Table 1. Crystal Data and Details of the Final Structure Refinement calculation for (6a*R*,12*R*)-**12**·HCl, (6a*R*,12*S*)-**12**·HCl, (6a*R*,12*S*)-**15**·2HCl·$H_2O$, (6a*R*,12*S*)-**16**·HCl·MeCN and (6a*R*,12*R*)-**17**·HCl.

| | (6a*R*,12*R*)-**12**·HCl | (6a*R*,12*S*)-**12**·HCl | (6a*R*,12*S*)-**15**·2HCl·$H_2O$ | (6a*R*,12*S*)-**16**·HCl·MeCN | (6a*R*,12*R*)-**17**·HCl |
|---|---|---|---|---|---|
| formula | $C_{18}H_{18}ClNO$ | $C_{18}H_{18}ClNO$ | $C_{18}H_{22}Cl_2N_2O$ | $C_{21}H_{23}ClN_2$ | $C_{20}H_{22}ClNO$ |
| formula weight | 299.78 | 299.78 | 353.28 | 338.86 | 327.84 |
| λ, Å (Mo *K*α) | 0.71073 | 0.71073 | 0.71073 | 0.71073 | 0.71073 |
| crystal system | orthorhombic | orthorhombic | orthorhombic | orthorhombic | monoclinic |
| space group | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_1$ |
| *a*, Å | 9.965(3) | 8.310(4) | 7.071(1) | 6.993(1) | 10.329(9) |
| *b*, Å | 12.101(5) | 11.833(3) | 10.893(1) | 14.988(3) | 7.109(3) |
| *c*, Å | 12.209(4) | 14.881(3) | 23.004(2) | 17.269(4) | 11.813(7) |
| *β* (deg) | 90 | 90 | 90 | 90 | 101.58(9) |
| *μ*, $mm^{-1}$ | 0.26 | 0.26 | 0.19 | 0.22 | 0.22 |
| $V_c$, $Å^3$ | 1472.3(8) | 1463.2(9) | 1771.9(3) | 1810.0(6) | 849.7(10) |
| *Z* | 4 | 4 | 4 | 4 | 2 |
| $D_c$, $g·cm^{-1}$ | 1.352(1) | 1.361(1) | 1.324(1) | 1.244(1) | 1.281(2) |
| *T*, K | 150(2) | 150(2) | 100(2) | 150(2) | 100(2) |
| *N* (measured) | 2483 | 2478 | 14016 | 3861 | 6520 |
| *N* (unique) | 2458 | 2453 | 3436 | 3645 | 3112 |
| *N* $[F_o > 4\sigma(F_o)]$ | 1679 | 1788 | 3006 | 2158 | 2089 |
| no. of parameters | 262 | 262 | 275 | 288 | 276 |
| *R* $[F_o > 4\sigma(F_o)]$ | 0.033 | 0.031 | 0.040 | 0.066 | 0.041 |
| *wR* ($F^2$) for all unique data | 0.081 | 0.079 | 0.105 | 0.186 | 0.091 |
| Weighting scheme, *w* where $P = (F_o^2 + 2F_c^2)/3$ | $1/[\sigma^2(F_o^2) + (0.0365P)^2 + 0.10P]$ | $1/[\sigma^2(F_o^2) + (0.0331P)^2 + 0.28P]$ | $1/[\sigma^2(F_o^2) + (0.0585P)^2]$ | $1/[\sigma^2(F_o^2) + (0.0854P)^2]$ | $1/[\sigma^2(F_o^2) + (0.0270P)^2]$ |
| Goodness-of-fit for all unique data | 1.04 | 1.06 | 1.05 | 1.05 | 0.87 |

Table 2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (6a*R*,12*R*)-**12**·HCl.

| Atom | x | y | z | $U_{eq}$ [Å$^2$] |
|---|---|---|---|---|
| Cl | 0.63572(7) | 0.40058(5) | 1.20840(5) | 0.0266(2) |
| O1 | 1.3259(2) | 0.6845(2) | 1.1581(2) | 0.0275(6) |
| N6 | 0.6683(2) | 0.5543(2) | 1.0113(2) | 0.0230(6) |
| C1 | 1.0838(2) | 0.6544(2) | 1.1978(2) | 0.0182(6) |
| C2 | 1.0213(3) | 0.7396(2) | 1.2549(2) | 0.0235(9) |
| C3 | 0.8842(3) | 0.7597(2) | 1.2354(2) | 0.0251(7) |
| C3A | 0.8105(2) | 0.7004(2) | 1.1573(2) | 0.0216(7) |
| C4 | 0.6615(3) | 0.7163(2) | 1.1394(2) | 0.0285(8) |
| C5 | 0.6155(3) | 0.6695(2) | 1.0308(2) | 0.0284(8) |
| C6A | 0.8193(2) | 0.5585(2) | 0.9993(2) | 0.0201(7) |
| C7 | 0.8791(3) | 0.4415(2) | 0.9804(2) | 0.0239(7) |
| C7A | 1.0298(3) | 0.4357(2) | 0.9998(2) | 0.0214(7) |
| C8 | 1.1184(3) | 0.3553(2) | 0.9621(2) | 0.0272(9) |
| C9 | 1.2523(3) | 0.3573(2) | 0.9971(2) | 0.0291(9) |
| C10 | 1.3028(3) | 0.4346(2) | 1.0720(2) | 0.0250(7) |
| C11 | 1.2146(3) | 0.5147(2) | 1.1093(2) | 0.0196(7) |
| C11A | 1.0835(3) | 0.5124(2) | 1.0707(2) | 0.0192(7) |
| C11B | 1.0071(2) | 0.5979(2) | 1.1221(2) | 0.0172(6) |
| C11C | 0.8748(3) | 0.6192(2) | 1.0969(2) | 0.0181(6) |
| C12 | 1.2277(2) | 0.6077(2) | 1.1943(2) | 0.0205(6) |
| C13 | 0.6019(3) | 0.5027(3) | 0.9137(2) | 0.0331(10) |

