Absolute Configuration of Small Molecules by Co-Crystallization
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**Experimental Procedures**

*Chemicals.* Chemicals were purchased from Sigma-Aldrich (Darmstadt, Germany) and were used without further purification. The syntheses of the tetraaryladmantanes (TAAs) 1,3,5,7-tetrakis(2,4-dimethoxyphenyl)adamantane (TDA) and 1,3,5,7-tetrakis(2,4-diethoxyphenyl)-adamantane (TEO) were performed following published protocols.\(^1\,^2\)

*Chromatography.* For column chromatography, silica gel 60 (0.040-0.063 nm particle size, Macherey-Nagel) was used. Thin layer chromatography (TLC) was performed on Merck Millipore aluminium sheets F\(_{254}\), visualized with UV light (254 nm) and stained with Seebach solution (25 g phosphormolybdic acid hydrate, 10 g cerium(IV) sulfate tetrahydrate, 60 mL conc. sulfuric acid, adjusted to 1 L with water).

*Melting point.* Measurements were performed with a melting point apparatus SMP 40 (Stuart, Staffordshire, UK).

*NMR.* Spectra were recorded on a Bruker AVANCE 300 MHz or 400 MHz spectrometer. The chemical shifts \(\delta\) are reported in ppm. The coupling constants \(J\) are given in Hz.

*Crystallography.* Diffraction data were collected on a KAPPA APEXII DUO diffractometer from Bruker (Karlsruhe, Germany) at 130 K or 135 K using Mo K\(\alpha\) (\(\lambda = 0.71073\) Å) or Cu K\(\alpha\) (\(\lambda = 1.54178\) Å). Cell refinement and data reduction were performed with the SAINT program package.\(^3\) Absorption correction was performed with SADBAS\(^3\). Structures were solved by direct methods using SHELXL97.\(^4\) An isotropic refinement by least-squares methods were also carried out in SHELXL97,\(^4\) followed by anisotropic refinements on F\(_2\) of all non-hydrogen atoms. The positions of the H-atoms were calculated geometrically with riding models. The crystallographic data reported have been deposited with the Cambridge Crystallographic Data Centre (CCDC). The graphics of crystal structures were generated with the programs Mercury 4.0.0 and VMD 1.9.3.

*Computational Strategy for Determining Absolute Configuration.* After the X-ray measurement of the crystal, during the first stage of the computational work, the intensity data appears to be centrosymmetric, although the encapsulated guest molecule is chiral. This is indicated by an \(e^2-1\) statistic value of approx. 1.0. This apparent finding should, of course, be ignored, as it does not properly reflect the structural reality. The apparent result is caused by the strong reflexes originating from host molecules that have established their positions with near-
centrosymmetric symmetry. First, it is necessary to refine the position of these host molecules. Trying to refine the pseudocentric host molecules in an acentric space group results in a co-variance conflict of their nearly centrosymmetric position. To resolve this conflict, it is necessary to introduce temporary restraints, especially in case of the displacement parameters. The shape of the guest molecule becomes distinguishable through the difference Fourier electron density map as the structural model converges. After localization and declaration of the positions of the chiral guest molecule, the temporary restraints can be removed from the refinement calculations. In difficult cases, it can be necessary to introduce additional restraints reflecting known structural properties of the analyte for refinement of the guest molecule(s), especially in case of disorder, where one guest molecule in the unit cell is less well ordered. The absolute structure parameters (e.g. the Flack parameter) are critical for determining that the correct absolute configuration of the guest molecule(s) has been found.
Synthesis of 1,3,5,7-Tetrakis(2-bromo-4-methoxyphenyl)adamantane (TBro)

The title compound was synthesized from 1,3,5,7-adamantanetetraol (TOA), which is accessible from 1,3,5,7-tetrabromo adamantane, which, in turn, is readily prepared from adamantane under Stetter conditions\(^1\). A mixture of TOA (100 mg, 0.5 mmol) and \(p\)-toluenesulfonic acid (95 mg, 0.5 mmol, 1 eq.) was treated with 3-bromoanisol (5.1 mL, 80 eq.). The resulting mixture was heated to 120 °C for 48 h in a Dean Stark apparatus. After cooling to room temperature, the reaction mixture was extracted with CH\(_2\)Cl\(_2\) (50 mL). The resulting solution was washed with saturated NaHCO\(_3\) solution (30 mL), and the aqueous phase was extracted again with CH\(_2\)Cl\(_2\) (30 mL). The combined organic phases were washed with HCl solution (2 M, 30 mL), brine (30 mL), dried over Na\(_2\)SO\(_4\), and concentrated under reduced pressure. The resulting dark brown oil was purified via column chromatography (petroleum ether / CH\(_2\)Cl\(_2\) 2:1 to 1:1 v/v). The solvent was removed under reduced pressure, yielding 86 mg (0.09 mmol, 20%) of 1,3,5,7-tetrakis(2-bromo-4-methoxyphenyl)adamantane as a colorless solid.

TLC (petroleum ether / CH\(_2\)Cl\(_2\) 1:1, v/v), \(R_f = 0.5\); melting point: 296°C; \(^1\)H-NMR (400 MHz, CDCl\(_3\)): \(\delta\) (ppm) = 7.29 (d, \(J = 9.1 \) Hz, 4 H), 7.12 (d, \(J = 2.7 \) Hz, 4 H), 6.77 (dd, \(J = 8.9 \) Hz, 4 H), 3.71 (s, 12 H), 2.64 (s, 12 H). \(^{13}\)C-NMR (75 MHz, CDCl\(_3\)): \(\delta\) (ppm) = 158.1, 138.2, 128.9, 122.4, 121.7, 112.9, 55.5, 41.4, 40.6. APCI-MS \(m/z\) calculated C\(_{38}\)H\(_{36}\)Br\(_4\)O\(_4\) [M\(^{+}\)]: 871.93, found: 871.93. IR (in CDCl\(_3\)): \(\tilde{\nu} = 2935, 2861, 2853, 1599, 1485, 1461, 1437, 1356, 1298, 1228, 1040, 1026, 842.

Spectra and the X-ray crystal structure of the solvate-free form, crystallized from acetic acid, are shown below (Figures S1-3).
NMR Spectra

Figure S1. $^1$H-NMR spectrum of 1,3,5,7-tetrakis(2-bromo-4-methoxyphenyl)adamante (TBro) (300 MHz, CDCl$_3$).

Figure S2. $^{13}$C-NMR spectrum of 1,3,5,7-tetrakis(2-bromo-4-methoxyphenyl)adamante (TBro) (75 MHz, CDCl$_3$).
X-ray Crystal structure
Deposition number CCDC 1970900

Figure S3. X-ray crystal structure of TBrø, re-crystallized from glacial acetic acid.

| Property                                      | Value                        |
|-----------------------------------------------|------------------------------|
| Empirical formula                            | C_{38}H_{36}Br_{4}O_{4}      |
| Formula weight                                | 876.31                       |
| Temperature                                   | 130(2) K                     |
| Wavelength                                    | 0.71073 Å                    |
| Crystal system, space group                   | Triclinic, P -1              |
| Unit cell dimensions                          | a = 14.1889(13) Å, alpha = 84.448(4) ° |
|                                              | b = 15.6498(14) Å, beta = 80.265(3) ° |
|                                              | c = 15.6962(14) Å, gamma = 89.794(4) ° |
| Volume                                        | 3418.8(5) Å³                 |
| Z, Calculated density                         | 4, 1.703 Mg/m³               |
| Absorption coefficient                        | 4.749 mm⁻¹                   |
| F(000)                                        | 1744                         |
| Crystal size                                  | 0.16 x 0.08 x 0.04 mm        |
| Theta range for data collection               | 1.31 to 25.04 °              |
| Limiting indices                              | -16<=h<=16, -18<=k<=18, -13<=l<=18 |
| Reflections collected / unique                | 42638 / 11994 [R(int) = 0.0820] |
| Completeness to theta = 25.04                 | 99.3 %                       |
| Absorption correction                         | Numerical                    |
| Max. and min. transmission                    | 0.9104 and 0.6792            |
| Refinement method                             | Full-matrix least-squares on F² |
| Data / restraints / parameters                | 11994 / 56 / 845             |
| Goodness-of-fit on F²                         | 1.041                        |
| Final R indices [I>2sigma(I)]                 | R1 = 0.0484, wR2 = 0.0656    |
| R indices (all data)                          | R1 = 0.1145, wR2 = 0.0727    |
| Largest diff. peak and hole                   | 1.090 and -0.667 e.A⁻³       |
**General Protocol for Thermal Co-Crystallization**

The following general protocol is for TEO and is representative for thermal crystallization with all three chaperones. For isothermal crystallization, see below (SCC method). To a sample of solid TEO (2 mg, 0.0025 mmol) in a glass vial (1 mL void volume) the liquid analyte (R)-methylbenzylamine (30 mg, 29 µL, 0.25 mmol) was added. The resulting suspension was briefly heated by placing the vial on a heater-stirrer or hot plate until a clear solution formed. To achieve this, the temperature of the hot plate was set to the boiling point of the analyte or a maximum of 150 °C. Then, the heating of the hot plate was switched off, and the solution was allowed to cool to room temperature with the vial on the plate. The set-up was left at room temperature overnight, and a suitable crystal was harvested and then analyzed by X-ray diffraction. Details of the crystallization runs for the analytes shown in Fig. 1 are listed in the following co-crystallization protocols below. The crystallographic results are briefly summarized in Table S1.
**Details for Co-Crystallizations Leading to the Structures Shown in Figures 2 and 3 of the manuscript**

Table S1. Typical amounts of TAA and liquid guest, as used for the crystallization experiments of Figures 2 and 3.

| Chaperone | [mg] | Analyte | [mg] | Crystal system | R1  | Flack parameter\(^a\) |
|-----------|------|---------|------|----------------|-----|---------------------|
| TEO 5     |      | hexamethylenediisocyanate | 50   | triclinic      | 0.0493 |
| TEO 5     |      | cyclopentylisocyanate     | 50   | triclinic      | 0.0556 |
| TEO 5     |      | phenylisocyanate          | 50   | triclinic      | 0.0421 |
| TEO 2     |      | (R)-(+)−α-methylbenzylamine | 30   | triclinic      | 0.0438 | 0.02(13) |
| TEO 2     |      | (S)-(−)−α-methylbenzylamine | 30   | triclinic      | 0.0382 | 0.14(16) |
| TEO 1     |      | (R)-(−)-phenylethanol     | 40   | triclinic      | 0.0484 | −0.1(3) |
| TEO 2     |      | (S)-(−)-phenylethanol     | 40   | triclinic      | 0.0578 | 0.0(5) |
| TEO 2     |      | (R)-2-butanol             | 50   | triclinic      | 0.0622 | −0.07(59) |
| TEO 2     |      | (R)-2-pentanol            | 50   | triclinic      | 0.0735 | −0.6(6) |
| TEO 1     |      | (S)-2-hexanol             | 50   | triclinic      | 0.0540 | −0.04(13) |
| TEO 1     |      | (S)-2-heptanol            | 50   | triclinic      | 0.0434 | −0.06(18) |
| TEO 2     |      | L-tert-leucine methyl ester | 60   | triclinic      | 0.0327 | 0.007(37) |
| TEO 3     |      | (R)-(−)-limonene          | 50   | monoclinic     | 0.0455 | 0.07(14) |
| TEO 3     |      | (S)-(−)-limonene          | 50   | monoclinic     | 0.0475 | 0.2(3) |
| TEO 3     |      | (R)-(−)-carvone           | 30   | triclinic      | 0.0430 | −0.04(12) |
| TEO 3     |      | (S)-(−)-carvone           | 30   | triclinic      | 0.0446 | 0.21(19) |
| TEO 3     |      | (−)-α-thujone             | 30   | triclinic      | 0.0491 | −0.07(20) |
| TEO 5     |      | [12]crown-4              | 50   | triclinic      | 0.0543 |
| TEO 3     |      | (−)-linalool              | 45   | triclinic      | 0.0775 | 0.0(4) |
| TEO 10    |      | nicotine                 | 30   | monoclinic     | 0.0484 | 0.00(8) |
| TEO 3     |      | eugenol                  | 30   | triclinic      | 0.0497 |
| TBro 3    |      | n-decane                 | 50   | triclinic      | 0.1121 |
| TBro 3    |      | geraniol                 | 45   | triclinic      | 0.0864 |
| TBro 2    |      | farnesol                 | 35   | triclinic      | 0.0742 |
| TBro 2    |      | α-humulene               | 45   | triclinic      | 0.0453 |
| TBro 2    |      | muscone                  | 45   | triclinic      | 0.0475 | 0.523(19)\(^b\) |
| TDA 5     |      | (R)-(−)-epichlorohydrine | 35   | triclinic      | 0.0476 | 0.13(15) |
| TDA 5     |      | (S)-(−)-epichlorohydrine | 35   | triclinic      | 0.0523 | 0.143(17) |

\(^a\) Numbers in parentheses are standard deviations. \(^b\) No absolute configuration assigned.
### Overview of Results from Crystallization Runs, Including Unsuccessful Experiments

