Trustees' Report and Financial Statements

For year ending 31st December 2021

CCDC

advancing structural science

About this report

The Trustees present their annual report together with the audited financial statements of the group and the company for the year 1 January 2021 to 31 December 2021. The Annual Report serves the purpose of both a Trustees' report and a Directors' report under company law.

The Trustees confirm that the Annual Report and financial statements of the company comply with the current statutory requirements, the requirements of the company's governing document, and the provisions of the Statement of Recommended Practice (SORP) applicable to charities preparing their accounts in accordance with the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) (effective 1 January 2019).

Contents

About the CCDC and its purpose

We shape the future:

With scientific software and high-quality data services that accelerate the discovery and development of new medicines, chemical products, and advanced materials.

By promoting collaboration across academia and industry globally to generate new discoveries and methods in structural science.

By inspiring and training a new generation of structural chemists worldwide through outreach and education.

What we do

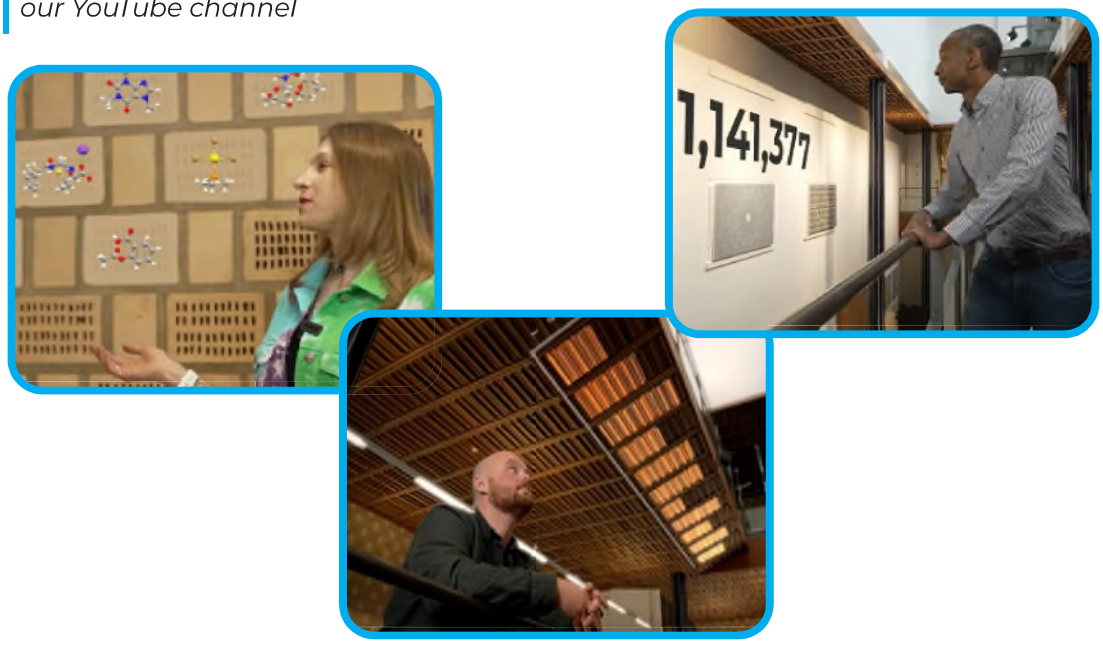
CCDC are world-leading experts in structural chemistry data, scientific software, and knowledge for materials and life science research and application.

We specialise in the collation, preservation, and application of scientific structural data for use in pharmaceutical discovery and manufacturing, materials development, and research and education.

We compile and distribute the Cambridge Structural Database (CSD), a certified trusted database of fully curated and enhanced organic and metal-organic high-quality structures, used by researchers across the globe.

Our cutting-edge scientific software empowers scientists and researchers to extract invaluable insights from the vast dataset, informing and accelerating their research and development.

Screenshots taken from our video "We are the CCDC" - available on our YouTube channel



What makes us different?

High-quality, trusted data

Each structure within the CSD undergoes extensive validation and cross-checking via automated workflows (utilising machine learning and semantic rules) and through manual curation by our expert chemists and crystallographers. This means you can trust that all the data within the CSD is accurate, consistent, and of highest quality.

Furthermore, we enrich all the data with bibliographic, chemical, and physical property information and a range of additional metadata. This adds further value to the original structural data and enables scientists (and machines) to interpret the structures in a chemically meaningful way.

Unique data

We enable researchers to publish data that otherwise would have remained unpublished, confidential, and unknown directly through the CSD. The CSD therefore contains data that isn't available anywhere else in the world.

Intelligent software and expertise

Our in-house software experts keep up to date with the latest developments in global data and software, applying their knowledge and expertise to develop robust systems that provide researchers with the tools to access, search, visualize, and meaningfully interpret the data within the CSD.

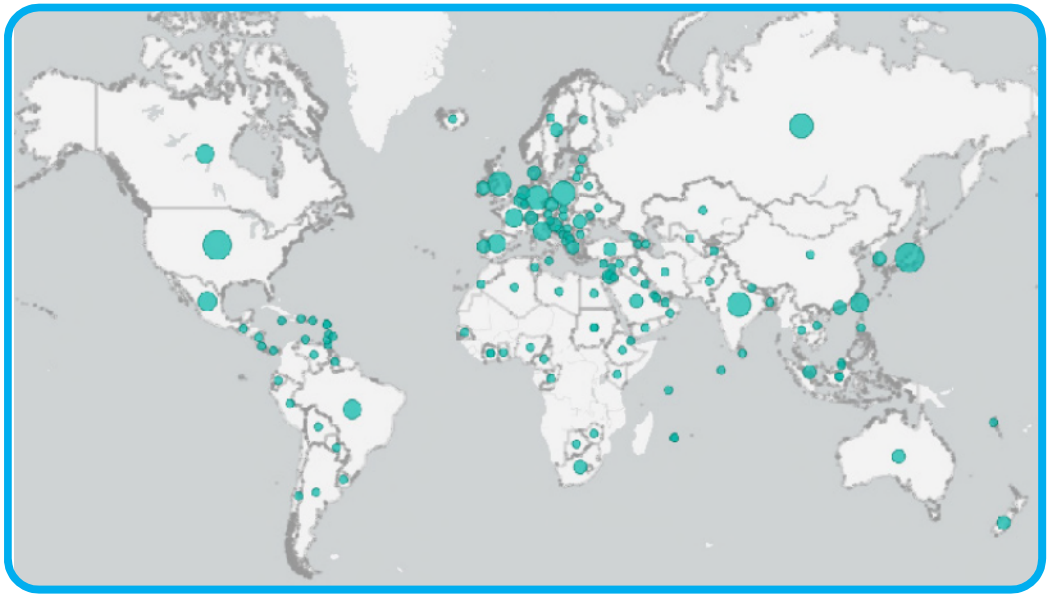
Knowledge

Using a novel application of existing and new algorithms and methods to explore the high-quality structural data and physicochemical properties within the CSD, we can extract scientific insights to advance structural science worldwide.

Supporting the community

We are committed to the advancement of chemistry for the public benefit, serving the global chemistry community by helping to address our customers' structural, physical, and chemical challenges through high-quality data, cutting-edge software, and specialist knowledge. We offer a selection of products and services free of charge for the benefit of the scientific community. Our services cover a wide range of crystallographic tools—from data collection, validation, and visualization to teaching, research, and analysis.

Representation of all application starts across our entire portfolio in 2021.
The larger dots indicate countries with a higher volume of application starts.



Our strategy: Advancing structural chemistry worldwide

The main objective of the not-for-profit charity is the general advancement and promotion of the science of chemistry and crystallography in all its branches for the public benefit.

The CCDC's strategy is to continue collecting, curating, making available, and learning from structural chemistry data on a deeper, faster, and more interlinked level, as well as gradually more in line with open and FAIR (Findable, Accessible, Interoperable, Reusable) requirements. We've set a goal to go from one million to over two million structures over the next five years. Both more complex molecules (for example, proteins, macromolecules, metal-organic frameworks, and polymers) and non-experimental data or theoretically calculated data (for example, crystal structure prediction landscapes and structures with density-functional theory with recalculated hydrogen positions) will be stored. This data growth, the inclusion of new types of structures, and the increased level of interlinking will be based on a new, presently evolving, foundational database architecture that is much more scalable and future-proof. Through updated editorial workflows and improved interactions with the wider scientific community and all depositors, we will capture and add more fields and metadata, as well as physicochemical data (such as melting points and solubility). We endeavour to lead structural scientific research by working with all our in-house scientists, our research partners, and our international academic network. By developing and supporting CCDC's industry-leading, scientific software suites and underlying high-quality and high-precision data, we will find new insights using novel techniques in machine learning and artificial intelligence. To this end, CCDC is constructing a distributed and heterogeneous, high-compute infrastructure using all our existing computational power. This system will use other cloud computing resources to expand elastically as needed for more scientific computations.