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

Table 3 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: (6a*R*,12*R*)-**12**·HCl.

| Atom | x | y | z | $U_{iso}$ [Å$^2$] |
|---|---|---|---|---|
| H1O | 1.336(3) | 0.736(3) | 1.205(3) | 0.044(10) |
| H2 | 1.066(3) | 0.787(3) | 1.308(3) | 0.037(8) |
| H3 | 0.840(3) | 0.816(2) | 1.280(2) | 0.026(7) |
| H4A | 0.613(3) | 0.685(3) | 1.199(3) | 0.041(9) |
| H4B | 0.638(3) | 0.798(2) | 1.138(2) | 0.033(8) |
| H5A | 0.637(3) | 0.715(2) | 0.970(2) | 0.030(8) |
| H5B | 0.519(4) | 0.663(3) | 1.027(3) | 0.041(9) |
| H6 | 0.650(3) | 0.509(2) | 1.073(3) | 0.032(8) |
| H6A | 0.830(2) | 0.604(2) | 0.935(2) | 0.015(6) |
| H7A | 0.854(3) | 0.418(2) | 0.906(2) | 0.022(7) |
| H7B | 0.834(3) | 0.390(2) | 1.028(2) | 0.025(7) |
| H8 | 1.091(3) | 0.301(2) | 0.911(2) | 0.031(8) |
| H9 | 1.310(3) | 0.300(2) | 0.968(2) | 0.030(8) |
| H10 | 1.395(3) | 0.433(2) | 1.104(2) | 0.026(8) |
| H12 | 1.250(3) | 0.573(2) | 1.268(2) | 0.027(7) |
| H13A | 0.618(3) | 0.424(3) | 0.916(3) | 0.044(10) |
| H13B | 0.501(4) | 0.513(3) | 0.920(3) | 0.060(11) |
| H13C | 0.636(3) | 0.538(2) | 0.847(2) | 0.025(7) |

Table 4 - Anisotropic Displacement Parameters for: (6a*R*,12*R*)-**12**·HCl.

| Atom | $U_{1,1}$ | $U_{2,2}$ | $U_{3,3}$ | $U_{2,3}$ | $U_{1,3}$ | $U_{1,2}$ |
|---|---|---|---|---|---|---|
| Cl | 0.0351(3) | 0.0250(3) | 0.0196(2) | 0.0039(3) | -0.0030(3) | -0.0018(3) |
| O1 | 0.0230(10) | 0.0272(10) | 0.0324(10) | -0.0039(9) | 0.0026(8) | -0.0077(8) |
| N6 | 0.0203(11) | 0.0293(10) | 0.0195(10) | 0.0057(9) | -0.0021(9) | -0.0040(9) |
| C1 | 0.0204(11) | 0.0183(10) | 0.0160(11) | 0.0019(9) | 0.0014(9) | -0.0013(9) |
| C2 | 0.031(2) | 0.0200(12) | 0.0194(11) | -0.0038(10) | 0.0017(11) | -0.0025(11) |
| C3 | 0.0308(15) | 0.0201(11) | 0.0245(12) | -0.0042(10) | 0.0082(11) | 0.0039(11) |
| C3A | 0.0215(12) | 0.0197(11) | 0.0237(12) | 0.0019(10) | 0.0038(10) | 0.0026(10) |
| C4 | 0.0230(14) | 0.0297(14) | 0.0329(14) | -0.0001(12) | 0.0013(12) | 0.0062(12) |
| C5 | 0.0209(14) | 0.0323(14) | 0.0321(14) | 0.0112(12) | -0.0001(13) | 0.0056(12) |
| C6A | 0.0190(12) | 0.0230(11) | 0.0182(11) | 0.0022(10) | 0.0021(10) | -0.0023(10) |
| C7 | 0.0278(13) | 0.0221(11) | 0.0219(11) | -0.0034(10) | -0.0008(12) | -0.0061(12) |
| C7A | 0.0306(14) | 0.0173(11) | 0.0163(11) | -0.0001(9) | 0.0033(10) | -0.0012(11) |
| C8 | 0.042(2) | 0.0181(11) | 0.0216(12) | -0.0035(10) | 0.0103(13) | 0.0007(13) |
| C9 | 0.037(2) | 0.0207(12) | 0.0296(14) | 0.0032(11) | 0.0128(13) | 0.0100(13) |
| C10 | 0.0235(13) | 0.0239(12) | 0.0275(13) | 0.0071(11) | 0.0063(12) | 0.0052(11) |
| C11 | 0.0216(13) | 0.0192(11) | 0.0181(11) | 0.0027(9) | 0.0035(10) | 0.0005(10) |
| C11A | 0.0234(13) | 0.0157(11) | 0.0184(11) | 0.0010(9) | 0.0046(10) | 0.0005(10) |
| C11B | 0.0205(11) | 0.0151(10) | 0.0160(10) | 0.0013(10) | 0.0014(9) | -0.0007(10) |
| C11C | 0.0191(11) | 0.0170(11) | 0.0183(10) | 0.0015(8) | 0.0027(10) | -0.0023(10) |
| C12 | 0.0187(11) | 0.0228(11) | 0.0201(11) | 0.0014(11) | 0.0008(9) | -0.0016(10) |
| C13 | 0.030(2) | 0.047(2) | 0.0223(13) | 0.0036(13) | -0.0070(12) | -0.0131(14) |

Table 5 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (6a*R*,12*S*)-**12**·HCl.