#### Table S2. Co-Crystallization Experiments Performed.

| Entry No. | Analyte                          | \( M_w \) [g/mol] | \( \log \text{P} \) | TEO (CCDC entry numbers) | TDA (CCDC entry numbers) | TBRO |
|-----------|----------------------------------|-------------------|---------------------|--------------------------|--------------------------|------|
| 1         | acetic acid                       | 60.1              | -0.23               | no incl.                 | no incl.                 | no incl. |
| 2         | propanol                          | 60.1              | 0.56                | no incl.                 | 1040366<sup>ref.1</sup> | -    |
| 3         | cyclopentadiene                   | 66.1              | 1.48                | no incl.                 | 1841018<sup>ref.6</sup> | -    |
| 4         | diethyl ether                     | 74.1              | 1.05                | 1978496                  | -                        | -    |
| 5         | 2-butanol                         | 74.1              | 0.92                | 1987497                  | 1040363<sup>ref.1</sup> | -    |
| 6         | (R)-2-butanol                     | 74.1              | 0.92                | 1994686                  | -                        | -    |
| 7         | trimethylphosphine                | 76.1              | -0.27               | 1978498                  | no incl.                 | -    |
| 8         | pyridine                          | 79.1              | 0.70                | 1978499                  | 1483183<sup>ref.7</sup> incl. conf.<sup>d</sup> | -    |
| 9         | dichloromethane                   | 84.9              | 1.51                | no incl.                 | 1040365<sup>ref.1, e</sup> no incl. | -    |
| 10        | (R)-2-pentanol                    | 88.1              | 1.48                | 1994687                  | -                        | -    |
| 11        | toluene                           | 92.1              | 2.39                | 1981377                  | 1918380                  | -    |
| 12        | (R)-epichlorohydrine              | 92.5              | 0.75                | 1970857                  | -                        | -    |
| 13        | (S)-epichlorohydrine              | 92.5              | 0.75                | 1970865                  | -                        | -    |
| 14        | aniline                           | 93.1              | 1.01                | 1978500                  | no incl.                 | -    |
| 15        | (S)-2-hexanol                     | 102.2             | 1.99                | 1994689                  | -                        | -    |
| 16        | p-xylene                          | 106.1             | 2.83                | 1521514<sup>ref.2</sup> | 1978501                  | -    |
| 17        | cyclopentlysilocyanate            | 111.1             | 1.47                | 1978246                  | no incl.                 | -    |
| 18        | (S)-2-heptanol                    | 116.2             | 2.49                | 1994690                  | -                        | -    |
| 19        | phenylisocyanate                  | 119.1             | 1.77                | 1978248                  | no incl.                 | -    |
| 20        | L-erythulose                      | 120.1             | -2.43               | no crystals              | no crystals              | no crystals |
| 21        | (R)-methylbenzylamine             | 121.2             | -0.20               | 1970890                  | -                        | -    |
| 22        | (S)-methylbenzylamine             | 121.2             | -0.20               | 1970891                  | -                        | -    |
| 23        | (R)-phenylethanol                 | 122.2             | 1.50                | 1970919                  | -                        | -    |
| 24        | (S)-phenylethanol                 | 122.2             | 1.50                | 1970892                  | -                        | -    |
| 25        | cinnamic aldehyde                 | 132.2             | 2.48                | no incl.                 | -                        | -    |
| 26        | \( \alpha \)-pinene               | 136.2             | 3.54                | incl. conf.<sup>d</sup>  | no incl.                 | -    |
| 27        | terpinene                         | 136.2             | 3.36                | incl. conf.<sup>d</sup>  | no incl.                 | -    |
| 28        | (R)-limonene                      | 136.4             | 3.62                | 1970875                  | -                        | -    |
| 29        | (S)-limonene                      | 136.4             | 3.62                | 1970877                  | -                        | -    |
| 30        | n-decane                          | 142.3             | 6.18                | no incl.                 | no incl.                 | 1970895 |
| 31        | methyl-L-pyroglutamate            | 143.1             | -0.33               | no crystals              | no crystals              | -    |
| 32        | L-tert-leucine methyl ester       | 145.2             | 0.74                | 1994691                  | -                        | -    |
| 33        | trans-anethole                    | 148.2             | 3.10                | 1978504                  | -                        | -    |
| 34        | (R)-carvone                       | 150.2             | 2.51                | 1970880                  | -                        | -    |
| 35        | (S)-carvone                       | 150.2             | 2.51                | 1970881                  | -                        | -    |
| 36        | (-)-\( \alpha \)-thujone         | 152.2             | 2.16                | 1970886                  | -                        | -    |
| 37        | (-)-linalool                      | 154.3             | 3.21                | 1970887                  | -                        | -    |
| 38        | (+)-rose oxide                    | 154.3             | 3.11                | no incl.                 | no incl.                 | no incl. |
| 39        | eucalyptol                        | 154.3             | 2.72                | incl. conf.<sup>d</sup>  | incl. conf.<sup>d</sup>  | -    |
| 40        | geraniol                          | 154.3             | 3.20                | no incl.                 | no incl.                 | 1970897 |
| 41        | citronellal                       | 154.3             | 3.60                | no incl.                 | no incl.                 | 1978505 |
| 42        | 2-decanol                         | 158.3             | 4.01                | -                        | -                        | incl. conf.<sup>d</sup> |
| 43        | nicotine                          | 162.2             | 1.09                | 1970888                  | incl. conf.<sup>d</sup>  | -    |
| 44        | eugenol                           | 164.2             | 2.10                | 1970893                  | -                        | -    |
| 45        | 1-(R)-nopol                       | 166.3             | 2.57                | no incl.                 | no incl.                 | no incl. |
| 46        | hexamethyleneisocyanate           | 168.2             | 1.38                | 1970894                  | -                        | -    |
| 47        | [12]crown-4                       | 176.2             | -0.64               | 1970889                  | 1978506                  | -    |
| 48        | geranyl acetate                   | 196.3             | 4.17                | incl. conf.<sup>d</sup>  | no incl.                 | -    |
| 49        | \( \alpha \)-humulene             | 204.4             | 5.30                | -                        | no incl.                 | 1970896 |
| 50        | [15]crown-5                       | 220.3             | -0.85               | no incl.                 | -                        | incl. conf.<sup>d</sup> |
| 51        | farnesol                          | 222.4             | 5.05                | -                        | -                        | 1970899 |
| 52        | muscone                           | 238.4             | 5.72                | -                        | -                        | 1978250<sup>f</sup> |

- **a)** Lipophilicity, calculated as described below (see Table S4).  
- **b)** CCDC entry numbers are given for runs that were successful and led to a high-resolution structure.  
- **c)** bar indicates that this combination of analyte/chaperone was not tested.  
- **d)** inclusion of a guest molecule was confirmed by X-ray, but no high resolution structure was obtained in the first run.  
- **e)** Crystals labile upon exposure to air.  
- **f)** Absolute configuration not assigned.
Results from Determining the Flack Parameter with the Parson Method and Inversion Tests for Critical Cases

Table S3. Flack parameters and results of inversion tests for crystalline inclusion complexes of TEO and different analytes.

| Entry | Analyte                  | χ(μ)  | χ(μ) Parsons* | χ(μ) inversion of coordinates* |
|-------|--------------------------|-------|---------------|-------------------------------|
| 1     | (S)-(−)-α-methylbenzylamine | 0.14(16) | 0.107(85)     | 0.864(86)                     |
| 2     | (R)-(−)-phenylethanol     | -0.1(3)  | -0.13 (30)    | 1.11 (30)                     |
| 3     | (R)-2-pentanol            | -0.6(6)  | -0.59(67)     | 1.52 (68)                     |
| 4     | (S)-(−)-limonene          | 0.2(3)   | 0.15 (26)     | 0.77 (26)                     |
| 5     | (−)-linalool              | 0.0(4)   | 0.04 (37)     | 0.80 (38)                     |

* Test performed with Parsons’ method.
**Additional Results for Spectroscopy cum Crystallization (SCC)**

**Preparation of finely powdered TEO.** A sample of TEO (50 mg, 0.065 mmol) was dissolved in dichloromethane (1 mL), and the solvent was allowed to evaporate at room temperature. The resulting crystals were dried under vacuum (10⁻² mbar). The resulting solid was ground to a finely powdered material with pestle and mortar, and used for isothermal crystallization experiments.

**Isothermal Crystallization.** A sample of nicotine (3 mg, 0.0018 mmol) was dissolved in CD₂Cl₂ (0.2 mL) and was analysed via NMR spectroscopy. The solvent was allowed to evaporate with the help of a nitrogen steam directed onto the surface of the solution for 1 h, and the resulting liquid was treated with finely powdered TEO (1 mg, 1.3 µmol). The mixture was allowed to stand at room temperature for 16 h, and a crystal was selected and then analyzed by X-ray diffraction. This method was also used to prepare a co-crystal with (R)-carvone. The amount of the analyte in this case was 5 mg. The procedure for the co-crystallization of nicotine is shown in Fig. 3 in the main manuscript, a flow chart of the additional experiment with (R)-carvone is shown below (Figure S4).

![Flow chart of the SCC protocol for (R)-carvone as analyte. After NMR, the solvent was allowed to evaporate (a), and finely powdered TEO was added (b). The mixtures were allowed to stand overnight at 20 °C, and a suitable crystal was picked (c), of which X-ray analysis was performed (d), giving the structure shown on the left. Completing the protocol took 3 days, including wait times, handling and computational time.](image-url)

**Figure S4.** Flow chart of the SCC protocol for (R)-carvone as analyte. After NMR, the solvent was allowed to evaporate (a), and finely powdered TEO was added (b). The mixtures were allowed to stand overnight at 20 °C, and a suitable crystal was picked (c), of which X-ray analysis was performed (d), giving the structure shown on the left. Completing the protocol took 3 days, including wait times, handling and computational time.
X-Ray Crystal Structures

Isothermal crystallization

TEO with encapsulated hexamethylenediisocyanate

Deposition number CCDC 1970894

Empirical formula \( \text{C}_{54} \text{H}_{70} \text{N}_{9} \)

Chemical formula moiety \( \text{C}_{50} \text{H}_{64} \text{O}_{8}, 1.5 (\text{C}_{10} \text{H}_{12} \text{O}) \)

Formula weight 877.11

Temperature 130(2) K

Wavelength 0.71073 Å

Crystal system, space group Triclinic, \( P -1 \)

Unit cell dimensions
\( a = 10.1437(6) \) Å, alpha = 107.893(4)°
\( b = 15.1863(11) \) Å, beta = 90.807(4)°
\( c = 16.2657(11) \) Å, gamma = 92.248(3)°

Volume 2381.7(3) Å³

Z, Calculated density 2, 1.223 Mg/m³

Absorption coefficient 0.082 mm⁻¹

F(000) 946

Crystal size 0.46 x 0.33 x 0.33 mm

Theta range for data collection 1.32 to 30.55°

Limiting indices -13<=h<=14, -21<=k<=21, -23<=l<=23

Reflections collected / unique 63863 / 14341 [R(int) = 0.0295]

Completeness to theta = 28.40 98.1 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7459 and 0.7216

Refinement method Full-matrix least-squares on F²

Data / restraints / parameters 14341 / 8 / 594

Goodness-of-fit on F² 1.036

Final R indices [I>2sigma(I)] R1 = 0.0493, wR2 = 0.1245

R indices (all data) R1 = 0.0775, wR2 = 0.1361

Largest diff. peak and hole 0.425 and -0.443 e.Å⁻³
Thermal crystallization

TEO with encapsulated diethylether
Deposition number CCDC 1978496

Empirical Formula  \( \text{C}_54\text{H}_{74}\text{O}_9 \)
Chemical formula moiety  \( \text{C}_{50}\text{H}_{64}\text{O}_8, \text{C}_4\text{H}_{10}\text{O} \)
Formula Weight  867.13
Temperature  130(2) K
Wavelength  0.71073 Å
Crystal system, Space group  Triklin, \( P \)-1
Unit cell dimensions  \( a = 14.4213(15) \text{ Å}, \alpha = 66.074(4)° \)
\( b = 14.4361(16) \text{ Å}, \beta = 81.034(4)° \)
\( c = 15.3195(18) \text{ Å}, \gamma = 61.878(5)° \)
Volume  2568.6(5) \( \text{Å}^3 \)
Z, calculated density  2, 1.121 Mg / m\(^3\)
Absorption coefficient  0.075 mm\(^{-1}\)
\( F(000) \)  940
Crystal size  0.25 x 0.08 x 0.08 mm
Theta range for data collection  1.46 to 25.07 deg.
Limiting indices  \(-17\leq h \leq 17, -17\leq k \leq 17, -18\leq l \leq 18 \)
Reflections collected / unique  33872 / 9050 [R(int) = 0.0709]
Completeness to theta = 25.07  99.2 %
Absorption correction  Semi-empirical from equivalents
Max. and min. transmission  0.7452 and 0.6961
Refinement method  Full-matrix least-squares on \( F^2 \)
Data / restraints / parameters  9050 / 110 / 615
Goodness-of-fit on \( F^2 \)  1.033
Final R indices [I>2\sigma(I)]  \( R_1 = 0.0564, \text{wR}2 = 0.1031 \)
R indices (all data)  \( R_1 = 0.1394, \text{wR}2 = 0.1168 \)
Extinction coefficient  0.0019(4)
Largest diff. peak and hole  0.336 and -0.284 e\( \text{Å}^{-3} \)
TEO with encapsulated butanol
Deposition number CCDC 1987497

