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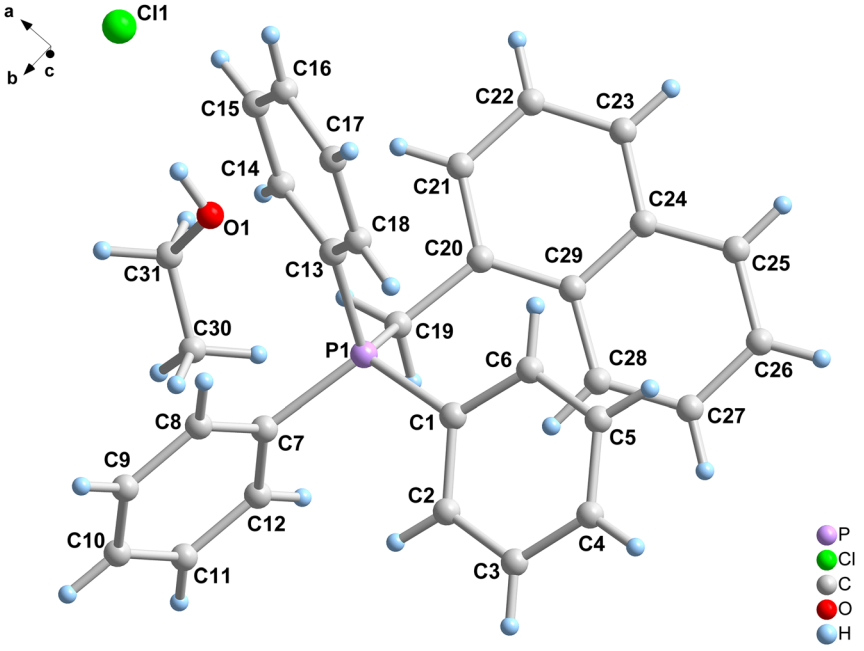
# Crystal structure of (1-naphthalen-1-yl-methyl) triphenylphosphonium chloride ethanol solvate, $C_{31}H_{30}ClOP$

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**Abstract**

$C_{31}H_{30}ClOP$, orthorhombic, $Pna2_1$ (no. 33), $a$ = 16.4933(2) Å, $b$ = 9.8603(2) Å, $c$ = 16.1472(3) Å, $V$ = 2626.00(8) Å$^3$, $Z$ = 4, $R_{gt}$ ($F$) = 0.0770, $wR_{ref}$ ($F^2$) = 0.2238, T = 298 K.

**CCDC no.:** 2414999

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Clear light white plate |
| Size: | 0.03 × 0.02 × 0.01 mm |
| Wavelength: | Cu $K\alpha$ radiation (1.54184 Å) |
| $\mu$: | 2.02 mm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku Synergy, $\varphi$ and $\omega$ scans |
| $\theta_{max}$, completeness: | 74.0°, 100 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 24415, 5172, 0.076 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 4706 |
| $N(param)_{refined}$: | 309 |
| Programs: | Rigaku,[1] Olex2,[3] SHELX[2,4] |

## 1 Source of materials

The (1-naphthylmethyl)triphenylphosphonium chloride (0.5 mmol) was carefully dissolved in 15 mL of ethanol to form a clear, homogeneous solution. The resulting solution was then left undisturbedly at room temperature in a covered vessel to prevent contamination. After several days, block-shaped single crystals of the desired compound were observed.