| Atom | x | y | z | $U_{eq}$ [Å$^2$] |
|---|---|---|---|---|
| Cl | 0.11979(7) | 0.42755(5) | 0.36765(4) | 0.0268(1) |
| O1 | -0.4776(2) | 0.54288(15) | 0.05834(13) | 0.0348(5) |
| N6 | 0.0494(3) | 0.1901(2) | 0.29805(13) | 0.0251(6) |
| C1 | -0.4009(3) | 0.3764(2) | 0.14687(14) | 0.0241(6) |
| C2 | -0.4962(3) | 0.3668(2) | 0.2229(2) | 0.0315(7) |
| C3 | -0.4357(3) | 0.3099(2) | 0.2975(2) | 0.0343(8) |
| C3A | -0.2826(3) | 0.2599(2) | 0.2995(2) | 0.0282(7) |
| C4 | -0.2118(4) | 0.2052(3) | 0.3819(2) | 0.0373(8) |
| C5 | -0.0698(4) | 0.1303(2) | 0.3582(2) | 0.0367(9) |
| C6A | -0.0253(3) | 0.2132(2) | 0.2076(2) | 0.0217(6) |
| C7 | 0.0885(3) | 0.2842(2) | 0.14752(15) | 0.0213(6) |
| C7A | 0.0067(3) | 0.3364(2) | 0.06602(14) | 0.0180(5) |
| C8 | 0.0807(3) | 0.3806(2) | -0.0101(2) | 0.0240(6) |
| C9 | -0.0098(3) | 0.4416(2) | -0.0727(2) | 0.0281(7) |
| C10 | -0.1742(3) | 0.4635(2) | -0.0611(2) | 0.0272(6) |
| C11 | -0.2492(3) | 0.4193(2) | 0.01373(14) | 0.0215(6) |
| C11A | -0.1571(3) | 0.3552(2) | 0.07294(14) | 0.0191(5) |
| C11B | -0.2487(3) | 0.3272(2) | 0.15079(14) | 0.0196(6) |
| C11C | -0.1886(3) | 0.2672(2) | 0.2225(2) | 0.0215(6) |
| C12 | -0.4203(3) | 0.4302(2) | 0.05342(15) | 0.0247(6) |
| C13 | 0.2023(4) | 0.1233(2) | 0.2914(2) | 0.0332(9) |

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

Table 6 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: (6a*R*,12*S*)-**12**·HCl.

| Atom | x | y | z | $U_{iso}$ [Å$^2$] |
|---|---|---|---|---|
| H1O | -0.520(4) | 0.560(3) | 0.008(2) | 0.052(10) |
| H2 | -0.602(3) | 0.402(2) | 0.2220(16) | 0.025(6) |
| H3 | -0.495(3) | 0.311(2) | 0.3481(16) | 0.027(7) |
| H4A | -0.183(3) | 0.271(2) | 0.4242(17) | 0.029(7) |
| H4B | -0.289(4) | 0.163(3) | 0.412(2) | 0.051(10) |
| H5A | -0.013(4) | 0.107(2) | 0.4129(19) | 0.035(7) |
| H5B | -0.104(3) | 0.061(2) | 0.3242(17) | 0.030(7) |
| H6 | 0.073(3) | 0.261(2) | 0.3214(15) | 0.020(6) |
| H6A | -0.040(3) | 0.1405(19) | 0.1791(15) | 0.014(6) |
| H7A | 0.182(3) | 0.2410(19) | 0.1340(15) | 0.017(6) |
| H7B | 0.133(3) | 0.345(2) | 0.1821(16) | 0.022(6) |
| H8 | 0.198(3) | 0.374(2) | -0.0199(16) | 0.018(6) |
| H9 | 0.043(3) | 0.472(2) | -0.1221(18) | 0.029(7) |
| H10 | -0.234(4) | 0.514(2) | -0.1013(18) | 0.039(8) |
| H12 | -0.497(4) | 0.384(2) | 0.0198(17) | 0.029(7) |
| H13A | 0.282(4) | 0.162(3) | 0.253(2) | 0.041(8) |
| H13B | 0.172(4) | 0.052(3) | 0.2667(19) | 0.044(9) |
| H13C | 0.241(4) | 0.115(3) | 0.351(2) | 0.045(9) |

Table 7 - Anisotropic Displacement Parameters for: (6a*R*,12*S*)-**12**·HCl.

| Atom | $U_{1,1}$ | $U_{2,2}$ | $U_{3,3}$ | $U_{2,3}$ | $U_{1,3}$ | $U_{1,2}$ |
|---|---|---|---|---|---|---|
| Cl | 0.0325(3) | 0.0203(2) | 0.0277(2) | -0.0041(2) | 0.0045(3) | -0.0018(2) |
| O1 | 0.0364(10) | 0.0332(9) | 0.0349(9) | -0.0128(8) | -0.0132(9) | 0.0178(8) |
| N6 | 0.0337(11) | 0.0153(8) | 0.0262(10) | 0.0033(8) | -0.0066(9) | -0.0009(8) |
| C1 | 0.0190(10) | 0.0254(10) | 0.0278(11) | -0.0069(9) | -0.0048(9) | -0.0034(9) |
| C2 | 0.0181(11) | 0.0387(13) | 0.0378(14) | -0.0150(11) | 0.0017(11) | -0.0048(11) |
| C3 | 0.0276(12) | 0.0457(15) | 0.0295(13) | -0.0089(12) | 0.0087(11) | -0.0146(12) |
| C3A | 0.0289(13) | 0.0273(11) | 0.0285(12) | -0.0006(10) | 0.0031(11) | -0.0127(10) |
| C4 | 0.0404(15) | 0.0412(14) | 0.0303(13) | 0.0119(12) | 0.0052(12) | -0.0161(13) |
| C5 | 0.050(2) | 0.0249(11) | 0.0351(13) | 0.0122(11) | -0.0064(14) | -0.0107(11) |
| C6A | 0.0262(11) | 0.0151(9) | 0.0238(10) | 0.0002(8) | -0.0049(10) | -0.0014(9) |
| C7 | 0.0215(11) | 0.0181(9) | 0.0242(11) | -0.0012(8) | -0.0016(9) | 0.0043(8) |
| C7A | 0.0206(10) | 0.0138(8) | 0.0197(9) | -0.0046(8) | -0.0005(9) | 0.0031(8) |
| C8 | 0.0245(11) | 0.0220(10) | 0.0255(11) | -0.0040(9) | 0.0018(9) | 0.0008(9) |
| C9 | 0.0375(13) | 0.0262(11) | 0.0206(10) | 0.0014(10) | 0.0041(10) | 0.0002(11) |
| C10 | 0.0375(13) | 0.0239(10) | 0.0203(10) | 0.0000(9) | -0.0086(10) | 0.0040(10) |
| C11 | 0.0215(10) | 0.0196(9) | 0.0234(10) | -0.0066(9) | -0.0060(9) | 0.0047(9) |
| C11A | 0.0219(10) | 0.0151(8) | 0.0204(9) | -0.0055(8) | -0.0023(8) | -0.0005(8) |
| C11B | 0.0191(9) | 0.0174(9) | 0.0222(11) | -0.0053(8) | -0.0005(8) | -0.0029(8) |
| C11C | 0.0218(10) | 0.0176(9) | 0.0252(11) | -0.0014(8) | -0.0012(9) | -0.0075(9) |
| C12 | 0.0208(10) | 0.0257(10) | 0.0276(10) | -0.0085(10) | -0.0082(9) | 0.0053(10) |
| C13 | 0.041(2) | 0.0242(12) | 0.0345(13) | 0.0025(11) | -0.0115(13) | 0.0111(12) |