Empirical Formula: $\text{C}_{54}\text{H}_{64}\text{O}_{9}$
Chemical formula moiety: $\text{C}_{50}\text{H}_{64}\text{O}_{8}$, $\text{C}_{4}\text{O}$
Formula Weight: 857.05
Temperature: 130(2) K
Wavelength: 0.71073 Å
Crystal system, Space group: Triklin, P-1
Unit cell dimensions:
- $a = 14.275(4)$ Å, $\alpha = 66.175(7)^\circ$
- $b = 14.417(3)$ Å, $\beta = 81.314(8)^\circ$
- $c = 15.299(4)$ Å, $\gamma = 62.635(7)^\circ$
Volume: $2555.5(11)$ Å$^3$
Z, calculated density: 2, 1.114 Mg / m$^3$
Absorption coefficient: 0.089 mm$^{-1}$
$F(000)$: 3104
Crystal size: 0.29 x 0.21 x 0.06 mm
Theta range for data collection: 1.54 to 25.06 deg.
Limiting indices: $-25 \leq h \leq 19, -20 \leq k \leq 20, -24 \leq l \leq 24$
Reflections collected / unique: 63363 / 13249 [$R(int) = 0.0825$]
Completeness to theta = 25.06: 99.7 %
Absorption correction: Semi-empirical from equivalents
Max. and min. transmission: 0.7381 and 0.7159
Refinement method: Full-matrix least-squares on $F^2$
Data / restraints / parameters: 13249 / 0 / 973
Goodness-of-fit on $F^2$: 1.020
Final R indices [I>2sigma(I)]: $R1 = 0.0483$, $wR2 = 0.0826$
R indices (all data): $R1 = 0.1189$, $wR2 = 0.0942$
Largest diff. peak and hole: 0.331 and -0.323 eÅ$^{-3}$
**TEO with encapsulated trimethylphosphine**

Deposition number CCDC 1978498

Empirical Formula  
\[ \text{C}_{53}\text{H}_{73}\text{O}_{8}\text{P} \]

Chemical formula moiety  
\[ \text{C}_{50}\text{H}_{64}\text{O}_{8}, \text{C}_{3}\text{H}_{9}\text{P} \]

Formula Weight  
869.08

Temperature  
130(2) K

Wavelength  
0.71073 Å

Crystal system, Space group  
Triklin, P-1

Unit cell dimensions  
\[ \begin{align*}
    a &= 14.2962(8) \text{ Å}, \alpha = 65.251(2)^\circ \\
    b &= 14.3687(7) \text{ Å}, \beta = 80.473(2)^\circ \\
    c &= 15.4169(8) \text{ Å}, \gamma = 62.881(2)^\circ 
\end{align*} \]

Volume  
2558.6(2) Å\(^3\)

Z, calculated density  
2, 1.128 Mg / m\(^3\)

Absorption coefficient  
0.104 mm\(^{-1}\)

F(000)  
940

Crystal size  
0.31 x 0.28 x 0.19 mm

Theta range for data collection  
1.46 to 26.49 deg.

Limiting indices  
-17 <= h <= 17, -17 <= k <= 16, -19 <= l <= 19

Reflections collected / unique  
37097 / 10490 [R(int) = 0.0391]

Completeness to theta = 26.49  
99.1 %

Absorption correction  
Semi-empirical from equivalents

Max. and min. transmission  
0.7454 and 0.7273

Refinement method  
Full-matrix least-squares on F\(^2\)

Data / restraints / parameters  
10490 / 18 / 571

Goodness-of-fit on F\(^2\)  
1.047

Final R indices [I>2sigma(I)]  
R1 = 0.0469, wR2 = 0.1099

R indices (all data)  
R1 = 0.0833, wR2 = 0.1213

Extinction coefficient  
0.0016(4)

Largest diff. peak and hole  
0.492 and -0.460 e.A\(^{-3}\)
# TEO with encapsulated pyridine

Deposition number CCDC 1978499

| Property                          | Value                          |
|----------------------------------|-------------------------------|
| Empirical Formula                | C<sub>55</sub>H<sub>69</sub>N O<sub>4</sub> |
| Chemical formula moiety          | C<sub>50</sub>H<sub>64</sub> O<sub>8</sub>, C<sub>5</sub> H<sub>5</sub> N |
| Formula weight                   | 872.11                         |
| Temperature                      | 130(2) K                       |
| Wavelength                       | 0.71073 Å                      |
| Crystal system, space group      | Triclinic, P -1                |
| Unit cell dimensions             | a = 14.2867(10) Å, alpha = 80.747(4) ° |
|                                  | b = 14.3851(11) Å, beta = 66.126(4) ° |
|                                  | c = 15.2332(11) Å, gamma = 62.413(3) ° |
| Volume                           | 2535.9(3) Å<sup>3</sup>        |
| Z, Calculated density            | 2, 1.142 Mg/m<sup>3</sup>      |
| Absorption coefficient           | 0.075 mm<sup>-1</sup>         |
| F(000)                           | 940                            |
| Crystal size                     | 0.41 x 0.38 x 0.17 mm          |
| Theta range for data collection  | 1.60 to 27.50 °                |
| Limiting indices                 | -18<=h<=18, -18<=k<=18, -17<=l<=19 |
| Reflections collected / unique   | 50597 / 11505 [R(int) = 0.0523] |
| Completeness to theta = 27.50    | 98.8 %                         |
| Absorption correction            | Semi-empirical from equivalents |
| Max. and min. transmission       | 0.7457 and 0.6633              |
| Refinement method                | Full-matrix least-squares on F<sup>2</sup> |
| Data / restraints / parameters   | 11505 / 6 / 585                |
| Goodness-of-fit on F<sup>2</sup> | 1.038                          |
| Final R indices [I>2sigma(I)]    | R1 = 0.0538, wR2 = 0.1316      |
| R indices (all data)             | R1 = 0.0938, wR2 = 0.1464      |
| Largest diff. peak and hole      | 0.360 and -0.303 e.A<sup>-3</sup> |
**TEO with encapsulated toluene**
Deposition number CCDC 1918377

```
Empirical formula       C_{57}H_{72}O_{8}
Chemical formula moiety C_{50}H_{64}O_{8}, C_{7}H_{8}
Formula weight         885.15
Temperature            130(2) K
Wavelength             0.71073 Å
Crystal system, space group Triclinic, \textit{P}-1
Unit cell dimensions   
a = 14.3582(10) Å,   \alpha = 66.280(4)°
b = 14.3961(10) Å,   \beta = 80.730(4)°
c = 15.2506(11) Å,   \gamma = 62.883(3)°
Volume                 2567.8(3) Å³
Z, Calculated density  2, 1.145 Mg/m³
Absorption coefficient 0.075 mm⁻¹
F(000)                 956
Crystal size           0.31 x 0.14 x 0.09 mm
Theta range for data collection 1.46 to 26.44°
Limiting indices      -17<=h<=17, -18<=k<=18, -18<=l<=19
Reflections collected / unique 50580 / 10471 \textit{[R(int) = 0.0580]}
Completeness to theta = 26.44 99.2 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7380 and 0.7064
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 10471 / 0 / 597
Goodness-of-fit on F² 1.022
Final R indices [I>2sigma(I)] R1 = 0.0503, wR2 = 0.0921
R indices (all data) R1 = 0.1024, wR2 = 0.1018
Extinction coefficient 0.0025(3)
Largest diff. peak and hole 0.353 and -0.250 e.A⁻³
```
TEO with encapsulated aniline
Deposition number CCDC 1978500

Empirical formula: C_{56}H_{71}NO_{8}
Chemical formula moiety: C_{50}H_{64}O_{8}, C_{6}H_{7}N
Formula Weight: 886.14
Temperature: 130(2) K
Wavelength: 0.71073 Å
Crystal system, Space group: Triclinic, P-1
Unit cell dimensions:
- a = 14.2548(8) Å, alpha = 80.693(4)°
- b = 14.3536(9) Å, beta = 66.400(3)°
- c = 15.2724(9) Å, gamma = 63.390(3)°
Volume: 2559.6(3) Å³
Z, calculated density: 2, 1.150 Mg / m³
Absorption coefficient: 0.076 mm⁻¹
F(000): 956
Crystal size: 0.88 x 0.59 x 0.37 mm
Theta range for data collection: 1.72 to 30.59 deg.
Limiting indices: -20≤h≤20, -20≤k≤20, -21≤l≤21
Reflections collected / unique: 78230 / 15465 [R(int) = 0.0340]
Completeness to theta = 30.59: 98.1%
Absorption correction: Semi-empirical from equivalents
Max. and min. transmission: 0.7461 and 0.7075
Refinement method: Full-matrix least-squares F²
Data / restraints / parameters: 15465 / 16 / 621
Godness-of-fit on F²: 1.036
Final R indices [I>2σ(I)]: R1 = 0.0526, wR2 = 0.1328
R indices (all data): R1 = 0.0833, wR2 = 0.1591
Largest diff. peak and hole: 0.431 and -0.390 e Å⁻³
TEO with encapsulated cyclopentylisocyanate
Deposition number CCDC 1978246

Empirical formula \( \text{C}_{56} \text{H}_{73} \text{N}_6 \text{O}_9 \)
Chemical formula moiety \( \text{C}_{30} \text{H}_{64} \text{O}_8, \text{C}_6 \text{H}_9 \text{N}_6 \text{O}_9 \)
Formula weight 904.15
Temperature 130(2) K
Wavelength 0.71073 Å
Crystal system, space group Triclinic, \( \text{P} - \text{1} \)
Unit cell dimensions \( a = 14.3202(7) \) Å, \( \alpha = 65.832(2) ^\circ \)
\( b = 14.3970(7) \) Å, \( \beta = 81.410(3) ^\circ \)
\( c = 15.4246(8) \) Å, \( \gamma = 62.634(2) ^\circ \)
Volume 2573.7(2) Å\(^3\)
Z, Calculated density 2, 1.167 Mg/m\(^3\)
Absorption coefficient 0.078 mm\(^{-1}\)
\( F(000) \) 976
Crystal size 0.36 x 0.24 x 0.11 mm
Theta range for data collection 1.45 to 28.33 °
Limiting indices -19<=h<=19, -19<=k<=19, -20<=l<=20
Reflections collected / unique 50800 / 12766 [R(int) = 0.0380]
Completeness to theta = 28.33 99.5 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7457 and 0.7295
Refinement method Full-matrix least-squares on \( F^2 \)
Data / restraints / parameters 12766 / 12 / 603
Goodness-of-fit on \( F^2 \) 1.045
Final R indices [I>2sigma(I)] \( R_1 = 0.0556, wR_2 = 0.1363 \)
R indices (all data) \( R_1 = 0.0903, wR_2 = 0.1478 \)
Largest diff. peak and hole 0.598 and -0.403 e.A\(^{-3}\)
TEO with encapsulated phenylisocyanate
Deposition number CCDC 1978248

Empirical formula          \[ C_{57} H_{69} N O_9 \]
Chemical formula moiety    \[ C_{50} H_{64} O_8, C_7 H_5 N O \]
Formula weight             912.13
Temperature                130(2) K
Wavelength                 0.71073 Å
Crystal system, space group Triclinic, P -1
Unit cell dimensions       
\[
\begin{align*}
  a &= 14.3343(12) \ \text{Å}, \quad \alpha = 81.323(3) \ ^\circ \\
  b &= 14.5135(13) \ \text{Å}, \quad \beta = 67.224(3) \ ^\circ \\
  c &= 15.2767(13) \ \text{Å}, \quad \gamma = 62.568(2) \ ^\circ 
\end{align*}
\]
Volume                     2599.4(4) Å³
Z, Calculated density      2, 1.165 Mg/m³
Absorption coefficient     0.078 mm⁻¹
F(000)                     980
Crystal size               0.51 x 0.12 x 0.11 mm
Theta range for data collection 1.45 to 25.40°
Limiting indices          
\[-17 \leq h \leq 17, -14 \leq k \leq 17, -18 \leq l \leq 18\]
Reflections collected / unique 33759 / 9452 [R(int) = 0.0273]
Completeness to theta = 25.40° 98.7 %
Absorption correction     Semi-empirical from equivalents
Max. and min. transmission 0.7452 and 0.7088
Refinement method          Full-matrix least-squares on F²
Data / restraints / parameters 9452 / 12 / 612
Goodness-of-fit on F²      1.042
Final R indices [I>2sigma(I)] R1 = 0.0421, wR2 = 0.1019
R indices (all data)        R1 = 0.0652, wR2 = 0.1094
Largest diff. peak and hole 0.487 and -0.354 e.Å⁻³
TEO with encapsulated trans-anethol
Deposition number CCDC 1978504