Furthermore, through our global education and outreach, we'll promote the power of structural science and train up the next generation of scientists and CCDC champions—ensuring better adoption of CCDC's software suites and data within both academia and industry.

Jürgen Harter, CEO of CCDC, showing the Olga Kennard Ewald Prize, awarded by the international Union of Crystallography IUCr in 2021

Our strategic aims, vision, and mission:

Collecting, curating, providing, and learning from structural chemistry data

Be the world's most comprehensive and trustworthy repository of structural chemistry knowledge for life and materials science research and application while establishing data trust through CCDC's adoption of the FAIR data principles and a philosophy of data openness.

Leading structural scientific research

Be recognised by industry as the "go-to" partner for structural science innovation (e.g., creation of digital drug design and manufacturing centres).

Enable world-class academic research that advances the application of structural knowledge via our growing global research network.

Creating new insights

Empower new scientific insights based on exploration of high-quality structural data.

Apply existing and new algorithms and methods—including artificial intelligence, machine learning, deep learning, statistics, and automation—in novel ways.

Creating and supporting industry leading software

Deliver a modern, cohesive, and reliable software ecosystem (cloud-based) that enables our users to gain new insights from structural data.

Enabling education and outreach

Be the world-leading provider of structural chemistry information for use in education to promote the power of structural science.

Supporting our people

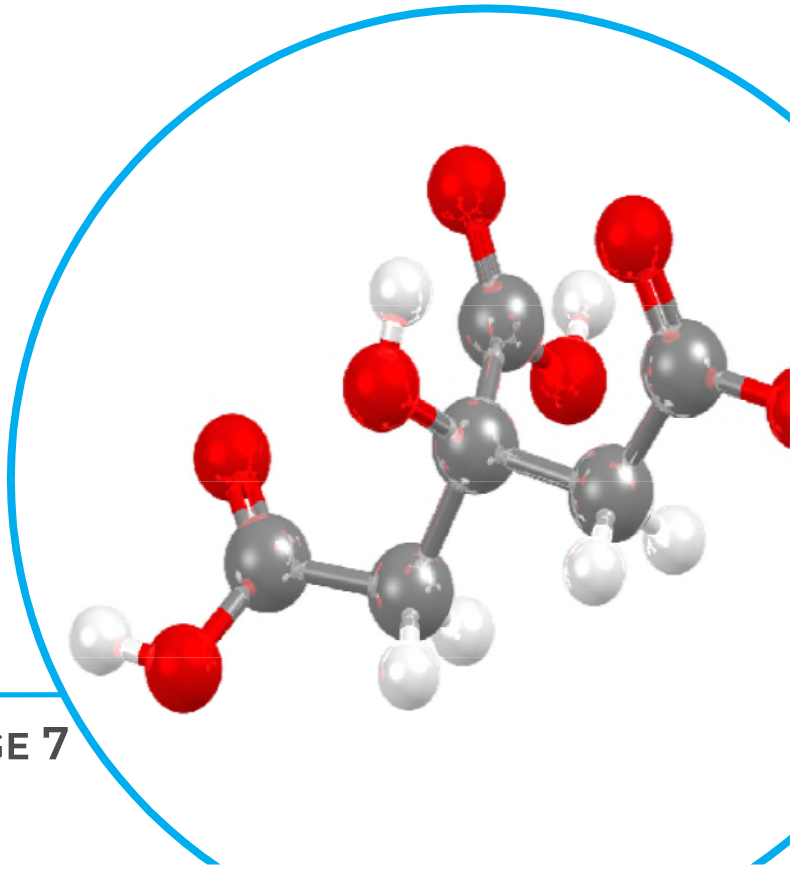
Live our values to be a healthy, happy, collaborative, productive, innovative, and fun place to work that values teamwork and delivers on goals with drive, urgency, energy, and pro-activity.

Customer centricity

Be customer-focused and deliver against requirements on time and on target.

Delivering sustainability

Generate sufficient funds to meet the needs of our industrial and academic customer bases.

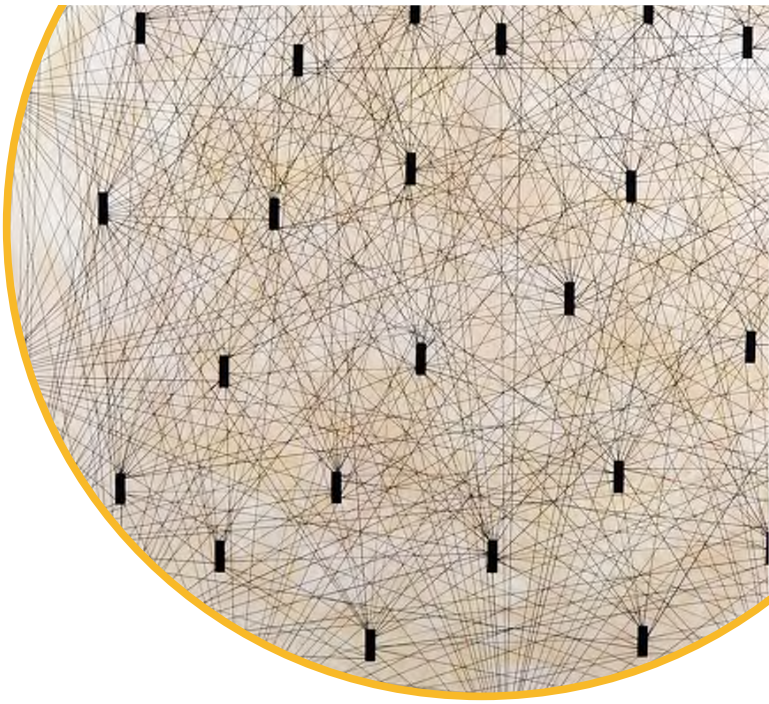


CSD STRUCTURE
Refcode: CITRAC

Our values

At the CCDC, our mission is to shape the future of structural science by accelerating the discovery and development of new medicines and chemical products by promoting collaboration across academia and industry and by inspiring a new generation of structural chemists globally through outreach and education.

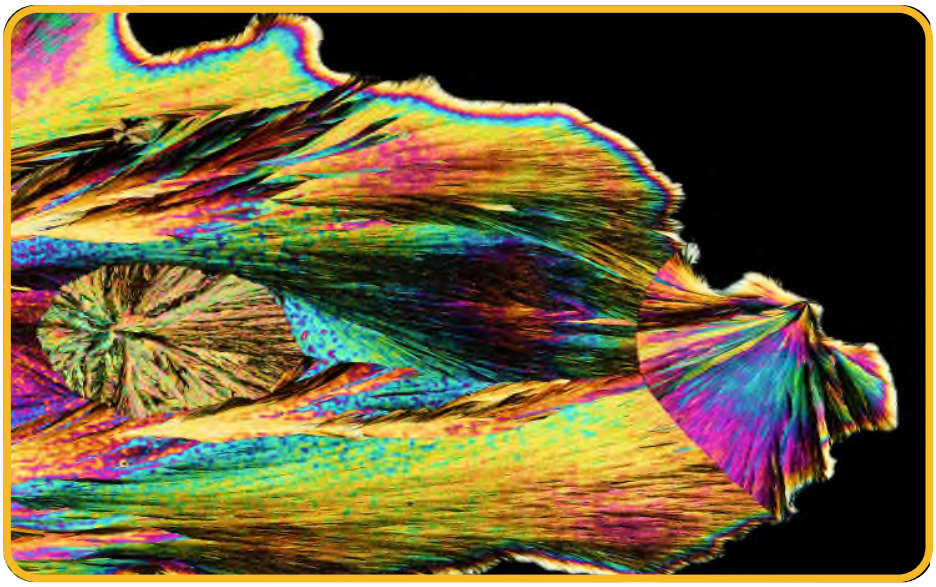
We have nine core values underpinning everything we do to ensure we achieve our mission. The CCDC and its staff live by the following nine principles and value statements, and over 2021 we have further embedded these values in the ways we work across all levels of the organisation.



Resonance by Clare Crouchman

Public Benefit

The CCDC Board of Trustees holds in high regard the principle of public benefIt and requires the CEO, wider senior leadership, and staff of the CCDC to pursue policies that demonstrate this. At its quarterly meetings, the Board of Trustees reviews ongoing charitable activities to ensure consistency with our charitable objects. The Board of Trustees is aware of the Charity Commission's guidance on public benefIt and has had regard to it in determining the Charity's aims and objectives and in the way it carries out its activities.



Crystal landscape by Alex Moldovan.

Community

We serve the global scientific community for the public benefit.

Collaboration

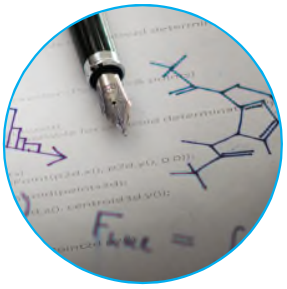
We work together and engage positively with others to achieve our goals.

Customer Centricity

We provide a quality product and service with an excellent customer experience.

Integrity

We act with integrity and communicate honestly and transparently.



