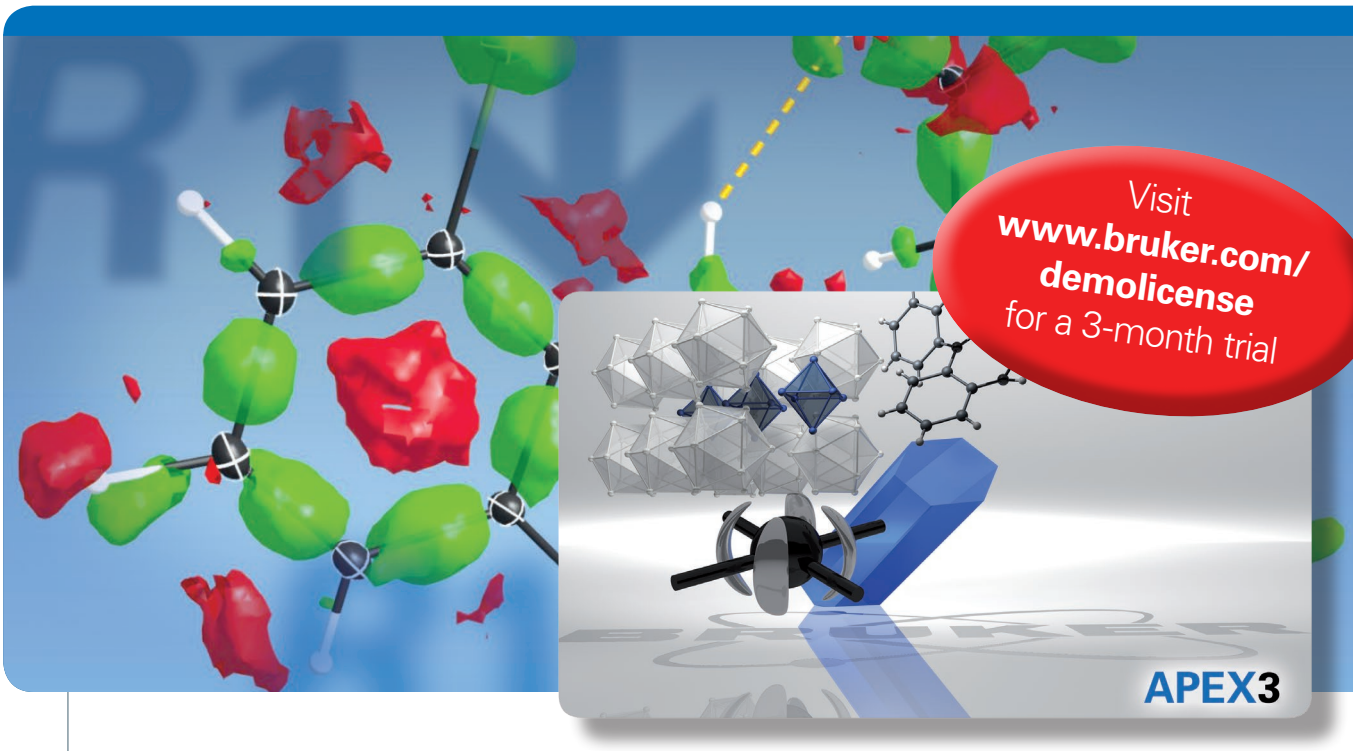


IDEAL – Invariom Derived Electron AnaLysis

Better Structures from Better Data

IDEAL, the new add-on to Bruker's APEX3 software for structure analysis, goes beyond the traditional Independent Atom Model (IAM) that has served crystallographers for more than 50 years. IDEAL uses IAM scattering factors, and in addition, models scattering contributions of bonds and lone pairs to improve structures.

Accurate, high-resolution data—readily available from Bruker's highly efficient instrumentation with large, sensitive detectors and high-intensity sources—benefits most from this method. IDEAL is easy-to-use within the APEX3 software suite and fully integrated into the IUCr's checkCIF routines. For the first time you do not have to choose to cut data to preserve a low structure reliability criteria *R*1, sacrificing additional information and overall structure quality.

IDEAL lets you have your cake and eat it too!

Better Data – Better Tools – Better Structures

The traditional Independent Atom Model (IAM) falls short in not describing electron density that Bruker's excellent data reveals. For the first time, IDEAL now provides an aspherical atom implementation with SHELXL, even for routine structural work.

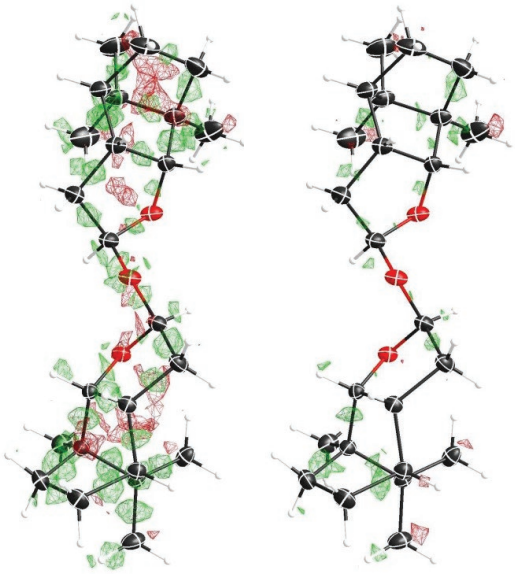
With IDEAL, it is finally possible to combine crystallographic and quantum chemical treatment of the organic solid state, for more precise and more accurate structures.

Information about the aspherical electron density has been derived from the Invariom Database, a collection of almost 3000 model compounds for which geometry and multipoles were determined computationally.

IDEAL uses pre-calculated fragment-based information applying fast fragment-matching algorithms to make computing most efficient.

IDEAL implements aspherical atom models using bond-oriented deformation density (BODD) and lone pair electron density (LONE).

- Extends the Independent Atom Model (IAM) for more accurate structures
- Fast – Relies on pre-computed database parameters, eliminating time-consuming quantum chemical computations
- For small-molecule and macromolecular diffraction data
- Intuitive and user-friendly implementation in APEX3
- Compatible with checkCIF



Methanobenzofuranyl-ether at 0.55Å. Left: IAM with *R*1= 2.68%. Right: IDEAL with improved difference density map and *R*1=2.29%.

	Formula	Radiation	Resolution	*R*1 IAM	*R*1 IDEAL
Sucrose	$C_{12}H_{22}O_{11}$	MoKα	0.4 A	1.84%	1.43%
Fluoro-Dioxololane	$C_{13}H_{21}FO_4$	CuKα	0.8 Å	2.95%	2.50%
Methylpiperazine	$C_5H_{12}N_2$	MoKα	0.5 Å	2.72%	2.35%
Ascorbic acid	$C_6H_8O_6$	MoKα	0.6 Å	3.00%	2.65%
Usnic acid	$C_{18}H_{16}O_7$	MoKα	0.55 Å	2.99%	2.51%
Usnic acid	$C_{18}H_{16}O_7$	CuKα	0.8 Å	2.68%	2.29%
Tartaric Acid	$C_4H_6O_6$	MoKα	0.4 Å	1.62%	1.41%
Alanine	$C_3H_7NO_2$	MoKα	0.37 A	2.09%	1.90%

Structure improvement for a variety of compounds with IDEAL refinement

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