Empirical formula \( \text{C}_{65} \text{H}_{82} \text{O}_{9.50} \)
Chemical formula moiety \( \text{C}_{50} \text{H}_{64} \text{O}_{8}, 1.5 (\text{C}_{10} \text{H}_{12} \text{O}) \)
Formula weight 1015.31
Temperature 130(2) K
Wavelength 0.71073 Å
Crystal system, space group Triclinic, \( P \)-1
Unit cell dimensions \( a = 10.1781(7) \) Å, \( \alpha = 102.758(3) \)°
\( b = 14.9909(9) \) Å, \( \beta = 98.736(4) \)°
\( c = 19.2143(13) \) Å, \( \gamma = 92.767(3) \)°
Volume 2815.9(3) Å³
Z, Calculated density 2, 1.197 Mg/m³
Absorption coefficient 0.079 mm⁻¹
\( F(000) \) 1096
Crystal size 0.40 x 0.30 x 0.13 mm
Theta range for data collection 1.57 to 28.40 °
Limiting indices \( -13 \leq h \leq 13, -20 \leq k \leq 19, -25 \leq l \leq 25 \)
Reflections collected / unique 61203 / 13964 \{R(int) = 0.0379\}
Completeness to theta = 28.40 98.8 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7457 and 0.7254
Refinement method Full-matrix least-squares on \( F^2 \)
Data / restraints / parameters 13964 / 113 / 855
Goodness-of-fit on \( F^2 \) 1.038
Final R indices \{I>2\sigma(I)\} \( R1 = 0.0452, \text{wR2} = 0.0930 \)
R indices (all data) \( R1 = 0.0843, \text{wR2} = 0.1020 \)
Largest diff. peak and hole 0.303 and -0.229 e.Å⁻³
**TEO with encapsulated eugenol**

Deposition number CCDC 1970893

| Property                        | Value                                      |
|---------------------------------|--------------------------------------------|
| Empirical formula               | C_{60}H_{76}O_{10}                         |
| Chemical formula moiety         | C_{50}H_{64}O_{8}, C_{10}H_{12}O_{2}       |
| Formula weight                  | 957.21                                     |
| Temperature                     | 130(2) K                                   |
| Wavelength                      | 0.71073 Å                                  |
| Crystal system, space group     | Triclinic, P -1                            |
| Unit cell dimensions            | a = 13.8726(7) Å, alpha = 83.624(3) °      |
|                                | b = 14.3311(7) Å, beta = 70.760(2) °       |
|                                | c = 15.5635(8) Å, gamma = 67.297(3) °      |
|                                | Volume = 2694.5(2) Å³                      |
| Z, Calculated density           | 2, 1.180 Mg / m³                           |
| Absorption coefficient          | 0.079 mm⁻¹                                 |
| F(000)                          | 1032                                       |
| Crystal size                    | 0.58 x 0.58 x 0.39 mm                      |
| Theta range for data collection | 1.68 to 30.54 °                            |
| Limiting indices                | -19<=h<=19, -20<=k<=20, -22<=l<=22          |
| Reflections collected / unique  | 65512 / 16433 [R(int) = 0.0380]            |
| Completeness to theta = 30.54   | 99.5 %                                     |
| Absorption correction          | Semi-empirical from equivalents            |
| Max. and min. transmission      | 0.7449 and 0.7193                          |
| Refinement method               | Full-matrix least-squares on F²            |
| Data / restraints / parameters  | 16433 / 41 / 682                           |
| Goodness-of-fit on F²           | 1.031                                      |
| Final R indices [I>2sigma(I)]   | R1 = 0.0497, wR2 = 0.1122                  |
| R indices (all data)            | R1 = 0.0873, wR2 = 0.1227                  |
| Largest diff. peak and hole     | 0.357 and -0.412 e.A⁻³                    |
**TEO with encapsulated [12]crown-4**

Deposition number CCDC 1970889

| Property                                      | Value                                      |
|-----------------------------------------------|--------------------------------------------|
| Empirical formula                            | C_{58}H_{80}O_{12}                         |
| Chemical formula moiety                      | C_{50}H_{64}O_{8}, C_{8}H_{16}O_{4}        |
| Formula weight                                | 969.22                                     |
| Temperature                                   | 130(2) K                                   |
| Wavelength                                    | 0.71073 Å                                  |
| Crystal system, space group                   | Triclinic, P -1                            |
| Unit cell dimensions                          | a = 14.4880(12) Å, alpha = 104.163(6) °    |
|                                              | b = 14.6428(12) Å, beta = 99.732(5) °      |
|                                              | c = 15.949(2) Å, gamma = 119.180(4) °      |
|                                              | 2693.0(5) Å^3                             |
| Volume                                        | 2, 1.195 Mg/m^3                            |
| Z, Calculated density                         | 0.082 mm^-1                                |
| Absorption coefficient                        | 1048                                       |
| F(000)                                        | 39955 / 10965 [R(int) = 0.0723]             |
| Crystal size                                  | 0.75 x 0.18 x 0.07 mm                      |
| Theta range for data collection               | 1.62 to 26.47 °                            |
| Limiting indices                              | -18<=h<=18, -18<=k<=18, -15<=l<=19         |
| Reflections collected / unique                | 98.5 %                                     |
| Completeness to theta = 26.47                 | Semi-empirical from equivalents            |
| Absorption correction                         | 0.7454 and 0.6967                          |
| Max. and min. transmission                    | Full-matrix least-squares on F^2           |
| Refinement method                             | 10965 / 146 / 748                          |
| Data / restraints / parameters                | 1.038                                       |
| Goodness-of-fit on F^2                        | R1 = 0.0543, wR2 = 0.0824                  |
| Final R indices [I>2sigma(I)]                 | R1 = 0.1355, wR2 = 0.0927                  |
| R indices (all data)                          | 0.399 and -0.228 e.A^-3                    |
**TEO with encapsulated (R)-(+)–α-methylbenzylamine**

Deposition number CCDC 1970890

| Property                                      | Value                                      |
|-----------------------------------------------|--------------------------------------------|
| Empirical formula                             | C_{58}H_{75}N_{5}O_{8}                     |
| Chemical formula moiety                       | C_{50}H_{64}O_{8}, C_{8}H_{11}N             |
| Formula weight                                | 914.19                                     |
| Temperature                                   | 130(2) K                                   |
| Wavelength                                    | 1.54178 Å                                  |
| Crystal system, space group                   | Triclinic, P 1                             |
| Unit cell dimensions                          | a = 14.3722(10) Å, alpha = 66.835(3) °     |
|                                              | b = 14.5566(11) Å, beta = 81.054(3) °     |
|                                              | c = 15.2786(11) Å, gamma = 62.648(2) °   |
| Volume                                        | 2608.9(3) Å \(^3\)                        |
| Z, Calculated density                         | 2.164 Mg/m\(^3\)                          |
| Absorption coefficient                        | 0.603 mm\(^{-1}\)                         |
| F(000)                                        | 988                                        |
| Crystal size                                  | 0.35 x 0.31 x 0.16 mm                      |
| Theta range for data collection               | 3.15 to 65.60 °                            |
| Limiting indices                              | -16 <= h <= 16, -16 <= k <= 17, -17 <= l <= 17 |
| Reflections collected / unique                | 78599 / 16301 [R(int) = 0.0373]            |
| Completeness to theta                         | 97.8 %                                     |
| Absorption correction                         | Semi-empirical from equivalents            |
| Max. and min. transmission                    | 0.7528 and 0.6401                          |
| Refinement method                             | Full-matrix least-squares on F\(^2\)       |
| Data / restraints / parameters                | 16301 / 20 / 1248                          |
| Goodness-of-fit on F\(^2\)                   | 1.040                                      |
| Final R indices [I>2sigma(I)]                 | R1 = 0.0348, wR2 = 0.0860                  |
| R indices (all data)                          | R1 = 0.0366, wR2 = 0.0875                  |
| Absolute structure parameter                  | 0.02(13)                                   |
| Extinction coefficient                        | 0.00183(9)                                 |
| Largest diff. peak and hole                   | 0.304 and -0.226 e.Å\(^3\)                |
TEO with encapsulated (S)-(-)-α-methylbenzylamine

Deposition number CCDC 1970891

Empirical formula $C_{58}H_{75}N\text{O}_4$
Chemical formula moiety $C_{50}\text{H}_{64}\text{O}_8, C_8\text{H}_{11}\text{N}$
Formula weight 914.19
Temperature 130(2) K
Wavelength 1.54178 Å
Crystal system, space group Triclinic, P 1
Unit cell dimensions $a = 14.3741(9)$ Å, $\alpha = 66.835(3)$ °
$b = 14.5412(9)$ Å, $\beta = 81.037(3)$ °
$c = 15.2939(10)$ Å, $\gamma = 62.669(4)$ °
Volume 2609.7(3) Å$^3$
Z, Calculated density 2, 1.163 Mg/m$^3$
Absorption coefficient 0.603 mm$^{-1}$
F(000) 988
Crystal size 0.30 x 0.27 x 0.13 mm
Theta range for data collection 3.14 to 65.58 °
Limiting indices $-16<=h<=16, -16<=k<=17, -17<=l<=17$
Reflections collected / unique 65878 / 16152 [R(int) = 0.0442]
Completeness to theta = 65.58 97.7 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7430 and 0.6648
Refinement method Full-matrix least-squares on F$^2$
Data / restraints / parameters 16152 / 35 / 1250
Goodness-of-fit on F$^2$ 1.026
Final R indices [I>2sigma(I)] $R_1 = 0.0382, wR_2 = 0.0968$
R indices (all data) $R_1 = 0.0454, wR_2 = 0.1014$
Absolute structure parameter 0.14(16)
Extinction coefficient 0.00110(8)
Largest diff. peak and hole 0.368 and -0.220 e.A$^{-3}$
TEO with encapsulated (S)-(-)-phenylethanol

Deposition number CCDC 1970892

Empirical formula

C_{58}H_{74}O_9

Chemical formula moiety

C_{50}H_{64}O_8, C_8H_{10}O

Formula weight

915.17

Temperature

135(2) K

Wavelength

1.54178 Å

Crystal system, space group

Triclinic, P1

Unit cell dimensions

a = 14.3361(6) Å, alpha = 66.353(3)°
b = 14.5857(7) Å, beta = 80.968(3)°
c = 15.2184(6) Å, gamma = 63.199(2)°

Volume

2600.8(2) Å³

Z, Calculated density

2, 1.169 Mg/m³

Absorption coefficient

0.615 mm⁻¹

F(000)

988

Crystal size

0.116 x 0.060 x 0.032 mm

Theta range for data collection

3.171 to 65.597°

Limiting indices

-16<=h<=16, -17<=k<=17, -17<=l<=14

Reflections collected / unique

41551 / 15528 [R(int) = 0.1143]

Completeness to theta = 65.597°

97.3%

Absorption correction

Semi-empirical from equivalents

Max. and min. transmission

0.8455 and 0.7667

Refinement method

Full-matrix least-squares on F²

Data / restraints / parameters

15528 / 82 / 1228

Goodness-of-fit on F²

1.054

Final R indices [I>2sigma(I)]

R1 = 0.0578, wR2 = 0.0946

R indices (all data)

R1 = 0.1342, wR2 = 0.1093

Absolute structure parameter

0.0(5)

Extinction coefficient

0.00057(7)

Largest diff. peak and hole

0.293 and -0.268 e.A⁻³
### TEO with encapsulated \((R)-(\pm)\)-phenylethanol

Deposition number CCDC 1970919

| Property                               | Value                        |
|----------------------------------------|------------------------------|
| Empirical formula                      | C_{58} H_{74} O_9            |
| Chemical formula moiety                | C_{50} H_{64} O_8, C_{8} H_{10} O |
| Formula weight                         | 915.17                       |
| Temperature                            | 135(2) K                     |
| Wavelength                             | 1.54178 Å                    |
| Crystal system, space group            | Triclinic, P1                |
| Unit cell dimensions                   | a = 14.3329(5) Å, alpha = 66.414(2) ° |
|                                        | b = 14.5859(5) Å, beta = 80.995(3) ° |
|                                        | c = 15.2067(6) Å, gamma = 63.215(2) ° |
| Volume                                 | 2599.80(17) Å³               |
| Z, Calculated density                  | 2, 1.169 Mg/m³                |
| Absorption coefficient                 | 0.615 mm⁻¹                   |
| F(000)                                 | 988                          |
| Crystal size                           | 0.120 x 0.051 x 0.047 mm     |
| Theta range for data collection        | 3.172 to 65.583 °            |
| Limiting indices                       | -16<=h<=16, -16<=k<=16, -17<=l<=17 |
| Reflections collected / unique         | 44215 / 15510 [R(int) = 0.0738] |
| Completeness to theta = 65.597         | 97.2 %                       |
| Absorption correction                  | Semi-empirical from equivalents |
| Max. and min. transmission             | 0.8532 and 0.7732            |
| Refinement method                      | Full-matrix least-squares on F^2 |
| Data / restraints / parameters         | 15510 / 88 / 1228            |
| Goodness-of-fit on F²                  | 1.040                        |
| Final R indices [I>2sigma(I)]          | R1 = 0.0484, wR2 = 0.0959    |
| R indices (all data)                   | R1 = 0.0872, wR2 = 0.1068    |
| Absolute structure parameter           | -0.1(3)                      |
| Extinction coefficient                 | 0.00063(9)                   |
| Largest diff. peak and hole            | 0.256 and -0.207 e.A⁻³       |
TEO with encapsulated (R)-2-butanol
Deposition number CCDC 1994686