Table 8 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (6a*R*,12*S*)-**15**·2HCl·$H_2O$.

| Atom | x | y | z | $U_{eq}$ [Å$^2$] |
|---|---|---|---|---|
| N6 | 0.2197(3) | -0.2423(2) | 0.40614(9) | 0.0134(5) |
| N14 | 0.2159(3) | -0.4161(2) | 0.10299(8) | 0.0140(6) |
| C1 | 0.2912(4) | -0.4268(2) | 0.21231(10) | 0.0129(6) |
| C2 | 0.2712(4) | -0.5464(2) | 0.23411(10) | 0.0136(7) |
| C3 | 0.2423(3) | -0.5609(2) | 0.29429(10) | 0.0136(7) |
| C3A | 0.2419(3) | -0.4610(2) | 0.33313(10) | 0.0115(6) |
| C4 | 0.2146(4) | -0.4745(2) | 0.39801(10) | 0.0143(7) |
| C5 | 0.2890(4) | -0.3634(2) | 0.43106(10) | 0.0157(7) |
| C6A | 0.2958(4) | -0.2244(2) | 0.34510(10) | 0.0130(6) |
| C7 | 0.2116(4) | -0.1087(2) | 0.31479(10) | 0.0149(7) |
| C7A | 0.2589(3) | -0.1032(2) | 0.24989(10) | 0.0146(7) |
| C8 | 0.2556(4) | 0.0004(2) | 0.21335(11) | 0.0162(8) |
| C9 | 0.2833(4) | -0.0140(2) | 0.15362(11) | 0.0174(7) |
| C10 | 0.3129(4) | -0.1285(2) | 0.12681(10) | 0.0167(7) |
| C11 | 0.3160(3) | -0.2315(2) | 0.16266(10) | 0.0124(7) |
| C11A | 0.2915(4) | -0.2138(2) | 0.22228(10) | 0.0124(6) |
| C11B | 0.2825(3) | -0.3307(2) | 0.25123(10) | 0.0126(6) |
| C11C | 0.2664(3) | -0.3418(2) | 0.31095(10) | 0.0113(6) |
| C12 | 0.3356(3) | -0.3713(2) | 0.15222(10) | 0.0123(7) |
| C13 | 0.2735(4) | -0.1388(2) | 0.44597(10) | 0.0178(8) |
| Ow | 0.0529(3) | 0.3660(2) | 0.51057(8) | 0.0253(6) |
| Cl1 | -0.21572(8) | -0.20571(5) | 0.40889(2) | 0.0140(2) |
| Cl2 | -0.19444(9) | -0.31403(5) | 0.08839(3) | 0.0183(2) |

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

Table 9 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: (6a*R*,12*S*)-**15**·2HCl·$H_2O$.

| Atom | x | y | z | $U_{iso}$ [Å$^2$] |
|---|---|---|---|---|
| H2 | 0.277(4) | -0.620(3) | 0.2111(11) | 0.0160 |
| H3 | 0.226(4) | -0.648(3) | 0.3092(11) | 0.0160 |
| H4A | 0.072(4) | -0.486(3) | 0.4058(12) | 0.0170 |
| H4B | 0.280(4) | -0.545(3) | 0.4118(12) | 0.0170 |
| H5A | 0.244(4) | -0.364(3) | 0.4718(12) | 0.0190 |
| H5B | 0.427(4) | -0.362(3) | 0.4280(12) | 0.0190 |
| H6 | 0.086(5) | -0.244(3) | 0.4049(12) | 0.0160 |
| H6A | 0.433(4) | -0.207(3) | 0.3498(11) | 0.0160 |
| H7A | 0.073(4) | -0.107(3) | 0.3186(12) | 0.0180 |
| H7B | 0.254(4) | -0.030(3) | 0.3321(11) | 0.0180 |
| H8B | 0.236(4) | 0.083(3) | 0.2270(12) | 0.0190 |
| H9 | 0.288(5) | 0.056(3) | 0.1301(12) | 0.0210 |
| H10 | 0.326(4) | -0.133(3) | 0.0843(13) | 0.0200 |
| H12 | 0.464(4) | -0.390(3) | 0.1415(12) | 0.0150 |
| H13A | 0.416(5) | -0.125(3) | 0.4465(13) | 0.0230 |
| H13B | 0.226(5) | -0.155(3) | 0.4855(13) | 0.0230 |
| H13C | 0.210(5) | -0.061(3) | 0.4300(12) | 0.0230 |
| H14A | 0.097(5) | -0.383(3) | 0.1046(12) | 0.0180 |
| H14B | 0.199(4) | -0.496(3) | 0.1042(12) | 0.0180 |
| H14C | 0.277(4) | -0.387(3) | 0.0671(12) | 0.0180 |
| H1W | -0.049(5) | 0.345(3) | 0.5241(14) | 0.0300 |
| H2W | 0.078(5) | 0.313(3) | 0.4856(14) | 0.0300 |

