

Crystal Structure Report for IALVB88 (Complex 10)

A specimen of $\text{C}_{30}\text{H}_{19}\text{EuO}_8$, approximate dimensions 0.038 mm x 0.079 mm x 0.295 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a D8 Venture system equipped with a multilayer monochromator and a Mo microfocus ($\lambda = 0.71073 \text{ \AA}$).

The total exposure time was 1.65 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 6112 reflections to a maximum θ angle of 25.00° (0.84 \AA resolution), of which 6112 were independent (average redundancy 1.000, completeness = 80.0%, $R_{\text{int}} = 13.66\%$, $R_{\text{sig}} = 12.96\%$) and 3719 (60.85%) were greater than $2\sigma(F^2)$. The final cell constants of $a = 11.1009(6) \text{ \AA}$, $b = 21.8025(12) \text{ \AA}$, $c = 18.7796(11) \text{ \AA}$, $\beta = 106.930(3)^\circ$, volume = $4348.2(4) \text{ \AA}^3$, are based upon the refinement of the XYZ-centroids of 22 reflections above $20 \sigma(I)$ with $3.797^\circ < 2\theta < 22.90^\circ$. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.853. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.4731 and 0.7461.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P 1 2_1/n 1$, with $Z = 4$ for the formula unit, $\text{C}_{30}\text{H}_{19}\text{EuO}_8$. The final anisotropic full-matrix least-squares refinement on F^2 with 568 variables converged at $R1 = 3.24\%$, for the observed data and $wR2 = 5.05\%$ for all data. The goodness-of-fit was 0.832. The largest peak in the final difference electron density synthesis was $1.069 \text{ e}/\text{\AA}^3$ and the largest hole was $-0.807 \text{ e}/\text{\AA}^3$ with an RMS deviation of $0.084 \text{ e}/\text{\AA}^3$. On the basis of the final model, the calculated density was $1.669 \text{ g}/\text{cm}^3$ and $F(000)$, 2168 e^- .