Innovation

We push boundaries in all that we do and creatively advance understanding.

Passion

We are enthusiastic about the services we provide and committed to the people we help.

Quality

We are experts in our field, producing trusted resources for our community and customers.

Agility

We act in flexible and efficient ways, with a sense of urgency and turn around requests as fast as possible without compromise to quality.

Diversity

We believe in diversity and inclusion, and we work to create a culture of belonging, where everyone is welcome, valued and respected.

Delivering our vision

During 2021, the Cambridge Structural Database (CSD) grew to over 1.16 million entries and 1.13 million unique structures. This was an increase of over 63,000 entries in 2021 and an additional 25,000 existing entries were improved and enhanced through our annual CSD Improvements programme.

During the year, four data releases were delivered through our desktop software and users could access up to the minute data updates through our online services such as Access structures and WebCSD. The CSD continues to be a global community resource, and in 2021 alone deposited structures were determined by over 7,000 different crystallographers from over 80 different countries. The ability for researchers to publish directly through the CSD for free as CSD Communications helped support the amount of new crystal structures shared with the community. CSD Communications continued to be the number one way to share structural data with over 6,000 additional structures shared in this way during the year. The CCDC also supported researchers worldwide to help convert over 400 historical entries into the CSD from hardcopy, printed information.

With the continued growth of the database, the CCDC expanded our portfolio of targeted collections of data. 2021 saw the launch of four new collections, namely Electron Diffraction, Polymorphs, Hydrates, and High-Pressure subsets. These targeted datasets help provide easy access to highly relevant structures that can be hard to locate with simple searches and that are convenient starting points for further research and analysis. The subsets are often created with external collaborators who are experts in their fields. So, users benefit from both internal and external knowledge.

The value of one million plus crystal structures continued to be the subject of hundreds of articles worldwide, including 17 that were showcased through our Tools in Action series. In 2021, over 1,000 peer-reviewed articles by researchers in academia and industry cited the CSD reference paper highlighting the breadth of applications made possible with this data. Alongside its use in research, the value of using the CSD in education was highlighted by eight guest blogs in our CSD Educators series.

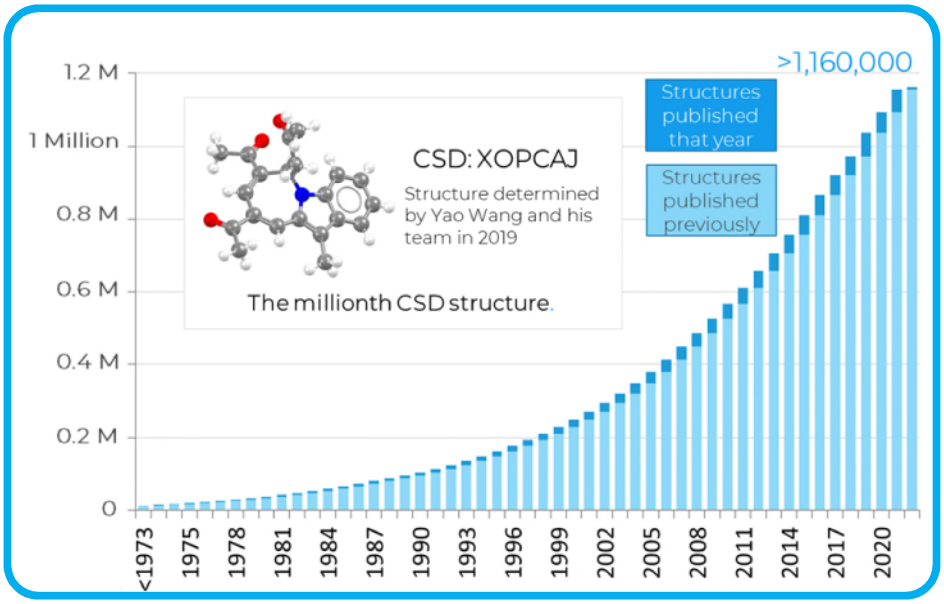
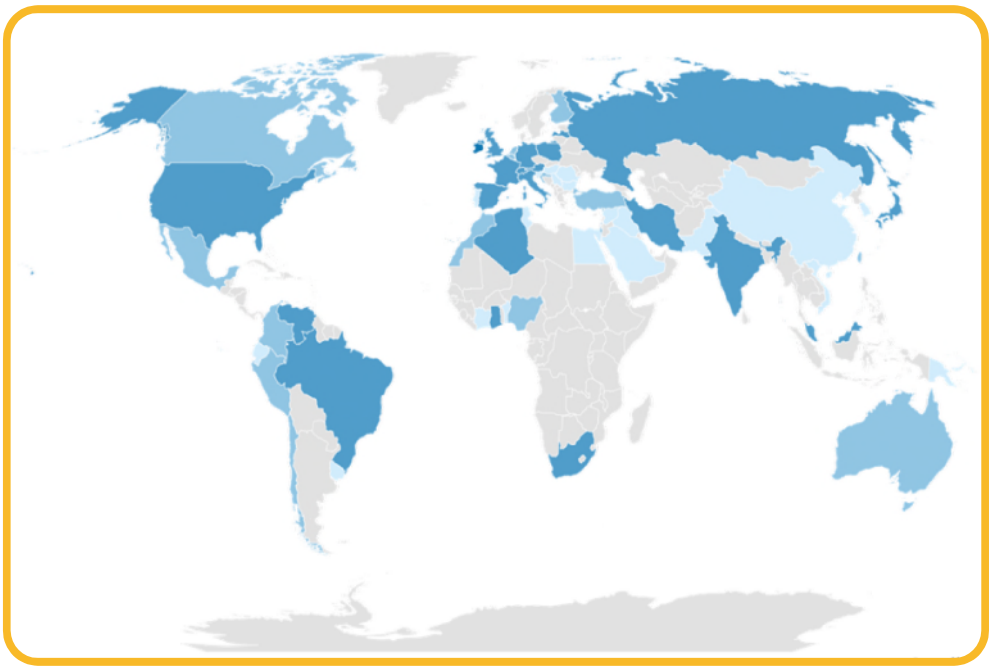


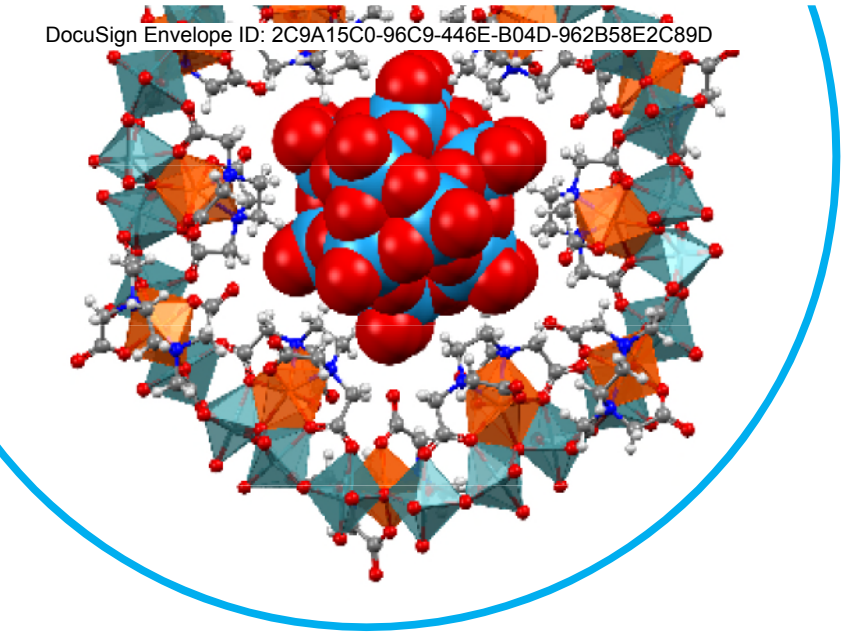
Chart showing the growth of the CSD.



Map showing attendees of the Virtual Workshops in 2021. The darker the blue more people attended, with light blue indicating at least one person joined from that country.

During the year, the CCDC continued to support our global scientific community virtually. We participated in many virtual international conferences, including the British Crystallographic Association (BCA) meeting, the American Crystallographic Association (ACA) meeting, the IUPAC World Congress, both the Spring and Fall American Chemical Society (ACS) meetings, the Italian Crystallographic Association meeting, the Brazilian Association of Crystallography meeting, the Research Data Alliance (RDA) Plenary meeting, and the Pan-African Conference on Crystallography. The CCDC also participated in the International Union of Crystallography (IUCr) Congress meeting, where the founder of the CSD, Dr Olga Kennard, was awarded the 12th Ewald Prize for her invaluable pioneering contribution to the development of crystallographic databases. Alongside participating in international conferences, the CCDC hosted several fully virtual User Group Meetings and a Science Day. These events were well attended with around 90 attendees and around 250 registrations on average each from users globally.