Empirical formula \( C_{54} H_{74} O_9 \)
Chemical formula moiety \( C_{50} H_{64} O_8, C_4 H_{10} O \)
Formula weight 867.13
Temperature 135(2) K
Wavelength 1.54178 Å
Crystal system, space group Triclinic, \( P1 \)
Unit cell dimensions
\( a = 14.2731(6) \) Å, \( \alpha = 66.167(4)^\circ \)
\( b = 14.4160(6) \) Å, \( \beta = 81.314(4)^\circ \)
\( c = 15.3122(8) \) Å, \( \gamma = 62.588(3)^\circ \)
Volume 2556.0(2) Å\(^3\)
Z, Calculated density 2, 1.127 Mg/m\(^3\)
Absorption coefficient 0.598 mm\(^{-1}\)
\( F(000) \) 940
Crystal size 0.322 x 0.063 x 0.055 mm
Theta range for data collection 3.158 to 65.599 °
Limiting indices \(-16<=h<=16, -16<=k<=16, -17<=l<=17\)
Reflections collected / unique 39266 / 15134 \( [R(int) = 0.1378] \)
Completeness to theta = 65.599 % 96.9 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7335 and 0.6470
Refinement method Full-matrix least-squares on \( F^2 \)
Data / restraints / parameters 15134 / 189 / 1152
Goodness-of-fit on \( F^2 \) 1.004
Final \( R \) indices \([I>2\sigma(I)]\) \( R1 = 0.0622, wR2 = 0.1102 \)
R indices (all data) \( R1 = 0.1580, wR2 = 0.1319 \)
Absolute structure parameter \(-0.07(59)\)
Extinction coefficient 0.00089(12)
Largest diff. peak and hole 0.363 and -0.242 e.A\(^{-3}\)
**TEO with encapsulated (R)-2-pentanol**
Deposition number CCDC 1994687

- **Empirical formula**: C_{55}H_{76}O_{9}
- **Chemical formula moiety**: C_{50}H_{64}O_{8}, C_{5}H_{12}O
- **Formula weight**: 881.15
- **Temperature**: 135(2) K
- **Wavelength**: 1.54178 Å
- **Crystal system, space group**: Triclinic, P1
- **Unit cell dimensions**: a = 14.3193(11) Å, alpha = 66.376(6)°
b = 14.4409(12) Å, beta = 81.325(7)°
c = 15.3156(12) Å, gamma = 62.583(6)°
- **Volume**: 2573.5(4) Å³
- **Z, Calculated density**: 2, 1.137 Mg/m³
- **Absorption coefficient**: 0.601 mm⁻¹
- **F(000)**: 956
- **Crystal size**: 0.101 x 0.051 x 0.040 mm
- **Theta range for data collection**: 3.15° to 65.59°
- **Limiting indices**: -16<=h<=16, -17<=k<=16, -17<=l<=17
- **Reflections collected / unique**: 42424 / 15327 [R(int) = 0.2217]
- **Completeness to theta = 65.599°**: 97.2 %
- **Absorption correction**: Semi-empirical from equivalents
- **Max. and min. transmission**: 0.8307 and 0.7336
- **Refinement method**: Full-matrix least-squares on F²
- **Data / restraints / parameters**: 15327 / 859 / 1169
- **Goodness-of-fit on F²**: 0.938
- **Final R indices [I>2sigma(I)]**: R1 = 0.0735, wR2 = 0.1219
- **R indices (all data)**: R1 = 0.2252, wR2 = 0.1521
- **Absolute structure parameter**: -0.6(6)
- **Extinction coefficient**: 0.00074(10)
- **Largest diff. peak and hole**: 0.440 and -0.294 e Å⁻³
**TEO with encapsulated (S)-2-hexanol**

Deposition number CCDC 1994689

| Property                                      | Value                                           |
|-----------------------------------------------|-------------------------------------------------|
| Empirical formula                            | C_{56}H_{78}O_{9}                              |
| Chemical formula moiety                      | C_{50}H_{64}O_8, C_6H_{14}O                     |
| Formula weight                                | 895.18                                         |
| Temperature                                   | 135(2) K                                       |
| Wavelength                                    | 1.54178 Å                                      |
| Crystal system, space group                   | Triclinic, P1                                  |
| Unit cell dimensions                          | a = 14.3846(5) Å, alpha = 66.280(2)°           |
| Volume                                        | b = 14.4844(5) Å, beta = 81.201(2)°             |
|                                               | c = 15.3876(6) Å, gamma = 62.364(3)°           |
|                                               | 2597.95(18) Å                                   |
| Z, Calculated density                         | 2, 1.144 Mg/m³                                  |
| Absorption coefficient                        | 0.602 mm⁻¹                                     |
| F(000)                                        | 972                                            |
| Crystal size                                  | 0.125 x 0.118 x 0.102 mm                       |
| Theta range for data collection               | 3.140 to 65.591 °                              |
| Limiting indices                              | -15<=h<=16, -17<=k<=16, -18<=l<=18              |
| Reflections collected / unique                | 64295 / 15687 [R(int) = 0.0626]                 |
| Completeness to theta                         | 97.8 %                                         |
| Absorption correction                         | Semi-empirical from equivalents                |
| Max. and min. transmission                    | 0.8642 and 0.7209                              |
| Refinement method                             | Full-matrix least-squares on F^2               |
| Data / restraints / parameters                | 15687 / 201 / 1192                             |
| Goodness-of-fit on F^2                        | 1.039                                          |
| Final R 30indices [I>2sigma(I)]              | R1 = 0.0540, wR2 = 0.1383                       |
| R 30ndices (all data)                         | R1 = 0.0694, wR2 = 0.1473                      |
| Absolute structure parameter                  | -0.04(13)                                      |
| Extinction coefficient                        | 0.00081(15)                                    |
| Largest diff. peak and hole                   | 0.775 and -0.397 e.A⁻³                         |
TEO with encapsulated (S)-2-heptanol

Deposition number CCDC 1994690

Empirical formula C_{53.50}H_{72}O_{8.50}
Chemical formula moiety C_{50}H_{64}O_{8} 0.5 (C_{7}H_{16}O)
Formula weight 851.11
Temperature 135(2) K
Wavelength 1.54178 Å
Crystal system, space group Triclinic, P1
Unit cell dimensions a = 10.0988(5) Å, alpha = 73.122(3)°
b = 15.4750(7) Å, beta = 88.900(3)°
c = 16.1909(8) Å, gamma = 87.936(2)°
Volume 2419.6(2) Å³
Z, Calculated density 2, 1.168 Mg/m³
Absorption coefficient 0.615 mm⁻¹
F(000) 922
Crystal size 0.242 x 0.052 x 0.049 mm
Theta range for data collection 2.852 to 66.410°
Limiting indices -11<=h<=11, -15<=k<=18, -19<=l<=18
Reflections collected / unique 46772 / 14660 [R(int) = 0.0603]
Completeness to theta = 66.410 96.7 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7475 and 0.6845
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 14660 / 3 / 1137
Goodness-of-fit on F² 1.028
Final R indices [I>2sigma(I)] R1 = 0.0434, wR2 = 0.1003
R indices (all data) R1 = 0.0683, wR2 = 0.1101
Absolute structure parameter -0.06(18)
Extinction coefficient 0.00079(14)
Largest diff. peak and hole 0.213 and -0.226 e.A⁻³
TEO with encapsulated \(L\)-\(\text{tert}\)-leucine methyl ester

Deposition number CCDC 1994691

**Empirical formula**  \(C_{57}H_{79}N_{10}O_{10}\)  
**Chemical formula moiety**  \(C_{50}H_{64}O_8, C_7H_{15}N_2O_2\)  
**Formula weight**  938.21  
**Temperature**  135(2) K  
**Wavelength**  1.54178 Å  
**Crystal system, space group**  Triclinic, \(P1\)  
**Unit cell dimensions**  
\[a = 14.3698(4) \text{ Å}, \quad \alpha = 65.5320(10) ^\circ\]  
\[b = 14.5423(5) \text{ Å}, \quad \beta = 82.4700(10) ^\circ\]  
\[c = 16.2653(5) \text{ Å}, \quad \gamma = 60.6560(10) ^\circ\]  
**Volume**  2685.66(15) \(\text{Å}^3\)  
**Z, Calculated density**  2, 1.160 \(\text{Mg/m}^3\)  
**Absorption coefficient**  0.625 \(\text{mm}^{-1}\)  
**\(F(000)\)**  1016  
**Crystal size**  0.305 x 0.283 x 0.227 mm  
**Theta range for data collection**  2.997 to 66.591 \(^\circ\)  
**Limiting indices**  
\(-17 \leq h \leq 16, -16 \leq k \leq 17, -19 \leq l \leq 19\)  
**Reflections collected / unique**  67367 / 16343 \([R(int) = 0.0320]\)  
**Completeness to theta = 66.591**  96.4 \%  
**Absorption correction**  Semi-empirical from equivalents  
**Max. and min. transmission**  0.7528 and 0.6775  
**Refinement method**  Full-matrix least-squares on \(F^2\)  
**Data / restraints / parameters**  16343 / 71 / 1306  
**Goodness-of-fit on \(F^2\)**  1.021  
**Final R indices \([I>2\sigma(I)]\)**  
\(R1 = 0.0327, \quad wR2 = 0.0893\)  
**R indices (all data)**  
\(R1 = 0.0346, \quad wR2 = 0.0910\)  
**Absolute structure parameter**  0.007(37)  
**Extinction coefficient**  0.00111(12)  
**Largest diff. peak and hole**  0.235 and -0.189 e.A\(^{-3}\)
**TEO with encapsulated (R)-(-)-limonene**

Deposition number CCDC 1970875

| Property                                      | Value                  |
|-----------------------------------------------|------------------------|
| Empirical formula                            | C_{55} H_{72} O_{8}    |
| Chemical formula moiety                      | 4 (C_{50} H_{64} O_{8}, 2 (C_{10} H_{16}) |
| Formula weight                               | 861.12                 |
| Temperature                                  | 130(2) K               |
| Wavelength                                   | 1.54178 Å              |
| Crystal system, space group                  | Monoclinic, P2(1)      |
| Unit cell dimensions                         |                         |
| a                                             | 19.3214(9) Å, alpha = 90° |
| b                                             | 22.7196(10) Å, beta = 92.722(3)° |
| c                                             | 22.6556(11) Å, gamma = 90° |
| Volume                                        | 9934.0(8) Å^3          |
| Z, Calculated density                        | 8, 1.152 Mg/m^3        |
| Absorption coefficient                       | 0.598 mm^{-1}          |
| F(000)                                        | 3728                   |
| Crystal size                                 | 0.321 x 0.135 x 0.060 mm |
| Theta range for data collection              | 2.289 to 66.468 °      |
| Limiting indices                             | -22<=h<=22, -27<=k<=25, -26<=l<=26 |
| Reflections collected / unique               | 152375 / 33235 [R(int) = 0.0573] |
| Completeness to theta = 66.468               | 98.2 %                 |
| Absorption correction                        | Numerical              |
| Max. and min. transmission                   | 0.9974 and 0.8852      |
| Refinement method                            | Full-matrix least-squares on F^2 |
| Data / restraints / parameters               | 33235 / 165 / 2401     |
| Goodness-of-fit on F^2                       | 1.045                  |
| Final R indices [I>2sigma(I)]                | R1 = 0.0455, wR2 = 0.1161 |
| R indices (all data)                         | R1 = 0.0679, wR2 = 0.1276 |
| Absolute structure parameter                 | 0.07(14)               |
| Extinction coefficient                       | n/a                    |
| Largest diff. peak and hole                  | 0.404 and -0.249 e.A^{-3} |
TEO with encapsulated (S)-(+) -limonene
Deposition number CCDC 1970877

Empirical formula \( C_{55} H_{72} O_{8} \)
Chemical formula moiety \( C_{50} H_{64} O_{8}, 0.5 (C_{10} H_{16}) \)
Formula weight 861.12
Temperature 130(2) K
Wavelength 1.54178 Å
Crystal system, space group Monoclinic, \( P2(1) \)
Unit cell dimensions
\[ a = 19.3017(10) \text{ Å}, \alpha = 90^\circ \]
\[ b = 22.6981(13) \text{ Å}, \beta = 92.715(3)^\circ \]
\[ c = 22.6394(12) \text{ Å}, \gamma = 90^\circ \]
Volume 9907.5(9) \( \text{Å}^3 \)
Z, Calculated density 8, 1.155 Mg/m³
Absorption coefficient 0.599 mm⁻¹
F(000) 3728
Crystal size 0.227 x 0.094 x 0.041 mm
Theta range for data collection 2.758 to 66.092°
Limiting indices -22<=h<=19, -26<=k<=26, -26<=l<=26
Reflections collected / unique 154257 / 33632 [R(int) = 0.0958]
Completeness to theta = 66.092 98.1 %
Absorption correction Numerical
Max. and min. transmission 0.9703 and 0.8861
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 33632 / 213 / 2374
Goodness-of-fit on F² 1.034
Final R indices [I>2sigma(I)] R1 = 0.0475, wR2 = 0.0897
R indices (all data) R1 = 0.1008, wR2 = 0.1020
Absolute structure parameter 0.2(3)
Extinction coefficient n/a
Largest diff. peak and hole 0.294 and -0.209 e.Å⁻³
TEO with encapsulated (R)-(−)-carvone
Deposition number CCDC 1970880

Empirical formula  
Chemical formula moiety  
Formula weight  
Temperature  
Wavelength  
Crystal system, space group  
Unit cell dimensions  
Volume  
Z, Calculated density  
Absorption coefficient  
F(000)  
Crystal size  
Theta range for data collection  
Limiting indices  
Reflections collected / unique  
Completeness to theta = 65.59°  
Absorption correction  
Max. and min. transmission  
Refinement method  
Data / restraints / parameters  
Goodness-of-fit on F²  
Final R indices [I>2sigma(I)]  
R indices (all data)  
Absolute structure parameter  
Extinction coefficient  
Largest diff. peak and hole