Table 10 - Anisotropic Displacement Parameters for: (6a*R*,12*S*)-**15**·2HCl·$H_2O$.

| Atom | $U_{1,1}$ | $U_{2,2}$ | $U_{3,3}$ | $U_{2,3}$ | $U_{1,3}$ | $U_{1,2}$ |
|---|---|---|---|---|---|---|
| N6 | 0.0123(10) | 0.0153(9) | 0.0127(9) | -0.0004(7) | 0.0006(9) | 0.0007(8) |
| N14 | 0.0146(11) | 0.0137(10) | 0.0136(10) | 0.0008(7) | -0.0024(9) | 0.0006(9) |
| C1 | 0.0082(11) | 0.0180(12) | 0.0124(10) | 0.0023(9) | -0.0012(10) | 0.0013(11) |
| C2 | 0.0093(12) | 0.0128(11) | 0.0186(11) | -0.0013(9) | -0.0016(10) | 0.0032(10) |
| C3 | 0.0097(14) | 0.0115(11) | 0.0196(12) | 0.0029(9) | -0.0001(9) | 0.0027(10) |
| C3A | 0.0074(12) | 0.0113(10) | 0.0157(11) | 0.0016(9) | -0.0005(9) | 0.0007(9) |
| C4 | 0.0164(13) | 0.0140(11) | 0.0126(12) | 0.0025(8) | 0.0000(11) | 0.0007(11) |
| C5 | 0.0163(12) | 0.0159(12) | 0.0148(11) | 0.0011(9) | -0.0005(11) | 0.0005(12) |
| C6A | 0.0108(11) | 0.0144(11) | 0.0138(11) | 0.0002(8) | 0.0007(10) | -0.0007(11) |
| C7 | 0.0143(13) | 0.0120(11) | 0.0183(12) | 0.0013(9) | -0.0004(11) | -0.0004(11) |
| C7A | 0.0099(13) | 0.0154(11) | 0.0186(11) | 0.0025(9) | -0.0024(10) | 0.0010(9) |
| C8 | 0.0112(14) | 0.0123(12) | 0.0250(13) | 0.0024(10) | -0.0008(11) | -0.0019(9) |
| C9 | 0.0118(12) | 0.0152(11) | 0.0252(13) | 0.0099(10) | -0.0024(12) | -0.0028(11) |
| C10 | 0.0110(13) | 0.0217(12) | 0.0174(12) | 0.0073(10) | -0.0013(11) | -0.0039(11) |
| C11 | 0.0054(12) | 0.0124(11) | 0.0193(12) | 0.0027(9) | -0.0016(10) | -0.0015(10) |
| C11A | 0.0069(11) | 0.0130(11) | 0.0173(11) | 0.0031(9) | -0.0036(10) | -0.0008(11) |
| C11B | 0.0077(11) | 0.0132(11) | 0.0170(11) | 0.0022(8) | -0.0013(10) | -0.0021(10) |
| C11C | 0.0075(11) | 0.0105(11) | 0.0158(11) | 0.0016(8) | -0.0008(9) | -0.0004(9) |
| C12 | 0.0092(12) | 0.0145(11) | 0.0131(11) | 0.0015(9) | -0.0016(9) | -0.0008(10) |
| C13 | 0.0221(15) | 0.0152(12) | 0.0161(12) | -0.0031(9) | -0.0006(11) | -0.0014(12) |
| Ow | 0.0219(11) | 0.0369(12) | 0.0170(10) | -0.0066(9) | 0.0036(8) | -0.0090(10) |
| Cl1 | 0.0122(3) | 0.0135(2) | 0.0162(3) | -0.0002(2) | 0.0008(2) | -0.0002(2) |
| Cl2 | 0.0143(3) | 0.0155(3) | 0.0251(3) | 0.0017(2) | -0.0006(3) | 0.0009(2) |

Table 11 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for (6a*R*,12*S*)-**16**·HCl·MeCN.

| Atom | x | y | z | $U_{eq}$ [Å$^2$] |
|---|---|---|---|---|
| N6 | 1.4856(5) | 0.5779(3) | 0.5637(2) | 0.0299(11) |
| C1 | 1.4843(6) | 0.4116(3) | 0.3205(2) | 0.0267(12) |
| C2 | 1.5035(7) | 0.4892(3) | 0.2774(3) | 0.0307(12) |
| C3 | 1.5063(7) | 0.5708(3) | 0.3165(3) | 0.0317(12) |
| C3A | 1.4844(6) | 0.5776(3) | 0.3969(2) | 0.0287(12) |
| C4 | 1.5028(8) | 0.6647(3) | 0.4407(3) | 0.0383(16) |
| C5 | 1.4159(9) | 0.6584(3) | 0.5207(3) | 0.0330(14) |
| C6A | 1.4145(7) | 0.4936(3) | 0.5252(3) | 0.0263(12) |
| C7 | 1.4898(6) | 0.4081(3) | 0.5657(3) | 0.0290(12) |
| C7A | 1.4711(6) | 0.3240(3) | 0.5161(2) | 0.0253(12) |
| C8 | 1.4785(7) | 0.2354(3) | 0.5406(3) | 0.0313(12) |
| C9 | 1.4786(7) | 0.1665(3) | 0.4865(3) | 0.0333(14) |
| C10 | 1.4837(7) | 0.1808(3) | 0.4074(3) | 0.0323(14) |
| C11 | 1.4773(7) | 0.2685(3) | 0.3807(3) | 0.0283(12) |
| C11A | 1.4654(6) | 0.3355(2) | 0.4374(3) | 0.0243(12) |
| C11B | 1.4662(5) | 0.4203(3) | 0.3999(2) | 0.0240(12) |
| C11C | 1.4603(6) | 0.5003(2) | 0.4397(3) | 0.0223(12) |
| C12 | 1.4903(7) | 0.3112(3) | 0.2996(2) | 0.0253(12) |
| C13 | 1.4247(8) | 0.5809(5) | 0.6480(3) | 0.0417(14) |
| C14 | 1.6772(7) | 0.2884(3) | 0.2583(3) | 0.0327(14) |
| N17 | 1.4477(10) | 0.8194(5) | 0.6994(5) | 0.111(3) |
| C15 | 1.4850(9) | 0.9785(4) | 0.6409(3) | 0.0460(18) |
| C16 | 1.4681(10) | 0.8899(5) | 0.6751(4) | 0.061(2) |
| Cl | 1.92018(14) | 0.58200(7) | 0.56327(7) | 0.0312(3) |