During 2021, the CCDC hosted nine free virtual workshops and delivered over 18 training sessions at international conferences and events, including many crystallography schools. The Virtual Workshops sessions were well attended from all over the world, with attendees from over 58 countries represented throughout the year. As well as supporting and hosting virtual global events, the CCDC established and enriched the educational resources we provide. These resources include guided step by step workshops, how to videos and social media software tips to help users explore the CSD and associated software. CSDU, a new collection of on-demand modules, with content comparable to that of live workshops and with a completion certificate to be earned at the end, was also launched in 2021. These on-demand courses go beyond our existing platform of self-guided workshops with focussed modules that include bite-sized videos, demonstrations, guided hands-on exercises and tests. They help to increase the accessibility of our training courses across different time-zones, competing schedules and different preferred learning styles of our user base. All the modules are free to access and are designed to help train the next generation of scientists in the value of structural data for research and education.



CSD STRUCTURE
Refcode: ASETEZ

We have also created new resources for chemistry and crystallography students and educators. These include two videos, covering challenging topics like chirality, symmetry operators and point groups, and an introductory short guide to the Crystallographic Information File (CIF), including CIF syntax. For younger aspiring scientists, we expanded the CCDC Home Learning collection with fun videos to introduce them to the wonders of crystals with simple experiments.

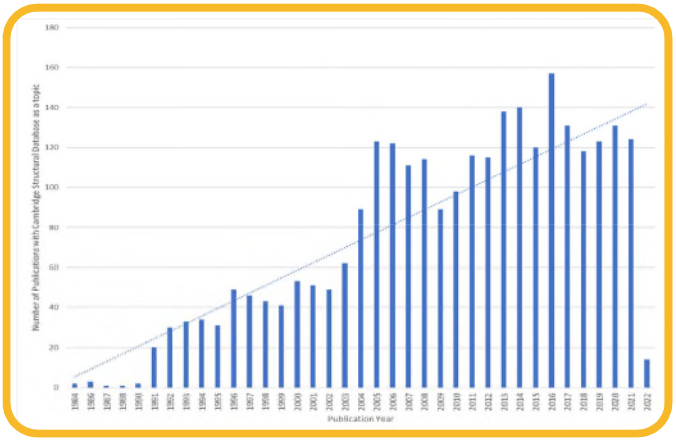
We continued to promote our Frank H. Allen International Research and Education (FAIRE) programme that provides free access to the CSD and associated software to scientists in eligible countries who may not otherwise have access. We have improved on facilitating the application process, for example by creating an online form. In 2021, four new institutions were awarded a campus-wide CSD license under the FAIRE programme. In the same year, over 50 peer-reviewed research articles were published because of our FAIRE programme - an outstanding result considering that the total number of publications up to 2020 was around 80.

The Russian invasion of Ukraine has forced the Centre to develop a response to this event through discussions between the ELT and the Board of Trustees. In this instance, the financial impact is small. The response has been to offer Ukraine the benefits of the FAIRE program due to the economic impact of the invasion. In the next Board meeting, the Trustees will develop a policy to offer guidance on how to respond when future geopolitical unrest occurs. In addition, the Risk Committee is adding the potential of global unrest to the risk register.

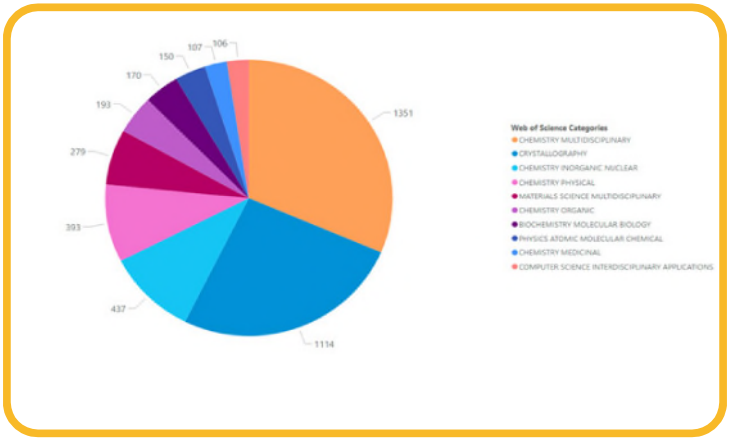
A previous CFC workshop.

Impact of the CCDC

Our data, software and services are used extensively both for industrial research and for academic endeavour. Users have published some 2,724 papers with a topic of “Cambridge Structural Database” since 1984, according to web of science. As can be seen from the histogram, the numbers of publications that cite the CSD as their topic of research have steadily increased since the year 2000.



Growth in publications with the CSD as their topic of research in Web of Science.



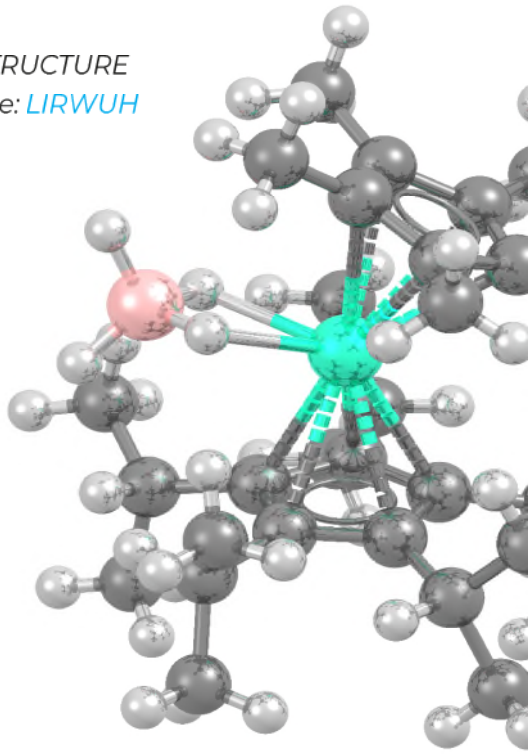
Pie Chart showing the common Web of Science categories.

Finally, the CSD has had a broad impact in 59 different topic areas. The topic areas that contain more than 100 papers are shown below. We note that while the high-ranking topics are dominated by chemistry and crystallography, the range of themes covered is far higher. For example, single papers have been published in areas such as toxicology or forensic analysis.

The impact of the CSD is truly global. Web of Science shows that publications with the CSD as a topic have emerged from 87 countries worldwide, shown in the map visualization below.

Map showing the countries that published papers based on the CSD.

CSD STRUCTURE
Refcode: LIRWUH



The Crystal Structure Prediction Blind Test

Visualization of the blind test.

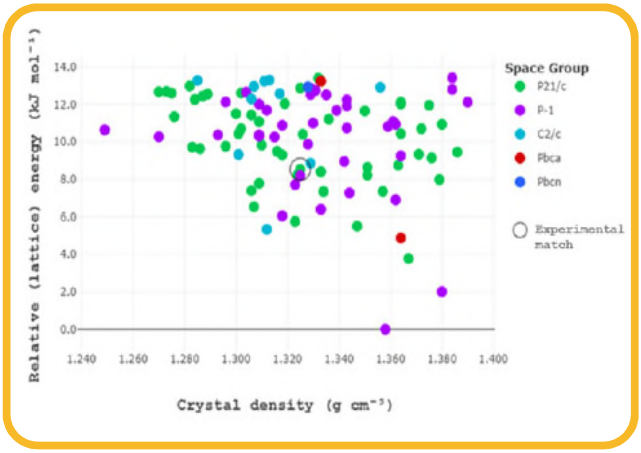
Crystal Structure Prediction (CSP) is a key scientific endeavour. The end goal of crystal structure prediction is to predict reliably all the crystalline forms that a compound can form starting from the 2D chemical diagram. CSP is of interest both academically, as an unsolved challenge, and industrially. Industry is interested in CSP for many reasons. In pharmaceutical development, understanding the polymorphic crystal landscape can help recognize the risks of moving forwards with a given form. In other scientific domains too, a CSP "landscape" (i.e., a prediction of all the structures that are energetically favourable) is potentially useful as it may suggest possible new forms that experimentalists can hunt for. Those new forms may have interesting new crystalline properties that consequently, could be new functional materials relevant to materials in optics, organic semiconducting, non-linear optics, gas separation, and more.

CCDC has run a series of high-profile benchmarks of CSP over the past 22 years. Rather like the Critical Assessment of Structure Prediction (CASP) protein folding tests, the CCDC CSP blind test challenges methods developers to predict unknown structures. Google DeepMind caused a stir at the last CASP test by achieving significant improvements to the results obtained due to methodological advances. We've seen more incremental improvements in CSP since 1999, with groups steadily achieving more success each time the test has been run.

In some ways, predicting a crystal structure of a small molecule is considerably harder than a test of protein folding because the required degree of accuracy is an order of magnitude higher for a prediction to be useful. In addition, the range of chemistries that need prediction for small molecules is far broader than the chemistry of polypeptides.

The process of the blind test is visualized above. Initially, CCDC sources a set of compounds with crystal structures. These structures are held back from deposition in the CSD and kept blind at CCDC. Participants are then set the challenge of predicting these structures. They submit their predictions to the team at CCDC who assess the results.
The CCDC team then presents findings back to the participants summarizing the overall achievements of the teams in a post-test meeting and paper.

