Structure Tables

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|  | **4060314-finalcif.cif** | **foobar.cif** | **ntd106c-P-1-final.cif** |
| Empirical formula | C40H36Au2Cl14F6NTl | C25H50Al1FGa1O5 | C18H19NO4 |
| Formula weight | 1739.30 | 172.81 | 313.34 |
| Temperature/K | 173(2) | 100(2) | 100(2) |
| Crystal system | ? | monoclinic | ? |
| Space group |  | *P*21*/c* (14) |  |
| *a*/Å | 12.0920(1) | 10.5086(3) | 7.9492(7) |
| *b*/Å | 28.5736(3) | 20.9035(5) | 8.9757(8) |
| *c*/Å | 15.4221(2) | 20.5072(5) | 11.3745(10) |
| α/° | 90.00 | 90 | 106.9740(10) |
| β/° | 107.365(1) | 94.1300(10) | 91.9630(10) |
| γ/° | 90.00 | 90 | 103.4560(10) |
| Volume/Å3 | 5085.66(9) | ? | 750.33(11) |
| *Z* | 4 | 4 | 2 |
| *ρ*calc g/cm3 | 2.272 | 0.255 | 1.387 |
| μ/mm-1 | ? | 0.914 | 0.098 |
| *F*(000) | ? | 319 | 332 |
| Crystal size/mm3 | ?×?×? | 0.4×0.3×0.21 | 0.18×0.15×0.15 |
| Crystal colour | ? | ? | colourless |
| Crystal shape | ? | ? | block |
| Radiation | ;  Mo *K\a  ;* (λ=?) | Mo*Kα* (λ=0.71073) | Mo*Kα* (λ=0.71073) |
| 2ϴ range/° | ? to ? | 3.89 to 56.24 | 3.76 to 53.46 |
| Index ranges | ≤ h ≤   ≤ k ≤   ≤ l ≤ | -13 ≤ h ≤ 8 -25 ≤ k ≤ 27 -27 ≤ l ≤ 26 | -10 ≤ h ≤ 10 -11 ≤ k ≤ 10 0 ≤ l ≤ 14 |
| Reflections collected | ? | 42245 | 15766 |
| Independent reflections | ? *R*int = ;  0.0376  ; *R*sigma = ? | 10786 *R*int = 0.0504 *R*sigma = 0.0585 | 3174 *R*int = 0.0327 *R*sigma = ? |
| Data / Restraints / Param. | ?/?/? | 10786/2419/933 | 3174/0/210 |
| Goodness-of-fit on *F*2 | ? | 0.999 | 1.036 |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = ? w*R*2 = ? | *R*1 = 0.0401 w*R*2 = 0.0862 | *R*1 = 0.0401 w*R*2 = 0.1072 |
| Final *R* indexes  [all data] | *R*1 = ? w*R*2 = | *R*1 = 0.0795 w*R*2 = 0.1014 | *R*1 = 0.0427 w*R*2 = 0.1096 |
| Largest peak/hole /eÅ3 | ?/? | 0.40/-0.69 | 0.32/-0.20 |
| Flack x parameter |  |  |  |