C₆₀H₇₈O₉  
C₅₀H₆₄O₈, C₁₀H₁₄O  
943.22  
130(2) K  
1.54178 Å  
Triclinic, P 1  
a = 14.4518(7) Å, alpha = 81.524(3)°  
b = 14.7500(8) Å, beta = 67.515(2)°  
c = 15.4109(8) Å, gamma = 61.964(2)°  
2677.0(2) Å³  
2, 1.170 Mg/m³  
0.611 mm⁻¹  
1020  
0.56 x 0.25 x 0.20 mm  
3.11 to 65.59°  
-16<=h<=16, -17<=k<=16, -17<=l<=18  
73965 / 16707 [R(int) = 0.0642]  
98.2%  
Semi-empirical from equivalents  
0.7528 and 0.6194  
Full-matrix least-squares on F²  
16707 / 260 / 1398  
1.027  
R₁ = 0.0430, wR₂ = 0.1137  
R₁ = 0.0472, wR₂ = 0.1171  
-0.04(12)  
0.00161(13)  
0.250 and -0.277 e.Å⁻³
**TEO with encapsulated (S)-(+-)carvone**

Deposition number CCDC 1970881

| Property                                      | Value                                      |
|-----------------------------------------------|--------------------------------------------|
| Empirical formula                            | C<sub>55</sub>H<sub>71</sub>O<sub>8.50</sub> |
| Chemical formula moiety                      | C<sub>50</sub>H<sub>64</sub>O<sub>8</sub>, 0.5 (C<sub>10</sub>H<sub>14</sub>O) |
| Formula weight                                | 868.12                                     |
| Temperature                                   | 130(2) K                                   |
| Wavelength                                    | 1.54178 Å                                  |
| Crystal system, space group                   | Triclinic, P 1                             |
| Unit cell dimensions                          | a = 10.0871(6) Å, alpha = 107.099(3) °     |
|                                              | b = 15.2707(9) Å, beta = 90.533(3) °       |
|                                              | c = 16.1833(10) Å, gamma = 90.788(2) °     |
| Volume                                        | 2382.2(2) Å<sup>3</sup>                   |
| Z, Calculated density                         | 2, 1.210 Mg/m<sup>3</sup>                 |
| Absorption coefficient                        | 0.636 mm<sup>-1</sup>                     |
| F(000)                                        | 938                                        |
| Crystal size                                  | 0.35 x 0.30 x 0.13 mm                      |
| Theta range for data collection               | 2.86 to 65.60 °                           |
| Limiting indices                              | -11<=h<=10, -17<=k<=17, -19<=l<=18         |
| Reflections collected / unique                | 78921 / 14708 [R(int) = 0.0433]            |
| Completeness to theta                         | 97.1 %                                     |
| Absorption correction                         | Semi-empirical from equivalents            |
| Max. and min. transmission                    | 0.7528 and 0.6624                          |
| Refinement method                             | Full-matrix least-squares on F<sup>2</sup>|
| Data / restraints / parameters                | 14708 / 634 / 1323                         |
| Goodness-of-fit on F<sup>2</sup>              | 1.032                                      |
| Final R indices [I>2sigma(I)]                 | R1 = 0.0446, wR2 = 0.1177                  |
| R indices (all data)                          | R1 = 0.0561, wR2 = 0.1373                  |
| Absolute structure parameter                  | 0.21(19)                                   |
| Extinction coefficient                        | 0.00162(15)                                |
| Largest diff. peak and hole                   | 0.652 and -0.354 e.A<sup>-3</sup>         |
TEO with encapsulated (-)-α-thujone
Deposition number CCDC 1970886

| Property                          | Value                          |
|----------------------------------|--------------------------------|
| Empirical formula                | C_{60}H_{80}O_{9}              |
| Chemical formula moiety          | C_{50}H_{64}O_{9}, C_{10}H_{16}O |
| Formula weight                   | 945.24                         |
| Temperature                      | 130(2) K                       |
| Wavelength                       | 1.54178 Å                      |
| Crystal system, space group      | Triclinic, P1                  |
| Unit cell dimensions             | a = 14.3565(10) Å, alpha = 65.845(4) ° |
|                                  | b = 14.7142(10) Å, beta = 80.977(5) ° |
|                                  | c = 15.9026(11) Å, gamma = 61.475(4) ° |
| Volume                           | 2690.0(3) Å³                   |
| Z, Calculated density            | 2, 1.167 Mg/m³                 |
| Absorption coefficient           | 0.608 mm⁻¹                     |
| F(000)                           | 1024                           |
| Crystal size                     | 0.18 x 0.08 x 0.05 mm          |
| Theta range for data collection  | 3.05 to 65.60 °                |
| Limiting indices                 | -16<=h<=16, -17<=k<=16, -18<=l<=18 |
| Reflections collected / unique   | 75610 / 16754 [R(int) = 0.1038] |
| Completeness to theta = 65.596   | 97.6 %                         |
| Absorption correction            | Semi-empirical from equivalents|
| Max. and min. transmission       | 0.7257 and 0.6550              |
| Refinement method                | Full-matrix least-squares on F²|
| Data / restraints / parameters   | 16754 / 517 / 1368             |
| Goodness-of-fit on F²            | 1.023                          |
| Final R indices [I>2sigma(I)]    | R1 = 0.0491, wR2 = 0.1000      |
| R indices (all data)             | R1 = 0.0922, wR2 = 0.1124      |
| Absolute structure parameter     | -0.07(20)                      |
| Extinction coefficient           | 0.00102(8)                     |
| Largest diff. peak and hole      | 0.247 and -0.241 e.A⁻³         |
**TEO with encapsulated nicotine**

Deposition number CCDC 1970888

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Empirical formula: $C_{55}H_{71}N_8O_8$

Chemical formula moiety: $C_{50}H_{64}O_8$, 0.5 ($C_{10}H_{14}N_2$)

Formula weight: 874.12

Temperature: 135(2) K

Wavelength: 1.54178 Å

Crystal system, space group: Monoclinic, $P2(1)$

Unit cell dimensions:
- $a = 19.2084(18)$ Å, $\alpha = 90^\circ$
- $b = 22.821(2)$ Å, $\beta = 93.583(5)^\circ$
- $c = 22.946(3)$ Å, $\gamma = 90^\circ$

Volume: 10039.1(18) Å$^3$

Z, Calculated density: 8, 1.157 Mg/m$^3$

Absorption coefficient: 0.605 mm$^{-1}$

$F(000)$: 3776

Crystal size: 0.467 x 0.278 x 0.124 mm

Theta range for data collection: 1.929 to 65.600°

Limiting indices:
- $-22 \leq h \leq 17$, $-26 \leq k \leq 26$, $-26 \leq l \leq 26$

Reflections collected / unique: 151397 / 33958 [$R(\text{int}) = 0.0629$]

Completeness to theta = 65.600°: 98.5%

Absorption correction: Semi-empirical from equivalents

Max. and min. transmission: 0.7528 and 0.6206

Refinement method: Full-matrix least-squares on $F^2$

Data / restraints / parameters: 33958 / 67 / 2385

Goodness-of-fit on $F^2$: 1.035

Final R indices [$I>2\sigma(I)$]: $R1 = 0.0484$, $wR2 = 0.1246$

R indices (all data): $R1 = 0.0697$, $wR2 = 0.1363$

Absolute structure parameter: 0.00(8)

Extinction coefficient: 0.00090(17)

Largest diff. peak and hole: 0.499 and -0.287 e Å$^{-3}$
**TEO with encapsulated (-)-linalool**

Deposition number CCDC 1970887

| Property                                      | Value                           |
|-----------------------------------------------|---------------------------------|
| Empirical formula                            | $C_{55}H_{73}O_{8.50}$          |
| Chemical formula moiety                      | $C_{50}H_{64}O_8, 0.5 (C_{10}H_{18}O)$ |
| Formula weight                               | 870.13                          |
| Temperature                                  | 130(2) K                        |
| Wavelength                                   | 1.54178 Å                       |
| Crystal system, space group                  | Triclinic, P1                   |
| Unit cell dimensions                         |                                 |
| Volume                                        | $5107.3(6)\,\text{Å}^3$         |
| Z, Calculated density                        | 4, 1.132 Mg/m$^3$               |
| Absorption coefficient                       | 0.593 mm$^{-1}$                 |
| F(000)                                        | 1884                            |
| Crystal size                                 | 0.190 x 0.188 x 0.084 mm        |
| Theta range for data collection              | 3.743 to 65.596 °               |
| Limiting indices                             | -17<=h<=17, -18<=k<=17, -25<=l<=26 |
| Reflections collected / unique               | 109929 / 31235 [R(int) = 0.1504] |
| Completeness to theta                        | 65.596                           |
| Absorption correction                        | Semi-empirical from equivalents |
| Max. and min. transmission                   | 0.7039 and 0.5969               |
| Refinement method                            | Full-matrix least-squares on F$^2$ |
| Data / restraints / parameters               | 31235 / 1505 / 2636             |
| Goodness-of-fit on F$^2$                     | 1.036                           |
| Final R indices [I>2sigma(I)]                | R1 = 0.0775, wR2 = 0.1722       |
| R indices (all data)                         | R1 = 0.1934, wR2 = 0.2090       |
| Absolute structure parameter                 | 0.0(4)                          |
| Extinction coefficient                       | 0.00070(10)                     |
| Largest diff. peak and hole                  | 0.395 and -0.316 e.A$^{-3}$     |
TBro with encapsulated \( n \)-decane

Deposition number CCDC 1970895

Empirical formula \( \text{C}_{48} \text{H}_{58} \text{Br}_{4} \text{O}_{4} \)
Chemical formula moiety \( \text{C}_{38} \text{H}_{36} \text{Br}_{4} \text{O}_{4}, \text{C}_{10} \text{H}_{22} \)
Formula weight 1018.58
Temperature 130(2) K
Wavelength 0.71073 Å
Crystal system, space group Triclinic, \( \text{P} -1 \)
Unit cell dimensions
\[ a = 13.0601(13) \, \text{Å}, \alpha = 102.679(4) \, ^\circ \]
\[ b = 15.6298(19) \, \text{Å}, \beta = 97.829(3) \, ^\circ \]
\[ c = 22.620(2) \, \text{Å}, \gamma = 98.592(3) \, ^\circ \]
Volume 4385.2(8) Å\(^3\)
\( Z \), Calculated density 4, 1.543 Mg/m\(^3\)
Absorption coefficient 3.714 mm\(^{-1}\)
\( F(000) \) 2072
Crystal size 0.40 x 0.16 x 0.04 mm
Theta range for data collection 1.45 to 25.00 \(^\circ\)
Limiting indices \(-11\leq h\leq 15, \ -18\leq k\leq 18, \ -26\leq l\leq 26\)
Reflections collected / unique 57590 / 15375 [\( R_{\text{int}} = 0.0717 \)]
Completeness to theta = 25.00 99.5 %
Absorption correction Numerical
Max. and min. transmission 0.8882 and 0.4192
Refinement method Full-matrix least-squares on \( F^2 \)
Data / restraints / parameters 15375 / 649 / 1018
Goodness-of-fit on \( F^2 \) 1.019
Final \( R \) indices [\( I > 2\sigma(I) \)] \( R_1 = 0.1121, \, wR_2 = 0.2720 \)
\( R \) indices (all data) \( R_1 = 0.1513, \, wR_2 = 0.2882 \)
Largest diff. peak and hole 5.755 and -1.050 e.Å\(^{-3}\)

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**TBro with encapsulated citronellal and water**

Deposition number CCDC 1978505

Identification code  s2452lm  
Empirical formula  C_{40.50}H_{40.50}Br_4O_{4.38}  
Chemical formula moiety  C_{38}H_{36}Br_4O_4, 0.25 (C_{10}H_{18}O), 0.125 (O)  
Formula weight  916.87  
Temperature  130(2) K  
Wavelength  0.71073 Å  
Crystal system, space group  Triclinic, P-1  
Unit cell dimensions  
\[ a = 14.6277(8) \text{ Å}, \quad \alpha = 92.209(3) ^\circ \]  
\[ b = 16.5250(9) \text{ Å}, \quad \beta = 101.630(3) ^\circ \]  
\[ c = 34.5118(18) \text{ Å}, \quad \gamma = 114.956(2) ^\circ \]  
Volume  7336.0(7) Å³  
Z, Calculated density  8, 1.660 Mg/m³  
Absorption coefficient  4.431 mm⁻¹  
F(000)  3668  
Crystal size  0.375 x 0.212 x 0.164 mm  
Theta range for data collection  1.373 to 26.438 °  
Limiting indices  -18<=h<=17, -20<=k<=20, -42<=l<=43  
Reflections collected / unique  108292 / 29902 [R(int) = 0.0404]  
Completeness to theta = 25.242  99.5 %  
Absorption correction  Numerical  
Max. and min. transmission  0.7183 and 0.4100  
Refinement method  Full-matrix least-squares on F²  
Data / restraints / parameters  29902 / 306 / 1880  
Goodness-of-fit on F²  1.037  
Final R indices [I>2sigma(I)]  R1 = 0.0489, wR2 = 0.1220  
R indices (all data)  R1 = 0.0801, wR2 = 0.1326  
Extinction coefficient  n/a  
Largest diff. peak and hole  3.849 and -2.069 e.A⁻³
**TBro with encapsulated geraniol**