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**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.82274 (9) | 0.63429 (18) | 0.34899 (14) | 0.0717 (5) |
| P1 | 0.49815 (7) | 0.68771 (12) | 0.54535 (15) | 0.0448 (3) |
| O1 | 0.6485 (3) | 0.7595 (7) | 0.3451 (4) | 0.0914 (17) |
| H1 | 0.696356 | 0.738837 | 0.350263 | 0.137* |
| C1 | 0.4140 (3) | 0.6445 (4) | 0.6101 (3) | 0.0517 (11) |
| C2 | 0.3653 (3) | 0.7464 (5) | 0.6428 (4) | 0.0618 (14) |
| H2 | 0.377330 | 0.836374 | 0.630803 | 0.074* |
| C3 | 0.2990 (4) | 0.7172 (6) | 0.6930 (5) | 0.0771 (19) |
| H3 | 0.266745 | 0.786320 | 0.714205 | 0.092* |
| C4 | 0.2823 (4) | 0.5821 (6) | 0.7108 (4) | 0.080 (2) |
| H4 | 0.239083 | 0.560539 | 0.745419 | 0.097* |
| C5 | 0.3295 (4) | 0.4789 (7) | 0.6774 (4) | 0.083 (2) |
| H5 | 0.316859 | 0.388837 | 0.688575 | 0.099* |
| C6 | 0.3955 (4) | 0.5097 (5) | 0.6272 (4) | 0.0687 (16) |
| H6 | 0.427189 | 0.440520 | 0.605182 | 0.082* |
| C7 | 0.5194 (3) | 0.8647 (5) | 0.5607 (3) | 0.0471 (11) |
| C8 | 0.5739 (3) | 0.9019 (5) | 0.6224 (4) | 0.0632 (15) |
| H8 | 0.602005 | 0.835675 | 0.651659 | 0.076* |
| C9 | 0.5862 (4) | 1.0383 (5) | 0.6404 (5) | 0.0780 (19) |
| H9 | 0.622368 | 1.063562 | 0.681802 | 0.094* |
| C10 | 0.5441 (5) | 1.1367 (6) | 0.5961 (5) | 0.084 (2) |
| H10 | 0.553046 | 1.228060 | 0.607102 | 0.101* |
| C11 | 0.4887 (5) | 1.0987 (5) | 0.5355 (5) | 0.082 (2) |
| H11 | 0.459853 | 1.164896 | 0.506987 | 0.098* |
| C12 | 0.4761 (4) | 0.9625 (4) | 0.5172 (4) | 0.0629 (14) |
| H12 | 0.439213 | 0.937203 | 0.476463 | 0.075* |
| C13 | 0.5855 (3) | 0.5907 (5) | 0.5758 (2) | 0.0518 (11) |
| C14 | 0.6509 (3) | 0.5868 (7) | 0.5215 (3) | 0.0657 (15) |
| H14 | 0.648646 | 0.633699 | 0.471580 | 0.079* |
| C15 | 0.7198 (3) | 0.5125 (8) | 0.5419 (4) | 0.081 (2) |
| H15 | 0.764088 | 0.510922 | 0.506320 | 0.097* |
| C16 | 0.7218 (4) | 0.4408 (8) | 0.6160 (3) | 0.087 (2) |
| H16 | 0.766492 | 0.386890 | 0.628403 | 0.104* |
| C17 | 0.6578 (4) | 0.4488 (8) | 0.6718 (4) | 0.0778 (19) |
| H17 | 0.660763 | 0.404104 | 0.722435 | 0.093* |
| C18 | 0.5892 (4) | 0.5238 (6) | 0.6515 (3) | 0.0634 (14) |
| H18 | 0.545998 | 0.529284 | 0.688426 | 0.076* |
| C19 | 0.4760 (3) | 0.6628 (6) | 0.4358 (4) | 0.0513 (11) |
| H19A | 0.429606 | 0.718678 | 0.421745 | 0.062* |
| H19B | 0.521792 | 0.696504 | 0.404192 | 0.062* |
| C20 | 0.4584 (2) | 0.5181 (5) | 0.4073 (3) | 0.0526 (12) |
| C21 | 0.5218 (3) | 0.4470 (5) | 0.3707 (4) | 0.0650 (14) |
| H21 | 0.572305 | 0.488024 | 0.365411 | 0.078* |
| C22 | 0.5106 (4) | 0.3155 (6) | 0.3417 (5) | 0.080 (2) |
| H22 | 0.552921 | 0.269184 | 0.316225 | 0.097* |
| C23 | 0.4353 (4) | 0.2540 (6) | 0.3515 (4) | 0.079 (2) |
| H23 | 0.427366 | 0.165619 | 0.333162 | 0.095* |
| C24 | 0.3717 (3) | 0.3243 (4) | 0.3886 (4) | 0.0651 (16) |
| C25 | 0.2981 (4) | 0.2577 (7) | 0.3997 (5) | 0.084 (2) |
| H25 | 0.292557 | 0.167984 | 0.383008 | 0.101* |
| C26 | 0.2329 (4) | 0.3248 (6) | 0.4358 (6) | 0.090 (2) |
| H26 | 0.184541 | 0.279111 | 0.445705 | 0.108* |
| C27 | 0.2407 (3) | 0.4609 (6) | 0.4570 (5) | 0.0765 (18) |
| H27 | 0.196618 | 0.508492 | 0.478137 | 0.092* |
| C28 | 0.3150 (2) | 0.5253 (6) | 0.4464 (4) | 0.0634 (14) |
| H28 | 0.319927 | 0.616139 | 0.461136 | 0.076* |
| C29 | 0.3822 (2) | 0.4580 (4) | 0.4142 (3) | 0.0569 (13) |
| C30 | 0.5710 (6) | 0.9455 (13) | 0.3016 (9) | 0.124 (4) |
| H30A | 0.572000 | 1.019889 | 0.263235 | 0.187* |
| H30B | 0.569095 | 0.980039 | 0.357175 | 0.187* |
| H30C | 0.523999 | 0.890656 | 0.291412 | 0.187* |
| C31 | 0.6418 (6) | 0.8660 (10) | 0.2913 (7) | 0.106 (3) |
| H31A | 0.642617 | 0.830926 | 0.235191 | 0.127* |
| H31B | 0.688803 | 0.924077 | 0.297914 | 0.127* |

## 2 Experimental details

Crystal data were collected using Rigaku,[1] the structure was determined by SHELXT program within Olex2 and refined by SHELXL.[2–4] The structural picture was finished using Diamond.[5]

## 3 Comment

In this paper, we report a compound that contains a (1-naphthylmethyl)triphenylphosphonium (**1NTP**) ion, one chloride ion and one ethanol molecule. The organic molecule **1NTP** has a positive charge, the free chloride ion serves as counter anion. The bond distances of **1NTP** are in normal range of literatures.[6–8]

**Author contributions:** All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

**Conflict of interest:** The authors declare no conflicts of interest regarding this article.

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