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|  | **p21c.cif** | **P21c-final.cif** | **p21c-finalcif.cif** |
| Empirical formula | C34H24AlF36GaO4 | C91H88O20 | C34H24AlF36GaO4 |
| Formula weight | 1277.23 | 1501.61 | 1277.23 |
| Temperature/K | 100(2) | 100(2) | 100(2) |
| Crystal system | monoclinic | ? | monoclinic |
| Space group | *P*21*/c* (14) |  | *P*21*/c* (14) |
| *a*/Å | 10.5086(3) | 16.6171(14) | 10.5086(3) |
| *b*/Å | 20.9035(5) | 16.4743(12) | 20.9035(5) |
| *c*/Å | 20.5072(5) | 28.964(3) | 20.5072(5) |
| α/° | 90 | 90.00 | 90 |
| β/° | 94.1300(10) | 103.218(4) | 94.1300(10) |
| γ/° | 90 | 90.00 | 90 |
| Volume/Å3 | 4493.0(2) | 7719.0(12) | 4493.0(2) |
| *Z* | 4 | 4 | 4 |
| *ρ*calc g/cm3 | 1.888 | 1.292 | 1.888 |
| μ/mm-1 | 0.821 | 0.091 | 0.821 |
| *F*(000) | 2512 | 3176 | 2512 |
| Crystal size/mm3 | ?×?×? | 0.22×0.13×0.07 | ?×?×? |
| Crystal colour | ? | colourless | ? |
| Crystal shape | ? | plate | ? |
| Radiation | Mo*Kα* (λ=0.71073) | Mo*Kα* (λ=0.71073) | Mo*Kα* (λ=0.71073) |
| 2ϴ range/° | 3.89 to 56.24 | 2.52 to 53.46 | 3.89 to 56.24 |
| Index ranges | -13 ≤ h ≤ 8 -25 ≤ k ≤ 27 -27 ≤ l ≤ 26 | -21 ≤ h ≤ 21 -20 ≤ k ≤ 20 -36 ≤ l ≤ 36 | -13 ≤ h ≤ 8 -25 ≤ k ≤ 27 -27 ≤ l ≤ 26 |
| Reflections collected | 42245 | 342741 | 42245 |
| Independent reflections | 10786 *R*int = 0.0504 *R*sigma = 0.0585 | 16388 *R*int = 0.0475 *R*sigma = ? | 10786 *R*int = 0.0504 *R*sigma = 0.0585 |
| Data / Restraints / Param. | 10786/1924/945 | 16388/291/1150 | 10786/1924/945 |
| Goodness-of-fit on *F*2 | 1.016 | 1.019 | 1.016 |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = 0.0400 w*R*2 = 0.0860 | *R*1 = 0.0420 w*R*2 = 0.1097 | *R*1 = 0.0400 w*R*2 = 0.0860 |
| Final *R* indexes  [all data] | *R*1 = 0.0795 w*R*2 = 0.1007 | *R*1 = 0.0576 w*R*2 = 0.1204 | *R*1 = 0.0795 w*R*2 = 0.1007 |
| Largest peak/hole /eÅ3 | 0.41/-0.69 | 0.31/-0.22 | 0.41/-0.69 |
| Flack x parameter |  |  |  |

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|  | **twin4.cif** |  |  |
| Empirical formula | C23H21NO |  |  |
| Formula weight | 327.41 |  |  |
| Temperature/K | ? |  |  |
| Crystal system | triclinic |  |  |
| Space group | *P-*1 (2) |  |  |
| *a*/Å | 8.1475(7) |  |  |
| *b*/Å | 9.4260(7) |  |  |
| *c*/Å | 11.6175(8) |  |  |
| α/° | 79.430(3) |  |  |
| β/° | 82.715(4) |  |  |
| γ/° | 79.618(3) |  |  |
| Volume/Å3 | 858.64(11) |  |  |
| *Z* | 2 |  |  |
| *ρ*calc g/cm3 | 1.266 |  |  |
| μ/mm-1 | 0.077 |  |  |
| *F*(000) | 348 |  |  |
| Crystal size/mm3 | 0.180×0.150×0.060 |  |  |
| Crystal colour | ? |  |  |
| Crystal shape | ? |  |  |
| Radiation | Mo*Kα* (λ=0.71073) |  |  |
| 2ϴ range/° | 3.58 to 55.02 |  |  |
| Index ranges | ? ≤ h ≤ ? ? ≤ k ≤ ? ? ≤ l ≤ ? |  |  |
| Reflections collected | 3952 |  |  |
| Independent reflections | 3952 *R*int = ? *R*sigma = 0.0162 |  |  |
| Data / Restraints / Param. | 3952/0/227 |  |  |
| Goodness-of-fit on *F*2 | 1.143 |  |  |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = 0.0540 w*R*2 = 0.1405 |  |  |
| Final *R* indexes  [all data] | *R*1 = 0.0594 w*R*2 = 0.1431 |  |  |
| Largest peak/hole /eÅ3 | 0.38/-0.27 |  |  |
| Flack x parameter |  |  |  |