We launched the latest test in October 2020 (7th blind test). The test has seven systems. Three are deemed methods development systems, whilst four are aimed specifically at the agrochemical and pharmaceutical industries. The test has progressed this year and the first phase closed. We have now launched the second phase of the test.



Energy-density visualisation of the solid form landscape of molecule XXIII from the 6th CSP Blind Test.

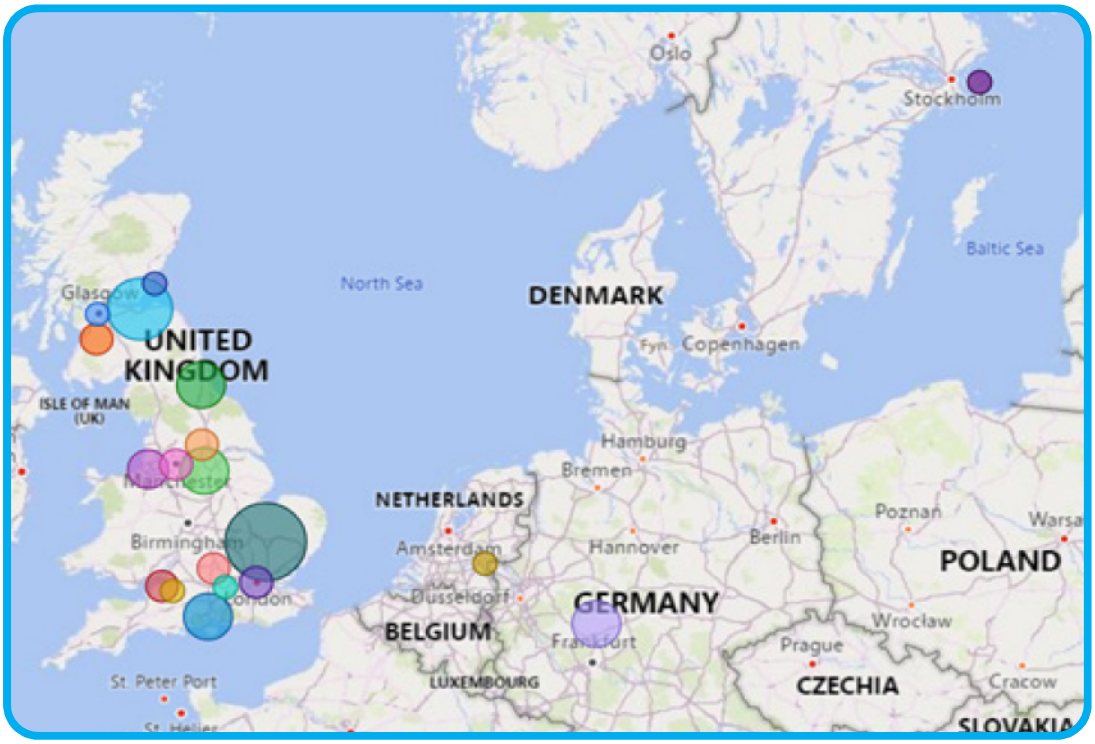
CCDC Studentship Program

The CCDC runs a vibrant and varied studentship programme. Typically, 9 to 12 students are in train at any one time. Currently we have 12 students active. We started 2 new PhDs in 2021 and provided additional sponsorship for a third student. CCDC typically acts as a co-sponsor of a student, contributing part of the fees and in-kind contribution via an industrial supervisor. The projects focus on areas of particular interest for CCDC. Two new students in 2022 will focus on database information content augmentation, for example. The historical network of European PhDs is shown below, colour coded by institution. The circle size indicates the degree of activity with the institute, vis-a-vis the number of students that have been hosted at the institute through time.

We have also had PhD students based in the USA historically. We are looking to expand our network in the coming years to include other countries. The PhD student projects cover a wide variety of topic areas. For example, this year we have had new projects starting in materials science, artificial intelligence for drug discovery, and in characterization of metal-organic frameworks.

2021 saw 2 new PhD student research projects starting.

Map showing the historical network of European PhDs. Colour coded by institution.



Key product releases

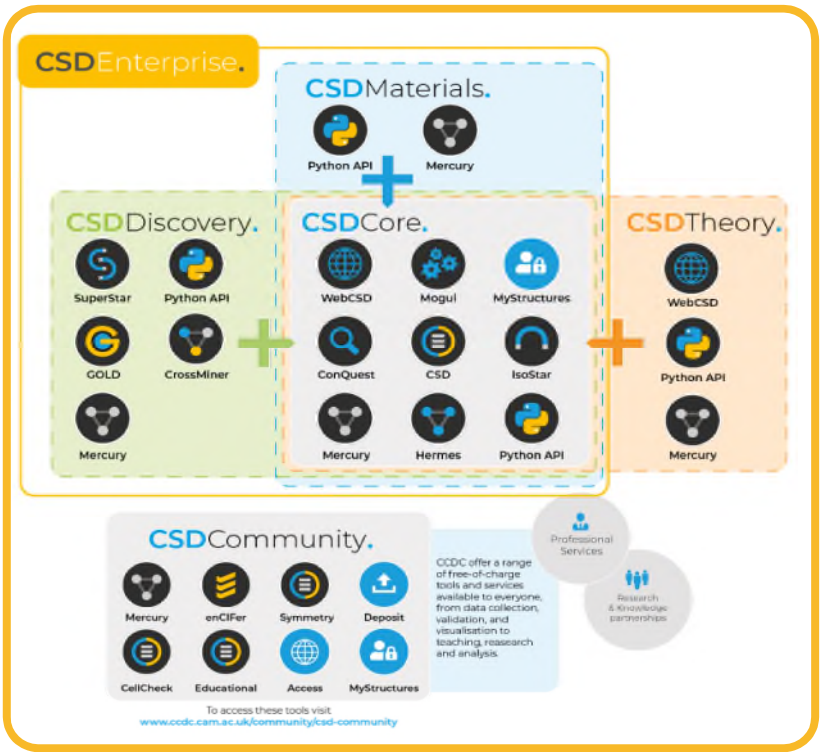
2021 saw six major releases across the desktop and web platforms, our first formal professional service launch, and seven further minor launches (including maintenance and data updates).

A key focus over 2021 was measuring the impact of each launch, plus the feedback from customers around our products, and using these data to optimize both what we're working on and how we communicate it to our user communities.

Ensuring CCDC data and tools are available to as wide a community as possible is a key driver for our developments. 2021 included significant database and architecture investment, as well as investment in the user experience (UX). The first iterations of these investments were delivered to customers via our Public WebCSD platform in May 2021 and the launch of a new product suite built entirely following our new UX approaches (CSD-Theory) happened in April 2021.

CSD-Community Updates

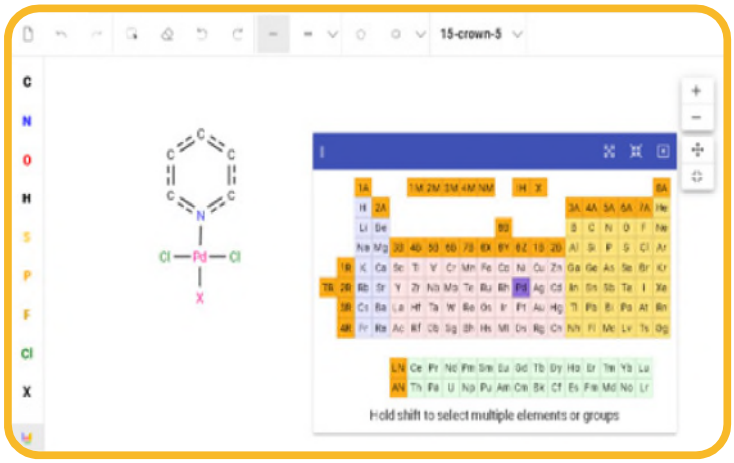
In 2021, we introduced some new capabilities for CSD-Community (i.e., free to access) users. In March 2021, we launched the CSD MOF Collection, which is freely available for non-commercial research, and helps support the use of CSD data in the fast-moving and impactful field of metal-organic framework research. MOF research continues in many directions, but these versatile materials are already in use in areas as diverse as gas storage, gas separation, energy storage, catalysis, batteries, semiconductors, and sensors. In December 2021, we also made some key structure editing capabilities within Mercury freely available, so CSD-Community users of Mercury can now edit structures manually or automatically to ensure they can achieve the best chemically meaningful analyses and visual representations of their structures.



Overview of the CCDC Product Portfolio, including the renamed CSD-Core suite at the heart.

