Advanced options of CrysAlis Pro including NoSpher A2 refinement of [Rh2(COOCH3)4]·2NCC6H4N(CH3)2

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Refinement of the title compound was accomplished using CrysAlis Pro. During peak picking and indexing, measured mosaicity down three orthogonal angles showed higher than expected values resulting in some unindexed reflections. Advanced options in the CrysAlisPro software package allowed us to adjust the reflection mask sizes to account for higher mosacity which resulted in lower overall R1 values and better statistics than in previous refinement instances where the higher mosaicity was not considered. A second refinement of single crystal diffraction data was performed with HAR (S. Cappelli & D. Jayatilaka) in NoSpherA2 (Kleemiss, F., Dolomanov, O. V., Bodensteiner, M., Peyerimhoff, N., Midgley, L., Bourhis, L. J., Genoni, A., Malaspina, L. A., Jayailaka, D., Spencer, J. L., White, F., Grundkötter-Stock, B., Steinhauer, S., Lentz, D., Puschmann, H. & Grabowsky, S. (2021). Chem. Sci. 12, 1675-1692) where tailor-made atomic scattering factors are used instead of the usual spherical description to describe more features of the diffraction data, e.g. bonds, lone pairs and charge transfer.