Deposition number CCDC 1970897

**Empirical formula**
\[ \text{C}_{40.50} \text{H}_{40.50} \text{Br}_4 \text{O}_{4.25} \]

**Chemical formula moiety**
\[ \text{C}_{38} \text{H}_{36} \text{Br}_4 \text{O}_4, 0.25 (\text{C}_{10} \text{H}_{18} \text{O}) \]

**Formula weight**
914.87

**Temperature**
130(2) K

**Wavelength**
1.54178 Å

**Crystal system, space group**
Triclinic, P -1

**Unit cell dimensions**
\[ \begin{align*}
a &= 14.2223(15) \text{ Å}, & \alpha &= 69.488(7) ^\circ \\
b &= 16.0866(18) \text{ Å}, & \beta &= 72.712(7) ^\circ \\
c &= 18.4078(16) \text{ Å}, & \gamma &= 70.073(8) ^\circ \\
\end{align*} \]

**Volume**
3632.0(6) Å³

**Z, Calculated density**
4, 1.673 Mg/m³

**Absorption coefficient**
5.744 mm⁻¹

**F(000)**
1830

**Crystal size**
0.09 x 0.06 x 0.02 mm

**Theta range for data collection**
5.24 to 65.60 °

**Limiting indices**
-16<=h<=16, -18<=k<=16, -21<=l<=21

**Reflections collected / unique**
45879 / 12186 [R(int) = 0.1661]

**Completeness to theta = 65.60**
97.2 %

**Absorption correction**
Semi-empirical from equivalents

**Max. and min. transmission**
0.7528 and 0.5922

**Refinement method**
Full-matrix least-squares on F²

**Data / restraints / parameters**
12186 / 264 / 1005

**Goodness-of-fit on F²**
1.032

**Final R indices [I>2sigma(I)]**
R1 = 0.0864, wR2 = 0.1770

**R indices (all data)**
R1 = 0.1795, wR2 = 0.2069

**Extinction coefficient**
0.00127(8)

**Largest diff. peak and hole**
2.192 and -1.871 e.A⁻³
TBro with encapsulated farnesol
Deposition number CCDC 1970899

Empirical formula: \( \text{C}_{41.75} \text{H}_{42.50} \text{Br}_4 \text{O}_{4.25} \)
Chemical formula moiety: \( \text{C}_{38} \text{H}_{36} \text{Br}_4 \text{O}_4, 0.25 (\text{C}_{15} \text{H}_{26} \text{O}) \)
Formula weight: 931.90
Temperature: 130(2) K
Wavelength: 0.71073 Å
Crystal system, space group: Triclinic, \( P-1 \)
Unit cell dimensions:
- \( a = 14.3460(5) \text{ Å}, \alpha = 68.445(2) ^\circ \)
- \( b = 16.7873(6) \text{ Å}, \beta = 70.241(2) ^\circ \)
- \( c = 18.1987(7) \text{ Å}, \gamma = 67.398(3) ^\circ \)
Volume: 3663.0(2) Å³
Z, Calculated density: 4, 1.690 Mg/m³
Absorption coefficient: 4.438 mm⁻¹
F(000): 1868
Crystal size: 0.30 x 0.28 x 0.16 mm
Theta range for data collection: 1.75 to 26.49 °
Limiting indices: \(-16\leq h\leq 17, -21\leq k\leq 21, -22\leq l\leq 22\)
Reflections collected / unique: 55437 / 14990 [\(R(int) = 0.0445\)]
Completeness to theta = 26.49: 99.0 %
Absorption correction: Numerical
Max. and min. transmission: 0.6049 and 0.3630
Refinement method: Full-matrix least-squares on \( F^2 \)
Data / restraints / parameters: 14990 / 119 / 1001
Goodness-of-fit on \( F^2 \): 1.045
Final R indices \([I>2\sigma(I)]\): \( R1 = 0.0742, wR2 = 0.1808 \)
R indices (all data): \( R1 = 0.1290, wR2 = 0.2022 \)
Largest diff. peak and hole: 3.429 and -2.738 e.Å⁻³
TBro with encapsulated α-humulene
Deposition number CCDC 1970896

Empirical formula  
C_{53}H_{60}Br_4O_{4.50}

Chemical formula moiety  
C_{38}H_{36}Br_4O_4, C_{15}H_{24}, 0.5 (O)

Formula weight  
1088.65

Temperature  
135(2) K

Wavelength  
1.54178 Å

Crystal system, space group  
Triclinic, P -1

Unit cell dimensions  
an = 13.5885(3) Å, alpha = 116.8980(10)°
b = 14.6230(4) Å, beta = 115.3810(10)°
c = 15.1073(4) Å, gamma = 90.364(2)°

Volume  
2342.82(10) Å³

Z, Calculated density  
2, 1.543 Mg/m³

Absorption coefficient  
4.556 mm⁻¹

F(000)  
1108

Crystal size  
0.09 x 0.06 x 0.04 mm

Theta range for data collection  
3.50 to 65.60°

Limiting indices  
-13<=h<=15, -17<=k<=16, -17<=l<=17

Reflections collected / unique  
31244 / 7866 [R(int) = 0.0476]

Completeness to theta = 65.60°  
97.3 %

Absorption correction  
Numerical

Max. and min. transmission  
0.8977 and 0.7311

Refinement method  
Full-matrix least-squares on F²

Data / restraints / parameters  
7866 / 18 / 577

Goodness-of-fit on F²  
1.043

Final R indices [I>2sigma(I)]  
R1 = 0.0453, wR2 = 0.1175

R indices (all data)  
R1 = 0.0565, wR2 = 0.1239

Largest diff. peak and hole  
1.274 and -1.109 e.Å⁻³
TBro with encapsulated muscone
Deposition number CCDC 1978250

Empirical formula: C₅₄ H₆₆ Br₄ O₅
Chemical formula moiety: C₃₈ H₃₆ Br₄ O₄, C₁₆ H₃₀ O
Formula weight: 1114.70
Temperature: 135(2) K
Wavelength: 1.54178 Å
Crystal system, space group: Triclinic, P1
Unit cell dimensions:
  a = 14.3013(5) Å, alpha = 74.570(2) °
  b = 14.3630(6) Å, beta = 64.730(2) °
  c = 14.4108(6) Å, gamma = 67.072(3) °
Volume: 2447.62(18) Å³
Z, Calculated density: 2, 1.512 Mg/m³
Absorption coefficient: 4.381 mm⁻¹
F(000): 1140
Crystal size: 0.097 x 0.083 x 0.046 mm
Theta range for data collection: 3.365 to 65.598 deg.
Limiting indices: -13<=h<=16, -16<=k<=16, -17<=l<=16
Reflections collected / unique: 54577 / 14806 [R(int) = 0.0548]
Completeness to theta = 65.598: 98.1 %
Absorption correction: Numerical
Max. and min. transmission: 0.8541 and 0.7286
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 14806 / 1069 / 1142
Goodness-of-fit on F²: 1.041
Final R indices [I>2sigma(I)]: R1 = 0.0475, wR2 = 0.1146
R indices (all data): R1 = 0.0712, wR2 = 0.1260
Absolute structure parameter: 0.523(19)
Extinction coefficient: n/a
Largest diff. peak and hole: 1.409 and -0.933 e.A⁻³
TDA with encapsulated toluene
Deposition number CCDC 1918380

Empirical formula \( \text{C}_{45.50} \text{H}_{52} \text{O}_{8} \)
Chemical formula moiety \( \text{C}_{42} \text{H}_{48} \text{O}_{8}, 0.5(\text{C}_7 \text{H}_8) \)
Formula weight 726.87
Temperature 100(2) K
Wavelength 0.71073 Å
Crystal system, space group Monoclinic, P 21/c
Unit cell dimensions
\[
a = 21.5613(11) \text{ Å}, \quad \alpha = 90^\circ \\
b = 16.8572(7) \text{ Å}, \quad \beta = 97.238(2)^\circ \\
c = 20.8779(8) \text{ Å}, \quad \gamma = 90^\circ 
\]
Volume 7527.9(6) Å\(^3\)
Z, Calculated density 8, 1.283 Mg/m\(^3\)
Absorption coefficient 0.087 mm\(^{-1}\)
F(000) 3112
Crystal size 0.72 x 0.38 x 0.15 mm
Theta range for data collection 1.76 to 26.40 °
Limiting indices -26<=h<=26, -21<=k<=16, -26<=l<=19
Reflections collected / unique 55761 / 15374 [R(int) = 0.0742]
Completeness to theta = 26.40 99.7 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7348 and 0.6936
Refinement method Full-matrix least-squares on F\(^2\)
Data / restraints / parameters 15374 / 0 / 981
Goodness-of-fit on F\(^2\) 1.032
Final R indices [I>2sigma(I)] R1 = 0.0504, wR2 = 0.0831
R indices (all data) R1 = 0.1162, wR2 = 0.0937
Largest diff. peak and hole 0.270 and -0.286 e.Å\(^{-3}\)
TDA with encapsulated p-xylene
Deposition number CCDC 1978501

Empirical formula \( \text{C}_{46} \text{H}_{53} \text{O}_8 \)
Chemical formula moiety \( \text{C}_{42} \text{H}_{48} \text{O}_8, 0.5(\text{C}_8 \text{H}_{10}) \)
Formula weight 733.88
Temperature 150(2) K
Wavelength 0.71073 Å
Crystal system, space group Monoclinic, \( \text{P} \ 21/c \)
Unit cell dimensions \( a = 21.673(2) \) Å, \( \alpha = 90^\circ \)
\( b = 16.9358(17) \) Å, \( \beta = 96.925(3)^\circ \)
\( c = 20.953(2) \) Å, \( \gamma = 90^\circ \)
Volume 7634.7(14) Å³
Z, Calculated density 8, 1.277 Mg/m³
Absorption coefficient 0.086 mm⁻¹
F(000) 3144
Crystal size 0.34 x 0.14 x 0.12 mm
Theta range for data collection 1.53 to 25.00°
Limiting indices \(-25<=h<=25, -18<=k<=20, -22<=l<=24\)
Reflections collected / unique 51836 / 13432 [R(int) = 0.1547]
Completeness to theta = 25.00 100.0 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.7254 and 0.6954
Refinement method Full-matrix least-squares on \( F^2 \)
Data / restraints / parameters 13432 / 0 / 991
Goodness-of-fit on \( F^2 \) 0.993
Final R indices [I>2sigma(I)] \( R1 = 0.0618, wR2 = 0.0704 \)
R indices (all data) \( R1 = 0.1932, wR2 = 0.0837 \)
Largest diff. peak and hole 0.305 and -0.273 eÅ⁻³
### TDA with encapsulated [12]crown-4

Deposition number CCDC 1978506

| Property                                      | Value                        |
|-----------------------------------------------|------------------------------|
| Empirical formula                            | $C_{54}H_{72}O_{14}$         |
| Chemical formula moiety                      | $C_{42}H_{48}O_{8}, 1.5(C_{8}H_{16}O_{4})$ |
| Formula weight                               | 945.12                       |
| Temperature                                  | 130(2) K                     |
| Wavelength                                   | 1.54178 Å                    |
| Crystal system, space group                  | Triclinic, $P - 1$           |
| Unit cell dimensions                         | $a = 13.8432(7) \text{ Å}, \alpha = 72.169(3)^\circ$ |
|                                              | $b = 13.9636(8) \text{ Å}, \beta = 69.907(2)^\circ$ |
|                                              | $c = 15.0421(8) \text{ Å}, \gamma = 68.486(3)^\circ$ |
| Volume                                        | 2485.8(2) Å$^3$              |
| Z, Calculated density                        | 2, 1.263 Mg/m$^3$            |
| Absorption coefficient                       | 0.737 mm$^{-1}$              |
| $F(000)$                                      | 1016                         |
| Crystal size                                 | 0.17 x 0.15 x 0.13 mm        |
| Theta range for data collection              | 3.20 to 65.59°               |
| Limiting indices                             | -16 <= h <= 16, -16 <= k <= 15, -17 <= l <= 16 |
| Reflections collected / unique               | 38156 / 8418 [R(int) = 0.0367] |
| Completeness to theta = 65.59°               | 97.9 %                       |
| Absorption correction                        | Numerical                    |
| Max. and min. transmission                   | 0.9978 and 0.8292            |
| Refinement method                            | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters               | 8418 / 262 / 721             |
| Goodness-of-fit on $F^2$                     | 1.040                        |
| Final R indices [I>2sigma(I)]                | R1 = 0.0371, wR2 = 0.0932    |
| R indices (all data)                         | R1 = 0.0466, wR2 = 0.0978    |
| Largest diff. peak and hole                  | 0.216 and -0.197 e.$\text{Å}^3$ |
**TDA with encapsulated (R)-(-)-epichlorohydrine**