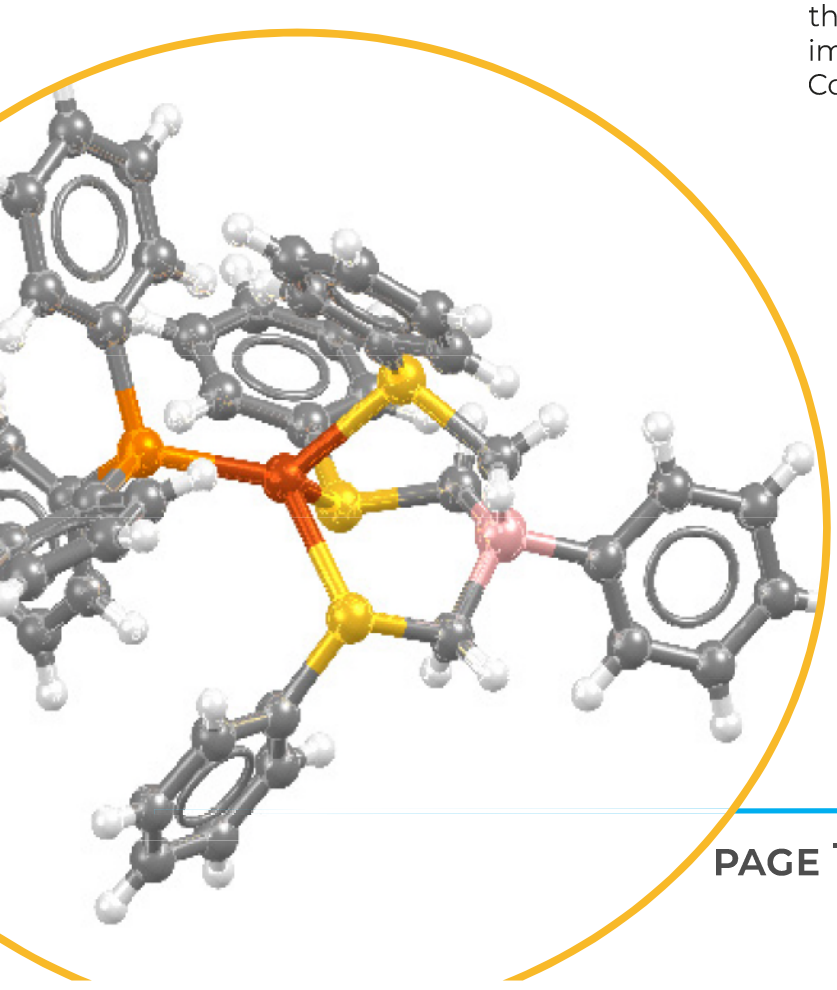
CSD-Core Updates

Within CSD-Core we had a strong focus in 2021 on building and launching key components that will form the basis of our new CSD Web Platform in the future. 2021 saw the full launch of our new CSD Sketcher in August 2021, which replaces the Elemental sketcher from Dotmatics in both our Public WebCSD platform and our On-Site WebCSD platform. (The sketcher was first released as an alpha version during 2020.) Developing our own CSD Sketcher has allowed the CCDC to much more effectively tailor sketching to 3D structural queries relevant to searching crystal structures, as well as handling simpler 2D chemical queries. In addiction to developing the user interface, the underlying database and architecture behind WebCSD are evolving. Through the Database Evolution project, we now have a faster, more maintainable, and more extensible system behind the WebCSD interface. We will continue to build on this platform in 2022, but we are already seeing some of the benefits of the database evolution within WebCSD. For example, we can now seamlessly improve and extend the platform behind the scenes with limited or no impact on the users.



CSD Sketcher: fully launched as version 1.0 in August 2021.

Alongside the focus on our developing web platform, we also introduced some impactful new capabilities within the rest of the CSD-Core suite. In December 2021, we extended the structure editing capabilities in Mercury to allow editing of covalent bond distances, giving users greater control over disordered structures and complex coordination chemistries. We also introduced four new CSD subsets (electron diffraction, polymorphs, hydrates, and high pressure) to help users filter the data that matters most to them, as well as improving the accessibility of subsets through ConQuest, Mercury, and the CSD Python API.



CSD STRUCTURE
Refcode: ACEKID

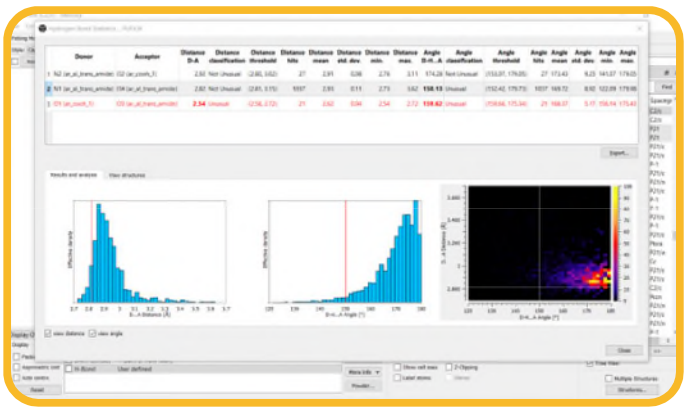
CSD-Discovery Updates

During July 2021, we delivered a range of impactful improvements in the Discovery area including a much more complete range of docking capabilities in the CSD Python API, a new method to generate 3D molecular structures from SMILES (Simplified Molecular-Input Line-Entry System) strings in the CSD Python API, and a new GOLD Cluster Computing package to support virtual screening on clusters. We continue to see a lot of interest from users in the application of GOLD on cluster and cloud platforms for docking on ultra-large scales.

In September 2021, we released significant changes to CSD-CrossMiner, our pharmacophore searching component that matches molecules to targets through intuitive, interactive data mining. These latest changes to CSD-CrossMiner included improvements to the user experience through optimizations in the user interface that were driven by direct customer feedback. We also increased the awareness and visibility around CSD-CrossMiner by integrating the program directly into the standard CCDC Portfolio installation and cross-linking with other parts of the portfolio. Finally, in December 2021, we introduced several changes to how we handle SMARTS and SMILES, making it easier than ever for cheminformatics teams to work with the CSD, Mercury, and the CSD Python API.

CSD-Materials Updates

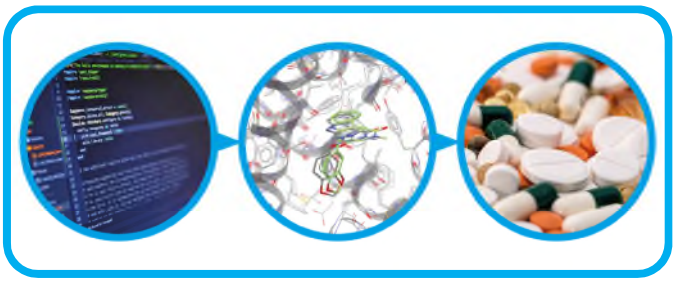
In September 2021, we launched a new Hydrogen Bond Statistics component in Mercury and the CSD Python API, delivering Mogul-like functionality for hydrogen bonds. This new CSD-Materials knowledge-driven component allows users to assess the stability of a given crystal structure by analysing the usual- or unusual-ness of the observed hydrogen bonds in the context of the over one million crystal structures in the CSD. In December 2021, we also completed the process of moving the program DASH, software focused on crystal structure solution from PXRD data, from a CSD-Materials component to become an open-source package. This change means the user community can freely use and extend the DASH software, while our team focuses on other developments within the CSD-Materials suite. This sharing of the DASH code with the community highlights the CCDC's support for community-driven approaches and open-source initiatives.



Hydrogen Bond Statistics: first launched in September 2021.

In September 2021, we also had the first formal launch of some of our professional services as a product: the Solid Form Snapshot and Solid Form Health Check. These allow organisations to better understand their solid forms, through applications of our expert solid form informatics approaches via reports and consultancy services. The Solid Form Snapshot provides a fast, standardised, data-driven report on a solid form to help assess risks and inform development. The Solid Form Health Check goes further to provide bespoke analysis of a solid form, including custom analyses, a more thorough report, and a tailored debrief meeting to present key findings and answer questions.

From data to drug.

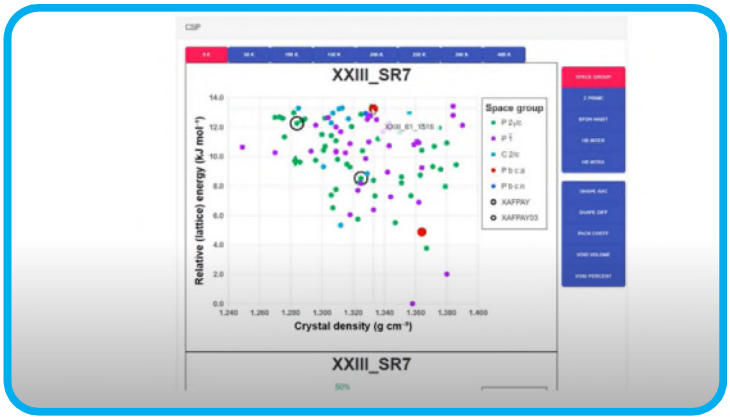


CSD-Theory Updates

2021 saw the first formal launch of CSD-Theory as a new product suite available to customers. This is the first new product suite launched by CCDC in a decade—the most recent new suite previously being CSD-Materials, which was first launched as the Materials Module of Mercury in 2007. CSD-Theory has been developed in close consultation with industrial customers. The product development was both funded and closely guided by the Crystal Structure Prediction Consortium (CSPC) Industry Partners made up of six global pharmaceutical organisations. At point of launch in April 2021, this innovative new platform provided the ability to capture proprietary CSP landscape data alongside experimental data within On-Site WebCSD. CSD-Theory sees the CCDC broadening its vision of making powerful use of collective data for science to incorporate not just experimental structures, but also predicted ones, further supporting the scientific community in generating insights.

