Structure Tables

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| --- | --- | --- | --- |
|  | **4060308.cif** | **4060310.cif** | **4060314.cif** |
| Empirical formula | C13H20NO5PSi2W | C34H26Cl2N2O7PRe | C40H36Au2Cl14F6NTl |
| Formula weight | 541.30 | 862.64 | 1739.30 |
| Temperature/K | 133(2) | 299(2) | 173(2) |
| Crystal system | ? | ? | ? |
| Space group |  |  |  |
| *a*/Å | 6.9618(4) | 8.792(2) | 12.0920(1) |
| *b*/Å | 9.6073(8) | 11.201(3) | 28.5736(3) |
| *c*/Å | 16.1541(9) | 17.928(4) | 15.4221(2) |
| α/° | 73.219(3) | 91.530(3) | 90.00 |
| β/° | 89.975(3) | 98.082(3) | 107.365(1) |
| γ/° | 81.823(3) | 109.195(3) | 90.00 |
| Volume/Å3 | 1022.98(12) | 1645.8(6) | 5085.66(9) |
| *Z* | 2 | 2 | 4 |
| *ρ*calc g/cm3 | 1.757 | 1.741 | 2.272 |
| μ/mm-1 | 5.860 | ? | ? |
| *F*(000) | 524 | ? | ? |
| Crystal size/mm3 | 0.16×0.15×0.08 | ?×?×? | ?×?×? |
| Crystal colour | colourless | ? | ? |
| Crystal shape | prism | ? | ? |
| Radiation | Mo*Kα* (λ=0.71073) | (λ=?) | (λ=?) |
| 2ϴ range/° | 2.64 to 60.06 | ? to ? | ? to ? |
| Index ranges | -9 ≤ h ≤ 9 -13 ≤ k ≤ 13 -22 ≤ l ≤ 22 | ≤ h ≤   ≤ k ≤   ≤ l ≤ | ≤ h ≤   ≤ k ≤   ≤ l ≤ |
| Reflections collected | 19997 | ? | ? |
| Independent reflections | 5954 *R*int = 0.0234 *R*sigma = ? | ? *R*int = ? *R*sigma = ? | ? *R*int = ? *R*sigma = ? |
| Data / Restraints / Param. | 5954/21/218 | ?/?/? | ?/?/? |
| Goodness-of-fit on *F*2 | 0.998 | ? | ? |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = 0.0159 w*R*2 = 0.0341 | *R*1 = ? w*R*2 = ? | *R*1 = ? w*R*2 = ? |
| Final *R* indexes  [all data] | *R*1 = 0.0185 w*R*2 = 0.0346 | *R*1 = ? w*R*2 = | *R*1 = ? w*R*2 = |
| Largest peak/hole /eÅ3 | 0.95/-0.55 | ?/? | ?/? |
| Flack x parameter |  |  |  |