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

Table 12 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: (6a*R*,12*S*)-**16**·HCl·MeCN.

| Atom | x | y | z | $U_{iso}$ [Å$^2$] |
|---|---|---|---|---|
| H2 | 1.555(8) | 0.485(3) | 0.217(3) | 0.0370 |
| H3 | 1.511(8) | 0.626(3) | 0.286(3) | 0.0380 |
| H4A | 1.658(8) | 0.692(3) | 0.450(3) | 0.0460 |
| H4B | 1.472(8) | 0.713(3) | 0.415(3) | 0.0460 |
| H5A | 1.264(8) | 0.653(3) | 0.518(3) | 0.0400 |
| H5B | 1.435(8) | 0.708(3) | 0.543(3) | 0.0400 |
| H6 | 1.614(7) | 0.573(3) | 0.571(3) | 0.0360 |
| H6A | 1.281(7) | 0.498(3) | 0.527(2) | 0.0360 |
| H7A | 1.428(7) | 0.398(3) | 0.613(3) | 0.0350 |
| H7B | 1.635(7) | 0.420(3) | 0.581(2) | 0.0350 |
| H8 | 1.487(8) | 0.230(3) | 0.593(3) | 0.0380 |
| H9 | 1.493(8) | 0.110(3) | 0.504(3) | 0.0400 |
| H10 | 1.490(8) | 0.134(3) | 0.373(3) | 0.0390 |
| H12 | 1.377(5) | 0.292(3) | 0.261(2) | 0.0300 |
| H13A | 1.500(9) | 0.535(4) | 0.678(3) | 0.0630 |
| H13B | 1.274(10) | 0.593(4) | 0.652(3) | 0.0630 |
| H13C | 1.472(10) | 0.635(4) | 0.665(3) | 0.0630 |
| H14A | 1.804(9) | 0.308(3) | 0.288(3) | 0.0490 |
| H14B | 1.686(9) | 0.328(4) | 0.212(3) | 0.0490 |
| H14C | 1.673(9) | 0.227(4) | 0.253(3) | 0.0490 |
| H15A | 1.377(10) | 1.013(4) | 0.677(3) | 0.0690 |
| H15B | 1.620(10) | 1.005(4) | 0.656(4) | 0.0690 |
| H15C | 1.496(10) | 0.968(4) | 0.588(4) | 0.0690 |

Table 13 - Anisotropic Displacement Parameters for: (6a*R*,12*S*)-**16**·HCl·MeCN.

| Atom | $U_{1,1}$ | $U_{2,2}$ | $U_{3,3}$ | $U_{2,3}$ | $U_{1,3}$ | $U_{1,2}$ |
|---|---|---|---|---|---|---|
| N6 | 0.0156(15) | 0.036(2) | 0.038(2) | -0.016(2) | -0.003(2) | -0.001(2) |
| C1 | 0.021(2) | 0.029(2) | 0.030(2) | -0.004(2) | -0.004(2) | -0.003(2) |
| C2 | 0.024(2) | 0.035(2) | 0.033(2) | 0.002(2) | -0.004(2) | 0.001(2) |
| C3 | 0.030(2) | 0.025(2) | 0.040(2) | 0.009(2) | -0.005(2) | 0.000(2) |
| C3A | 0.019(2) | 0.024(2) | 0.043(2) | -0.001(2) | -0.002(2) | -0.001(2) |
| C4 | 0.039(3) | 0.017(2) | 0.059(3) | 0.000(2) | 0.002(3) | 0.002(2) |
| C5 | 0.028(2) | 0.020(2) | 0.051(3) | -0.012(2) | 0.003(3) | 0.001(2) |
| C6A | 0.014(2) | 0.030(2) | 0.035(2) | -0.005(2) | 0.003(2) | -0.005(2) |
| C7 | 0.022(2) | 0.038(2) | 0.027(2) | 0.003(2) | 0.001(2) | 0.003(2) |
| C7A | 0.014(2) | 0.026(2) | 0.036(2) | 0.001(2) | 0.005(2) | -0.002(2) |
| C8 | 0.023(2) | 0.035(2) | 0.036(2) | 0.012(2) | 0.004(2) | 0.000(2) |
| C9 | 0.024(2) | 0.022(2) | 0.054(3) | 0.012(2) | 0.005(2) | -0.001(2) |
| C10 | 0.019(2) | 0.023(2) | 0.055(3) | -0.005(2) | 0.002(2) | -0.003(2) |
| C11 | 0.020(2) | 0.025(2) | 0.040(2) | 0.000(2) | -0.004(2) | -0.005(2) |
| C11A | 0.019(2) | 0.019(2) | 0.035(2) | -0.001(2) | 0.007(2) | -0.0005(15) |
| C11B | 0.015(2) | 0.023(2) | 0.034(2) | -0.001(2) | -0.002(2) | -0.003(2) |
| C11C | 0.014(2) | 0.021(2) | 0.032(2) | -0.001(2) | 0.000(2) | 0.0014(15) |
| C12 | 0.020(2) | 0.030(2) | 0.026(2) | -0.004(2) | -0.001(2) | 0.001(2) |
| C13 | 0.033(2) | 0.054(3) | 0.038(2) | -0.021(3) | 0.008(2) | -0.001(3) |
| C14 | 0.028(2) | 0.030(2) | 0.040(3) | 0.000(2) | 0.004(2) | 0.001(2) |
| N17 | 0.066(5) | 0.074(4) | 0.192(8) | 0.042(5) | -0.028(5) | 0.023(4) |
| C15 | 0.032(3) | 0.068(4) | 0.038(2) | -0.007(3) | 0.003(3) | -0.003(3) |
| C16 | 0.040(3) | 0.067(4) | 0.075(4) | 0.012(3) | -0.007(3) | 0.014(3) |
| Cl | 0.0190(4) | 0.0374(5) | 0.0373(5) | -0.0071(5) | -0.0006(5) | 0.0004(5) |