The CSD-Theory Web system allows easy viewing and understanding of landscapes, analysis to discover new insights, and easy sharing within a team via a simple URL. The CSD-Theory API component also allows easy access to prediction data, including metadata alongside experimental data, via the CSD Python API.

In December 2021, we also introduced the new CSD Landscape Generator in Mercury as a further component within the CSD-Theory suite that allows customers to generate a solid form landscape of any single- or multi-component system—quickly, easily, and empirically.



CSD-Theory Web interface: first launched in April 2021.

Looking Forward

A lot of the work on both product prototyping and product development that we have been carrying out in 2021 will be realised and delivered during 2022. We expect to see in 2022 advances across all our suites delivered through at least three major desktop releases, three major web releases, three specific data updates, and several minor maintenance releases or component launches. 2022 will bring the launch of another new product suite to further extend the CCDC Product Portfolio into new application areas while maintaining the CCDC's fundamental focus on the collective use of data to drive discovery. We will also continue to advance our key effort in building our future CSD Web Platform, which we'll develop on our evolving database architecture and in accordance with UX best practices. The new platform will be able to support both an increase in scale of data, as well as new data types, including protein structures alongside small-molecule structures.

CCDC office photograph - 2021

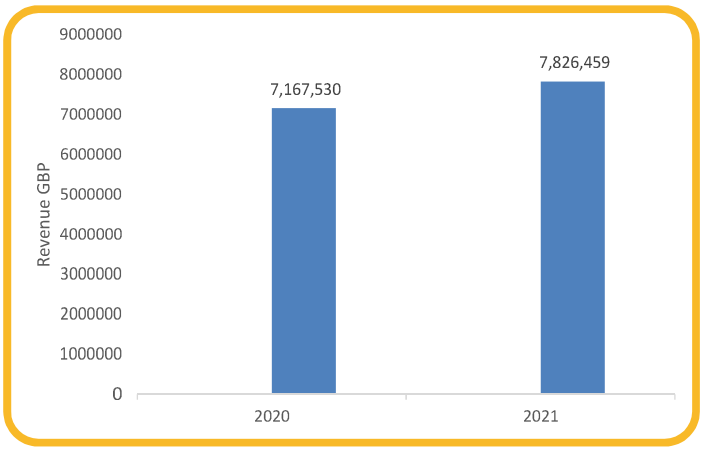
Financial review

A breakdown of the revenue.

Principal Funding

The CCDC's principal funds arise from the subscription fee to the CSD and its associated scientific software. Its subscribers are academic research institutions from around the globe and industrial companies, mainly within the biopharmaceutical and biotech sectors and growing into other sectors such as agrochemistry. The annual contributions requested from the worldwide academic community are significantly discounted as compared to the contributions requested from industrial customers, and special consideration is given to academic users with financial need in historically underrepresented nations. CCDC sets income from academic institutions at a level required to maintain the CSD data content. Income from non-academic users meets the costs of developing the database, enterprise architecture, and related software and enables the CCDC to invest in relevant scientific methods and applications' research and development. The CCDC received government grants for specific projects during 2021. It also received donations from its trading subsidiary, CCDC Services Ltd, under a Deed of Covenant. The CCDC holds an investment portfolio from which it receives dividends. The charity does not yet seek to raise funds from third parties by way of donations but has started to investigate this as an opportunity to underpin future growth plans.

Despite the pandemic, CCDC's performance continued to be strong. Driven by a strengthened Business Development team, we achieved a 9% growth compared to the prior year. The total revenue was £7,826,459 (2020: £7,167,530).



Graph showing the growth in revenue from 2020 to 2021.

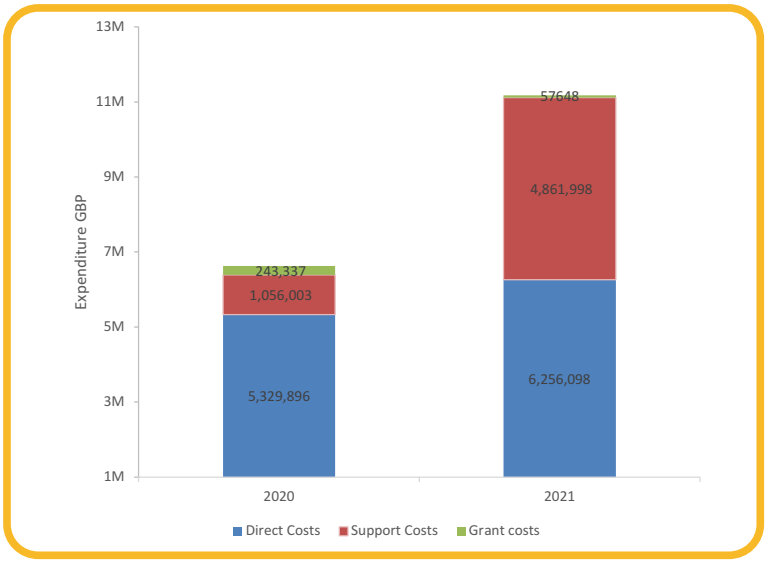
Expenditure

The activities undertaken in the year were carried out within the budget approved by the Trustees, and all the expenditures were spent for charitable purpose. The total expenditure in 2021 was £11,175,744, an increase of 69% on 2020 (£6,629,236).

The chart shows a signifIcant increase in support costs. This is due to a large increase in USS pension defIcit recovery cost based on the scheme's 2020 valuation.

Staff costs remain the largest expenditure for the CCDC. The total staff number increased from 79 to 97, between 1 January and 31 December 2021. Total staff costs in 2021 were £9,361,174 (2020: £5,118,289). This is an 79% increase from the previous year. The increase is not only due to increased number of employees, but also the USS pension debt recovery disclosure. USS is a multi-employer defIned benefIt scheme in which most of CCDC's staff participate. Given the mutual nature of the scheme, it is not possible to identify individual employer's share of assets and liabilities. The employers should account for the plan as if it were a defIned contribution plan. The 2020 valuation taken on 31 March 2020 shows a funding defIcit larger than the 2018 valuation. A funding plan has been agreed. Individual employers are required to recognize a liability for the contributions payable and the resulting expense in income statement. £3,270,557 were added to Staff Costs in the income statement.

The costs in maintaining IT systems, including software and hardware, increased to £351,317 (2020: £263,750). Cloud costs increased in 2021 to support several Microsoft Azure-based projects, including Licensing, Database Evolution, and GOLD Docking. Remote working and additional marketing efforts led to an increase in spending on communication, marketing, and collaborative working tools. We are confIdent that these investments will improve operational effIciency, meet the demand of our users by providing a flexible licensing system, and enable us to reach out to potential users more widely.



Total expenditure 2020 and 2021.

These investments follow our digital transformation theme and are made to enable future growth. Together with a network upgrade to 10Gb, we have enabled greater flexibility for remote/hybrid workers.

During 2021, the building was unoccupied for many months and staff worked remotely, successfully fulfIlling their roles. During Q4, we conducted a pilot study to assess staff appetite for returning to the building, for developing Covid-compliant protocols, and for preparing the building for full-occupancy at later date. The learnings from this pilot study will inform our hybrid working policy as we employ more people than the building can host.

Travel restrictions were still in place for the most part of the year. We continued running workshops, User Group Meetings, Consortium meetings, etc online. £64,790 were spent in 2021 on attending, sponsoring virtual events and other marketing activities, compared to £32,116 in 2020. This is at a lower level compared to pre-pandemic years.

The grants for hosting research students were £57,648 this year (2020: £243,337). We sponsored two new students during 2021, two less than anticipated.

One of the PhD project grant proposals, for which we were to provide top-up funds, did not end up getting funded. We also extended our support for the students whose studies were affected and prolonged by the pandemic. Currently, we are co-sponsoring 11 students from 8 UK universities.

Along with providing financial support through our FAIRE program, we also subsidised subscription fees for academic organisations worldwide. Including the financial aid provided through the FAIRE program, CCDC subsidized a total of £163,475 in 2021 (2020: £201,727).

The CCDC holds an investment portfolio that was affected by the performance of global market. It produced an unrealized gain of £945,035 (2020: loss £31,800). This brought the overall financial performance of the CCDC to a deficit of £2,404,250 in 2021 (2020: surplus £506,494).

Photograph of the top of CCDC building.