Deposition number CCDC 1970857

| Property                        | Value                                      |
|---------------------------------|--------------------------------------------|
| Empirical formula               | C_{44.25}H_{51.75}Cl_{0.75}O_{8.75}        |
| Chemical formula moiety         | C_{42}H_{48}O_{8}, 0.75 (C_{3}H_{5}Cl O)   |
| Formula weight                  | 750.19                                     |
| Temperature                     | 130(2) K                                   |
| Wavelength                      | 0.71073 Å                                  |
| Crystal system, space group     | Triclinic, P1                              |
| Unit cell dimensions            | a = 14.6308(6) Å, alpha = 67.971(2) °     |
|                                | b = 15.7942(6) Å, beta = 72.496(2) °     |
|                                | c = 20.4158(8) Å, gamma = 63.5760(10) °   |
| Volume                          | 3865.2(3) Å\(^3\)                        |
| Z, Calculated density           | 4, 1.289 Mg/m\(^3\)                      |
| Absorption coefficient          | 0.138 mm\(^{-1}\)                        |
| F(000)                          | 1600                                       |
| Crystal size                    | 0.520 x 0.398 x 0.260 mm                   |
| Theta range for data collection | 1.501 to 28.386 °                         |
| Limiting indices                | -19<=h<=19, -21<=k<=21, -27<=l<=27          |
| Reflections collected / unique  | 151840 / 38362 [R(int) = 0.0248]           |
| Completeness to theta = 25.242  | 99.9 %                                     |
| Absorption correction           | Semi-empirical from equivalents            |
| Max. and min. transmission      | 0.7457 and 0.6979                          |
| Refinement method               | Full-matrix least-squares on F\(^2\)      |
| Data / restraints / parameters  | 38362 / 543 / 2103                         |
| Goodness-of-fit on F\(^2\)      | 1.031                                      |
| Final R indices [I>2sigma(I)]   | R1 = 0.0476, wR2 = 0.1231                  |
| R indices (all data)            | R1 = 0.0646, wR2 = 0.1319                  |
| Absolute structure parameter    | 0.130(15)                                  |
| Extinction coefficient          | n/a                                        |
| Largest diff. peak and hole     | 0.921 and -0.664 e.Å\(^{-3}\)             |
**TDA with encapsulated (S)-(+) -epichlorohydrine**

Deposition number CCDC 1970865

![Image of the compound](image)

**Empirical formula**: $C_{44.25}H_{51.75}Cl_{0.75}O_{8.75}$

**Chemical formula moiety**: $C_{42}H_{48}O_{8}, 0.75 (C_3H_5ClO)$

**Formula weight**: 750.19

**Temperature**: 130(2) K

**Wavelength**: 1.54178 Å

**Crystal system, space group**: Triclinic, P1

**Unit cell dimensions**
- $a = 14.6556(4)$ Å, $\alpha = 67.955(2)$°
- $b = 15.8195(4)$ Å, $\beta = 72.452(2)$°
- $c = 20.4399(5)$ Å, $\gamma = 63.567(3)$°

**Volume**: 3881.3(2) Å³

**Z, Calculated density**: 4, 1.284 Mg/m³

**Absorption coefficient**: 1.170 mm⁻¹

**F(000)**: 1600

**Crystal size**: 0.104 x 0.065 x 0.058 mm

**Theta range for data collection**: 2.363 to 65.600°

**Limiting indices**: -16<=h<=17, -18<=k<=18, -24<=l<=24

**Reflections collected / unique**: 69380 / 23274 [R(int) = 0.0722]

**Completeness to theta = 65.600**: 97.0 %

**Absorption correction**: Semi-empirical from equivalents

**Max. and min. transmission**: 0.7449 and 0.6810

**Refinement method**: Full-matrix least-squares on F²

**Data / restraints / parameters**: 23274 / 564 / 2103

**Goodness-of-fit on F²**: 1.043

**Final R indices [I>2sigma(I)]**: R1 = 0.0523, wR2 = 0.1206

**R indices (all data)**: R1 = 0.0912, wR2 = 0.1365

**Absolute structure parameter**: 0.143(17)

**Extinction coefficient**: n/a

**Largest diff. peak and hole**: 0.638 and -0.541 e.A⁻³
Crystal Structures of isothermally crystallized co-crystals
TEO with encapsulated nicotine
Deposition number CCDC 1970909

Empirical formula  
Chemical formula moiety  
Formula weight  
Temperature  
Wavelength  
Crystal system, space group  
Unit cell dimensions  
Volume  
Z, Calculated density  
Absorption coefficient  
F(000)  
Crystal size  
Theta range for data collection  
Limiting indices  
Reflections collected / unique  
Completeness to theta = 65.600%  
Absorption correction  
Max. and min. transmission  
Refinement method  
Data / restraints / parameters  
Goodness-of-fit on F^2  
Final R indices [I>2sigma(I)]  
R indices (all data)  
Absolute structure parameter  
Extinction coefficient  
Largest diff. peak and hole  

C_{55}H_{71}N_{6}O_{8}  
C_{50}H_{64}O_{8}, 0.5 (C_{10}H_{14}N_{2})  
874.12  
135(2) K  
1.54178 Å  
Monoclinic, P2(1)  
a = 19.1940(7) Å, alpha = 90°  
b = 22.865(8) Å, beta = 93.545(2)°  
c = 22.9437(7) Å, gamma = 90°  
10033.1(6) Å^3  
8, 1.157 Mg/m^3  
0.606 mm^{-1}  
3776  
0.229 x 0.154 x 0.101 mm  
2.733 to 65.595°  
-22<=h<=22, -26<=k<=26, -21<=l<=27  
137552 / 33774 [R(int) = 0.0460]  
98.2%  
Numerical  
0.9723 and 0.8207  
Full-matrix least-squares on F^2  
33774 / 63 / 2367  
1.035  
R1 = 0.0449, wR2 = 0.1012  
R1 = 0.0613, wR2 = 0.1086  
0.09(8)  
0.000060(10)  
0.527 and -0.285 e Å^{-3}
TEO with encapsulated (R)-(-)-carvone

Deposition number CCDC 1970898

Empirical formula \( \text{C}_{55} \text{H}_{71} \text{O}_{8.50} \)

Chemical formula moiety \( \text{C}_{50} \text{H}_{64} \text{O}_8, \text{C}_{10} \text{H}_{14} \text{O} \)

Formula weight 868.11

Temperature 135(2) K

Wavelength 1.54178 Å

Crystal system, space group Triclinic, \( \text{P}_1 \)

Unit cell dimensions \( a = 10.0867(4) \) Å, \( \alpha = 107.075(2) \)°
\( b = 15.2641(6) \) Å, \( \beta = 90.511(3) \)°
\( c = 16.1720(7) \) Å, \( \gamma = 90.799(2) \)°

Volume 2379.71(17) Å³

Z, Calculated density 2, 1.212 Mg/m³

Absorption coefficient 0.637 mm⁻¹

F(000) 938

Crystal size 0.174 x 0.110 x 0.044 mm

Theta range for data collection 2.859 to 65.565°

Limiting indices \(-11 \leq h \leq 11, \ -17 \leq k \leq 14, \ -18 \leq l \leq 18\)

Reflections collected / unique 53928 / 13947 \[ R(\text{int}) = 0.0582 \]

Completeness to theta = 65.565° 96.3%

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.7528 and 0.6627

Refinement method Full-matrix least-squares on \( F^2 \)

Data / restraints / parameters 13947 / 706 / 1323

Goodness-of-fit on \( F^2 \) 1.049

Final R indices \([I>2\sigma(I)]\) \( R1 = 0.0508, \ wR2 = 0.1163 \)

R indices (all data) \( R1 = 0.0794, \ wR2 = 0.1277 \)

Absolute structure parameter 0.05(16)

Extinction coefficient 0.00101(15)

Largest diff. peak and hole 0.509 and -0.288 e.A⁻³
TEO with encapsulated limonene (racemic)

Empirical formula  
Chemical formula moiety  
Formula weight  
Temperature  
Wavelength  
Crystal system, space group  
Unit cell dimensions  
Volume  
Z, Calculated density  
Absorption coefficient  
F(000)  
Crystal size  
Theta range for data collection  
Limiting indices  
Reflections collected / unique  
Completeness to theta  
Absorption correction  
Max. and min. transmission  
Refinement method  
Data / restraints / parameters  
Goodness-of-fit on F²  
Final R indices [I>2sigma(I)]  
R indices (all data)  
Largest diff. peak and hole
**Calculated logP Values and Molecular Weights of all TAA Co-Crystals Reported to Date**

The octanol–water partition coefficients (logP) values were calculated with the software Molinspiration. A table of the molecules plotted in Figure S5 is listed in Table S4, below.

**Table S4.** Molecular weights and calculated logP values of the co-crystals of TDA, TEO and TBro.

| TAA    | Guest             | Molecular weight [g/mol] | Calculated logP    | Reference |
|--------|-------------------|--------------------------|--------------------|-----------|
| TDA    | epichlorohydrin   | 92.5                     | 0.75               | -*        |
| TDA    | nitromethane      | 61.04                    | 0.1                | 1         |
| TDA    | dichloromethane   | 84.93                    | 1.51               | 1         |
| TDA    | acetone           | 58.08                    | 0.23               | 1         |
| TDA    | acetonitrile      | 41.05                    | 0.47               | 1         |
| TDA    | p-xylene          | 106.16                   | 2.83               | 2         |
| TDA    | chloroform        | 119.38                   | 2.09               | 1         |
| TDA    | 2-butanol         | 74.12                    | 0.92               | 1         |
| TDA    | benzoyl chloride  | 140.57                   | 2.39               | 1         |
| TDA    | benzene           | 78.11                    | 1.94               | 1         |
| TDA    | hexane            | 86.18                    | 4.16               | 1         |
| TDA    | [12]-crown-4      | 176.21                   | -0.64              | -*        |
| TDA    | ethanol           | 46.07                    | 0.06               | 1         |
| TDA    | 2-propanol        | 60.10                    | 0.42               | 1         |
| TDA    | nitrobenzene      | 123.11                   | 1.9                | 1         |
| TDA    | cyclopentadiene   | 66.10                    | 1.48               | 6         |
| TDA    | trifluorobenzene  | 132.08                   | 2.36               | 1         |
| TDA    | piperidin         | 85.15                    | 0.66               | 7         |
| TDA    | styrene           | 104.15                   | 2.79               | 7         |
| TDA    | toluene           | 92.14                    | 2.39               | -*        |
| TDA    | anisol            | 108.14                   | 1.99               | 7         |
| TDA    | dimethylsulfoxide | 78.13                    | -0.69              | 7         |
| TDA    | pyrrolidine       | 71.12                    | 0.50               | 7         |
| TDA    | pyridine          | 79.10                    | 0.70               | 7         |
| TDA    | trimethylpyrazine | 122.17                   | 0.90               | 7         |
| TDA    | morpholine        | 87.10                    | -0.41              | 7         |
| TDA    | furfural          | 96.08                    | 0.98               | 7         |
| TDA    | acetyl chloride   | 78.49                    | 1.17               | 7         |
| TDA    | trimethylphosphate| 140.08                   | -0.43              | 7         |
| TEO    | trimethylphosphate| 76.08                    | -0.27              | -*        |
| TEO  | 1-butanol      | 74.12 | 1.12 | -* |
|------|----------------|-------|------|----|
| TEO  | 2-butanol      | 74.12 | 0.92 | -* |
| TEO  | benzene        | 78.11 | 1.94 | 2  |
| TEO  | 2-pentanol     | 88.12 | 1.48 | -* |
| TEO  | toluene        | 92.14 | 2.39 | -* |
| TEO  | diethylether   | 74.12 | 1.05 | -* |
| TEO  | aniline        | 93.12 | 1.01 | -* |
| TEO  | 2-hexanol      | 102.17| 1.99 | -* |
| TEO  | 2-heptanol     | 116.20| 2.49 | -* |
| TEO  | terpinene      | 136.24| 3.36 |    |
| TEO  | α-pinene       | 136.24| 3.54 |    |
| TEO  | pyrrolidine    | 71.12 | 0.50 | 2  |
| TEO  | acetone        | 58.08 | 0.23 | 2  |
| TEO  | eugenol        | 164.20| 2.10 | -* |
| TEO  | phenylethanol  | 122.17| 1.50 | -* |
| TEO  | methylbenzylamine | 121.18 | -0.20 | -* |
| TEO  | limonene       | 136.24| 3.62 | -* |
| TEO  | tert-leucine methyl ester | 145.20 | 0.74 | -* |
| TEO  | carvone        | 150.22| 2.51 | -* |
| TEO  | trans-anethol  | 148.22| 3.10 | -* |
| TEO  | (-)-α-thujon   | 152.24| 3.10 | -* |
| TEO  | [12]-crown-4   | 176.21| -0.64| -* |
| TEO  | (-)-linalool   | 154.25| 3.21 | -* |
| TEO  | nicotine       | 162.23| 1.09 | -* |
| TEO  | hexamethylenediisocyanate | 168.20 | 1.38 | -* |
| TEO  | cyclopentylisocyanate | 111.14 | 1.47 | -* |
| TEO  | phenylisocyanate | 119.12 | 1.77 | -* |
| TEO  | p-xylene       | 106.16| 2.83 | 2  |
| TEO  | 2-methyl-2-butanol | 88.15 | 1.30 | 2  |
| TEO  | dioxane        | 88.11 | -0.23| 2  |
| TBro | geraniol       | 154.25| 3.20 | -* |
| TBro | farnesol       | 222.37| 5.05 | -* |
| TBro | citronellal    | 154.25| 3.60 | -* |
| TBro | humulene       | 204.35| 5.30 | -* |
| TBro | muscone        | 238.41| 5.72 | -* |
| TBro | n-decane       | 142.29| 6.18 | -* |

- * This work.
Figure S5. Structural breadth of the chaperone effect: diversity of analytes co-crystallized with TDA, TEO or TBro visualized as a plot of calculated lipophilicities (logP values) of analytes vs their molecular weight.
References for Supporting Information

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