Table 14 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (6a*R*,12*R*)-**17**·HCl.

| Atom | x | y | z | $U_{eq}$ [Å$^2$] |
|---|---|---|---|---|
| Cl | -0.34348(8) | 0.75792(11) | -0.37031(7) | 0.0208(2) |
| O | 0.3891(2) | 0.2395(3) | -0.1354(2) | 0.0199(7) |
| N6 | -0.3082(3) | 0.3292(4) | -0.3666(2) | 0.0155(10) |
| C1 | 0.1787(3) | 0.3502(4) | -0.2647(3) | 0.0141(10) |
| C2 | 0.1879(3) | 0.3528(4) | -0.3809(3) | 0.0185(11) |
| C3 | 0.0711(3) | 0.3475(4) | -0.4659(3) | 0.0167(11) |
| C3A | -0.0563(3) | 0.3302(4) | -0.4411(3) | 0.0155(10) |
| C4 | -0.1833(3) | 0.3358(5) | -0.5292(3) | 0.0167(11) |
| C5 | -0.3006(3) | 0.2541(6) | -0.4850(3) | 0.0168(11) |
| C6A | -0.1882(3) | 0.2660(5) | -0.2784(3) | 0.0136(11) |
| C7 | -0.1896(3) | 0.3402(5) | -0.1562(3) | 0.0171(11) |
| C7A | -0.0551(3) | 0.3279(4) | -0.0728(3) | 0.0145(10) |
| C8 | -0.0306(4) | 0.3264(4) | 0.0481(3) | 0.0184(11) |
| C9 | 0.1004(3) | 0.3295(4) | 0.1119(3) | 0.0179(11) |
| C10 | 0.2118(4) | 0.3426(4) | 0.0603(3) | 0.0184(11) |
| C11 | 0.1888(3) | 0.3438(4) | -0.0599(3) | 0.0156(10) |
| C11A | 0.0572(3) | 0.3311(4) | -0.1198(3) | 0.0148(10) |
| C11B | 0.0517(3) | 0.3315(4) | -0.2424(3) | 0.0152(10) |
| C11C | -0.0646(3) | 0.3162(4) | -0.3235(3) | 0.0138(11) |
| C12 | 0.2806(4) | 0.3691(4) | -0.1490(3) | 0.0177(12) |
| C13 | -0.4357(3) | 0.2657(6) | -0.3360(3) | 0.0219(12) |
| C14 | 0.3451(4) | 0.5630(5) | -0.1377(4) | 0.0203(12) |
| C15 | 0.3502(4) | 0.0444(5) | -0.1382(4) | 0.0247(13) |

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

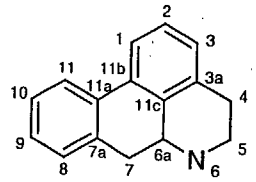
Table 15 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: (6a*R*,12*R*)-**17**·HCl.

| Atom | x | y | z | $U_{iso}$ [Å$^2$] |
|---|---|---|---|---|
| H2 | 0.277(4) | 0.349(4) | -0.403(3) | 0.0220 |
| H3 | 0.075(3) | 0.333(4) | -0.550(3) | 0.0200 |
| H4A | -0.178(3) | 0.273(5) | -0.607(3) | 0.0200 |
| H4B | -0.202(4) | 0.472(4) | -0.557(3) | 0.0200 |
| H5A | -0.394(3) | 0.289(4) | -0.539(3) | 0.0200 |
| H5B | -0.293(3) | 0.103(4) | -0.470(3) | 0.0200 |
| H6 | -0.302(4) | 0.476(4) | -0.361(3) | 0.0190 |
| H6A | -0.196(3) | 0.119(4) | -0.279(3) | 0.0160 |
| H7A | -0.254(3) | 0.269(5) | -0.117(3) | 0.0210 |
| H7B | -0.217(4) | 0.471(4) | -0.158(3) | 0.0210 |
| H8 | -0.116(3) | 0.315(4) | 0.087(3) | 0.0220 |
| H9 | 0.117(3) | 0.319(4) | 0.201(3) | 0.0210 |
| H10 | 0.303(4) | 0.337(4) | 0.112(3) | 0.0220 |
| H13A | -0.448(4) | 0.338(5) | -0.265(3) | 0.0290 |
| H13B | -0.507(4) | 0.295(5) | -0.399(3) | 0.0290 |
| H13C | -0.423(4) | 0.123(5) | -0.327(3) | 0.0290 |
| H14A | 0.401(4) | 0.579(5) | -0.196(3) | 0.0260 |
| H14B | 0.273(4) | 0.675(4) | -0.157(3) | 0.0260 |
| H14C | 0.400(4) | 0.587(5) | -0.053(3) | 0.0260 |
| H15A | 0.429(4) | -0.033(5) | -0.128(4) | 0.0320 |
| H15B | 0.281(4) | 0.014(5) | -0.215(4) | 0.0320 |
| H15C | 0.315(5) | 0.000(5) | -0.058(4) | 0.0320 |

