel organic field-effect transistors under ambient conditions. *J. Mater. Chem. C.* **2024**, *12*, 3854–3864.
6. Bomben, A.; Selva, M.; Tundo, P.; Valli, L. A continuous flow *O*-methylation of phenols with dimethyl carbonate in a continuously fed stirred tank reactor. *Ind. Eng. Chem. Res.* **1999**, *38*, 2075–2079.
7. Balsama, S.; Beltrame, P.; Beltrame, P. L.; Carniti, P.; Forni, L.; Zuretti, G. Alkylation of phenol with methanol over zeolites. *Appl. Catal.* **1984**, *13*, 161–170.
8. Beltrame, P.; Beltrame, P. L.; Carniti, P.; Castelli, A.; Forni, L. Alkylation of phenol with anisole over zeolites or γ -alumina. *Appl. Catal.* **1987**, *29*, 327–334.
9. Chada, R.R.; Ketike, T.; Boilla, A.R.; Gangadharam, S.D.; Kamaraju, S.R.R.; Burri, D.R. Preparation and characterization of lanthanum phosphate catalysts for *O*-methylation of phenol to anisole in gas phase. *Mol. Catal.* **2017**, *438*, 224–229.
10. Zhu, X.; Mallinson, R.G.; Resasco, D.E. Role of transalkylation reactions in the conversion of anisole over HZSM-5. *Appl. Catal., A* **2010**, *379*, 172–181.
11. Sad, M.E.; Padró, C.L.; Apesteguía, C.R. Study of the phenol methylation mechanism on zeolites HBEA, HZSM5 and HMCM22. *J. Mol. Catal. A: Chem.* **2010**, *327*, 63–72.
12. Mordí, R.C.; Fields, R.; Dwyer, J. Thermolysis of alkyl aryl ethers catalysed by HZSM-5, P-HZSM-5, H-Theta-1, H-Y and H-Mordenite zeolites. *J. Mol. Catal.* **1994**, *92*, 51–65.
13. Marczewski, M.; Bodibo, J.-P.; Guisnet, M. Alkylation of aromatics: Part I. Reaction network of the alkylation of phenol by methanol on ushy zeolite. *J. Mol. Catal.* **1989**, *50*, 211–218.
14. Tinaco-Sáenz, R.; Alcantara-Avila, J.R.; Mansouri, S.S.; Sánchez-Ramírez, E.; Ramírez-Márquez, C.; Segovia-Hernández, J.G. Design and optimization of an inherently safe and sustainable process for the separation of anisole. *J. Loss Prev. Process Ind.* **2022**, *80*, 104899.
15. Sholl, D.; Lively, R. Seven chemical separations to change the world. *Nature* **532**, 435–437.
16. Lin, J.-M.; He, C.-T.; Liao, P.-Q.; Lin, R.-B.; Zhang, J.-P. Structural, energetic, and dynamic insights into the abnormal xylene separation behavior of hierarchical porous crystal. *Sci. Rep.* **2015**, *5*, 11537.
17. Barton, B.; Senekal, U.; Hosten, E.C. Host compound DED: Guest accommodation type, noncovalent host...guest interactions, crystal densities, and thermal stabilities ensure high host selectivities for 4-methylanisole in anisole and methylanisole mixtures. *Cryst. Growth Des.* **2023**, *23*, 602–611.
18. Barton, B.; Pohl, P.L.; Hosten, E.C. Complexes of host compound (–)-(2*R*,3*R*)-2,3-dimethoxy-1,1,4,4-tetraphenylbutane-1,4-diol (DMT) with guests anisole and the methyl-substituted anisoles: Host selectivity, thermal and single crystal diffraction considerations. *J. Incl. Phenom. Macrocycl. Chem.* **2018**, *92*, 357–367.
19. Barton, B.; Trollip, D.B.; Hosten, E.C. Host behaviour of two tricyclic fused systems in mixed anisole guest solvents. *CrystEngComm* **2023**, *25*, 3013–3024.
20. Vorgers, J.A.; Barton, B.; McClelland, C.W.; Hosten, E.C. Peroxides as host compounds: An investigation of the host ability and selectivity of di-(9-(*p*-trifluoromethylphenyl)xanthen-9-yl) peroxide in anisole/methylanisole mixtures. *Cryst. Growth Des.* **2025**, *25*, 6999–7011.
21. Lehn, J.-M. *Supramolecular Chemistry Concepts and Perspectives*, VCH Verlagsgesellschaft mbH, Weinheim

(Bundesrepublik Deutschland), 1st edn., **1995**.

22. Steed, J.W.; Atwood, J.L. *Supramolecular Chemistry*, Wiley, 3rd Edn., **2022**.

23. Groenewaldt, J.-L.; Barton, B.; Hosten, E.C. The selectivity behaviour of 9,9'-bifluorenyl-9,9'-diol as a host compound for highly efficient separations of mixed pyridines. *CrystEngComm* **2025**, *27*, 4176–4188.

24. Bruker, A. *APEX2, SADABS and SAINT*; Bruker AXS Inc., Madison (WI), USA, **2010**.

25. Sheldrick, G.M. SHELXT - Integrated space-group and crystal-structure determination. *Acta Crystallogr., Sect. A: Found. Adv.* **2015**, *71*, 3–8.

26. Sheldrick, G.M. Crystal structure refinement with SHELXL. *Acta Crystallogr., Sect. C: Struct. Chem.* **2015**, *71*, 3–8.

27. Hübschle, C.B.; Sheldrick, G.M.; Dittrich, B. ShelXle: A Qt graphical user interface for SHELXL. *J. Appl. Crystallogr.* **2011**, *44*, 1281–1284.

28. Bruker, A. *APEX4, SADABS and SAINT*; Bruker AXS Inc., Madison, Wisconsin, USA, **2012**.

29. Farrugia, L.J. WinGX and ORTEP for Windows: An update. *J. Appl. Cryst.* **2012**, *45*, 849–854.

30. Weber, E.; Nitsche, S.; Wierig, A.; Csöregi, I. Inclusion compounds of diol hosts featuring two 9-hydroxy-9-fluorenyl or analogous groups attached to linear spacer units. *Eur. J. Org. Chem.* **2002**, 856–872.

31. Pivovar, A.M.; Holman, K.T.; Ward, M.D. Shape-selective separation of molecular isomers with tunable hydrogen-bonded host frameworks. *Chem. Mater.* **2001**, *13*, 3018–3031.

32. Sykes, N.M.; Su, H.; Weber, E.; Bourne, S.A.; Nassimbeni, L.R. Selective enclathration of methyl- and dimethylpiperidines by fluorene hosts. *Cryst. Growth Des.* **2017**, *17*, 819–826.

33. MacRae, C.F.; Sovago, I.; Cottrell, S.J.; Galek, P.T.A.; McCabe, P.; Pidcock, E.; Platings, M.; Shields, G.P.; Stevens, J.S.; Towler, M.; Wood, P.A. Mercury 4.0: From visualization to analysis, design and prediction. *J. Appl. Crystallogr.* **2020**, *53*, 226–235.

34. Spek, A.L. PLATON SQUEEZE: A tool for the calculation of the disordered solvent contribution to the calculated structure factors. *Acta Crystallogr.* **2015**, *C71*, 9–18.

35. Bourne, S.A.; Charles, J.; Luigi, M.; Weber, E.; Skobridis, K.; Toda, F. Complexation with hydroxy host compounds. Part. 4. Structures and thermal stabilities of inclusion compounds with dioxane as the guest. *J. Chem. Soc., Perkin trans. 2* **1991**, 1707–1713

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