Table 16 - Anisotropic Displacement Parameters for: (6a*R*,12*R*)-**17**·HCl.

| Atom | $U_{1,1}$ | $U_{2,2}$ | $U_{3,3}$ | $U_{2,3}$ | $U_{1,3}$ | $U_{1,2}$ |
|---|---|---|---|---|---|---|
| Cl | 0.0256(4) | 0.0165(3) | 0.0179(4) | -0.0006(4) | -0.0011(3) | 0.0006(4) |
| O | 0.0181(12) | 0.0118(10) | 0.0290(14) | -0.0015(12) | 0.0027(11) | -0.0010(11) |
| N6 | 0.018(2) | 0.0126(12) | 0.015(2) | -0.0008(12) | 0.0010(13) | 0.0018(11) |
| C1 | 0.017(2) | 0.0099(13) | 0.014(2) | 0.0044(13) | 0.0000(15) | -0.0004(14) |
| C2 | 0.018(2) | 0.0150(15) | 0.022(2) | 0.004(2) | 0.003(2) | 0.0045(15) |
| C3 | 0.020(2) | 0.0160(14) | 0.013(2) | 0.0023(15) | 0.001(2) | 0.0015(15) |
| C3A | 0.018(2) | 0.0128(13) | 0.014(2) | 0.0029(13) | -0.0012(15) | 0.0024(13) |
| C4 | 0.018(2) | 0.0185(15) | 0.012(2) | 0.0032(14) | -0.001(2) | 0.0011(15) |
| C5 | 0.017(2) | 0.0187(14) | 0.013(2) | -0.004(2) | -0.0012(14) | 0.000(2) |
| C6A | 0.013(2) | 0.0127(14) | 0.013(2) | 0.002(2) | -0.0021(13) | 0.000(2) |
| C7 | 0.019(2) | 0.0139(14) | 0.017(2) | -0.0040(14) | 0.000(2) | -0.0011(15) |
| C7A | 0.016(2) | 0.0113(13) | 0.014(2) | 0.0024(13) | -0.002(2) | -0.0015(14) |
| C8 | 0.025(2) | 0.0110(14) | 0.019(2) | -0.0006(14) | 0.004(2) | -0.0002(15) |
| C9 | 0.025(2) | 0.0150(14) | 0.013(2) | -0.0010(14) | 0.002(2) | -0.0022(14) |
| C10 | 0.021(2) | 0.0104(14) | 0.022(2) | 0.0013(15) | 0.000(2) | -0.0013(15) |
| C11 | 0.017(2) | 0.0105(13) | 0.019(2) | 0.0002(14) | 0.003(2) | -0.0021(14) |
| C11A | 0.019(2) | 0.0089(12) | 0.017(2) | 0.0009(13) | 0.005(2) | -0.0009(13) |
| C11B | 0.019(2) | 0.0101(13) | 0.016(2) | 0.0008(13) | 0.002(2) | -0.0020(14) |
| C11C | 0.015(2) | 0.0108(15) | 0.015(2) | 0.0012(12) | 0.0015(15) | 0.0023(11) |
| C12 | 0.021(2) | 0.007(2) | 0.024(2) | 0.0028(13) | 0.002(2) | 0.0026(13) |
| C13 | 0.015(2) | 0.026(2) | 0.025(2) | 0.003(2) | 0.005(2) | -0.004(2) |
| C14 | 0.019(2) | 0.012(2) | 0.030(2) | 0.000(2) | 0.005(2) | -0.003(2) |
| C15 | 0.031(3) | 0.0053(14) | 0.035(2) | 0.000(2) | 0.000(2) | 0.001(2) |

Table 17. Conformational features of selected aporphine derivatives included in the Cambridge Structural Database. The aporphine derivatives are substituted with hydrogen either at the C1 or at the C11 position.




| | 1 | 2 | 3 | 4 | 5 | 6 | 6a | 7 | 8 | 9 | 10 | 11 | Torsion angle,[a] C11-C11a-C11b-C1, (deg) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ACLAUR[1] | OCOMe | OMe | | | | COMe, H | | | | OH | OMe | | -25.7, -25.2 |
| ACNORT[2] | OMe | OMe | | OCOMe | | COMe | | | | -O-$CH_2$-O- | | | 23.8 |
| APOMRC[3] | | | | | | Me, H | | | | | OH | OH | 22.4, 26.3 |
| BOJIU10[4] | OMe | OMe | | OH | | Me | | | | OMe | OMe | | 30.0 |
| BOTYAK[5] | OMe | OMe | | | | —C(=CH—COOMe)—C(=CH—COOMe)— | | | | | | | 23.9 |
| BULMUQ[6] | OMe | OMe | | | | Me, Me | | OH | | OMe | OMe | | -27.4, 21.5 |
| FIXSAG[7] | -O-$CH_2$-O- | | | | OH | Me, Me | | | | | | | -17.8 |
| HIHXUR[8] | OMe | OH | | | | Me, H | | | | OH | OMe | | 27.8 |
| ISBOLD10[9] | OH | OMe | | | | Me, H | | | | OH | OMe | | 20.5 |
| LAUREL[10] | OH | OMe | | | | H | | | | OH | OMe | | -25.5 |
| LEUCOX10[9] | -O-$CH_2$-O- | | | | | Me, H | | | OH | OMe | OMe | | 15.0 |
| TICVAC[11] | OMe | OMe | | | | CHO | | | | | | | 23.5 |
| YONPAS[12] | | | | | | Me, H | | | | | Me | OH | -30.5, -22.6 |
| | | | | | | | | | | | Mean ( \| torsion angle \| ) | | 24 (4) |

[a] Torsion angles with negative sign correspond to the 6a*R* configuration in apomorphine, whereas angles with positive sign correspond to 6a*S*.

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