Investment policy

Since 1987, CCDC has looked to build up its reserves to provide financial stability and to enable it to fund its research and development activities. The primary objective of the investment policy is to preserve the capital and income in the investment portfolio from inflation.

In 2015, the Board of Trustees reviewed the investment policy. As a result, Newton Investment Management Ltd were appointed as our investment managers and the monies were moved from the incumbent Investment Manager and invested into Newton Growth and Income Fund for Charities.

The investment policy sets no specific ethical constraints on the investment portfolio. However, the portfolio should be invested in a socially responsible manner and the investment manager of the portfolio is expected to consider environmental, social, and governance (ESG) issues in their investment analysis and decision-making process, engaging with company management where appropriate.

It is the practice that the investment advisers attend regular meetings of the Board of Trustees and report on the progress of the fund, and of the CCDC's investment into it. Detailed written reports are produced on a quarterly basis that value the portfolio and record its respective performance statistics. An integral part of the regular meetings is a detailed discussion on the content of the report with particular reference to the performance aspect. The table below shows the fund's performance in the last five years.

Funds performance calendar years in %

Fund performance calendar years %					
	2021	**2020**	**2019**	**2018**	**2017**
Newton Growth and Income Fund for Charities - Net	18.54	1.55	18.34	-1.08	13.14
Newton Growth and Income Fund for Charities - Gross	19.24	2.16	19.05	-0.49	13.82
Performance Benchmark	13.34	1.06	16.72	-5.06	10.21

The Executive Team at the CCDC review monthly reports from the investment managers. The Trustees will review the performance of the investment portfolio on a half-yearly basis. A more formal independent review of the investment manager and investment policy will be carried out at least every five years or more frequently if the circumstances require. An independent review was carried out during 2020. The Board were satisfied with the performance of Newton Growth & Income Fund for Charities. It was decided to continue investing with Newton.

The global market recovered steadily during 2021, influenced by the roll-out of vaccines. The Fund produced a positive return and outperformed its performance benchmark. At the end of the year, the value of the portfolio was at £6,869,644, which represented an unrealised gain of £945,035. CCDC's investment strategy is investing for the long term. During the year, we received £139,470 investment income, which was not reinvested (2020: £116,960).

Reserves

CCDC's Reserves Policy is to maintain sufficient levels of reserves to enable normal operating activities to continue over a period of at least six months should a shortfall in income occur; the policy should take account of potential risks and contingencies that may arise from time to time. CCDC's reserves policy requires the retention of income sufficient to encompass:

- The balance on tangible and intangible fixed assets for use by the Charity to avoid having to liquidate functional assets to release cash less all loans associated directly with these assets.
- To cover 50% of the direct costs and support costs, agreed in the budget or at meetings of the Board of Trustees.
- Funds to enable designated expenses and provisions that are anticipated to be greater than £200,000 less any external funding of them.

The reserves policy is reviewed annually to take into consideration perceived risks and opportunities.

At the end of 2021, CCDC's free reserve was £1,824k (2020: £4,427k). This is equivalent to 2 months of operating costs, lower than 50% of 2022 budgeted costs.

Our present reserves and funds position.

	31 Dec 2021
Unrestricted Reserves	**£5,126k**
Designated Funds	
Fixed Asset Fund	£2,003k
Research and Development Fund	£173k
Sponsorship and Outreach Fund	£118k
Pension provision Fund	£908k
Sustainability Fund	£100k
Free Reserves	**£1,824k**

Structure, management, and governance

CCDC was incorporated as a Company Limited by Guarantee on 18 August 1987. It has no share capital and is a registered charity. The guarantee of each member is £1. The governing documents are the Articles of Association of the company (as amended May 2010).

In addition to CCDC, the charity operates the following subsidiaries:

CCDC Services Ltd (formerly CCDC Software Ltd.)

a wholly owned trading subsidiary of the CCDC. It was established in 1998 to deliver bespoke software development as necessary to meet the requirements of CCDC's charitable status. Since 2015, its trading activities have evolved towards professional services from software development. 2019 was the first year when all its revenues arose from professional services, which includes Digital Drug Design & Manufacturing Centres. The CCDC's Board of Trustees and the Director of CCDC Software Ltd approved of the name change to best reflect the trading activities of the company in May 2019. The name change was officially registered with Companies House on 28 July 2019. The company is located at the same address as CCDC. The Directors of CCDC Services Limited consist of two trustees of the CCDC, an external Non-Executive Director, and the Chief Executive Officer of the CCDC. The Directors meet at least once a year. The Directors of the CCDC Services Limited do not receive remuneration for their service. An executive summary report of the key activities and performance of the entity is provided into the main Board of Trustees' meeting.

CCDC Inc. – established 9 September 2013 as a New Jersey company.

CCDC Inc. is a standard US Corporation, wholly owned by the CCDC, whose directors include a Trustee of the CCDC who does not receive remuneration and two external Non-Executive Directors with an annual remuneration of $5,000. Day-to-day management has been delegated to the General Manager. CCDC Inc. was established to provide scientific technical services to the CCDC user communities across the Americas, which represents almost 40% of the worldwide total revenues. CCDC Inc.'s activities are guided by a service level agreement (SLA). All legal and other agreements with users remain with the CCDC and CCDC Services Limited. The Directors meet once a year, usually in April. An executive summary report of the key activities and performance of the entity is provided at the main Board of Trustees' meeting.

An office was originally established within University of Rutgers, at the Centre for Integrative Proteomics Research. As we continue to grow our US-user community, we believe the needs of our users can be better served by retaining a core sales and support team in a virtual office to provide the rapid response they demand. This would also allow flexibility to locate US staff closer to the user community. A virtual office was established in July 2018. CCDC Inc.'s staff are located across the US.

Starting from 1 January 2020, CCDC Inc. has a business office address at 1 International Place, Suite 1400, Boston, MA 02110, USA. It has since moved to 1 Boston Place, Suite 2600, Boston, MA 02108, USA. It provides conferencing facilities and other administrative services.

Governance

The Charity is governed by the Board of Trustees who delegate operational management to the Chief Executive Officer (CEO), supported by an Executive Leadership Team (ELT) covering all functions of the organisation, as well as a Wider Management Team (XMT), the Operational Management Team (OMT), Product Management Board (PMB), Technical Review Board (TRB), Data Review Board (DRB), Science Research Council (SRC), Knowledge Management Team (KMT), and the new Project Management Office (PMO). Other cross-functional teams or groups, such as the Wellbeing Committee and Culture Team, also exist. Following a review, improvements to the organisational structure of the Science and Operations functions of the CCDC has been undertaken.

In accordance with governing documents, potential Trustees are appointed by the Board based on recommendations by the Nominations Committee and on their specific skills, location, and diversity. Potential Trustees are sent an induction pack covering their obligations under Charity and Company Law, Articles of Association, Memorandum of Association and Codes of Practice, company policies, and a non-disclosure agreement. Potential Trustees are invited to attend Board meetings as observers. After that, the Board of Trustees and the individual consider their suitability to act as a Trustee ahead of their formal acceptance to the post at the Annual General Meeting (AGM). Upon acceptance and appointment, Trustees receive an induction to the business, which covers key aspects of the organisation, its operations, and salient Health and Safety information.

The Board of Trustees usually meets at the CCDC twice per annum in May and November, with two further virtual meetings in February and August. Due to the pandemic all Board meetings were held virtually during 2021. Working to a standing agenda, the meetings with the CEO and the ELT provide oversight on the performance and progress of the Charity in line with strategy. Progress reports from all functions are presented to the Board at these meetings. In addition, the Board also receives monthly management account reports, which include the investment performance and cash balances. The opportunity for all staff to interact with the Trustees is always encouraged and pre-COVID-19 was specifically addressed as part of the on-site meetings. As soon as the restrictions on travel are relaxed, anticipated to be May 2022, these interactions will resume. All staff members have the option to ask questions in quarterly Q&A sessions at All-Staff meetings, where some trustees are usually present as well.

In addition to the Board meetings, the Board members hold regular, quarterly, telephone update calls with the CEO to address any matters arising from the meetings in a timely manner, to address any issues that need action, or to discuss trends and any matters of interest to the advancement of the charity. In special cases, extra joint calls were convened as needed.

During 2021, meetings of the Board Committees, Nomination, Audit, Risk, and Remuneration were held in accordance with their terms of reference.

Nomination Committee

The purpose of the Nominations Committee is primarily to ensure that:

- The Board and its committees should have the appropriate balance of skills, experience, independence, and knowledge of CCDC to enable them to discharge their respective duties and responsibilities effectively.
- There should be a formal, rigorous, and transparent procedure for the appointment of new trustees to the Board of CCDC.
- There should be an efficient, fair, and thorough process on which the Nominations Committee leads for recommendations of appointments to the Board.

Audit Committee

The purpose of the Audit Committee is to ensure the Charity's annual accounts, budgets, forecasts, and plans are reflected accurately by management accounts and other financial reports presented to them by the finance team.

Remuneration Committee

The purpose of the Remuneration Committee is to provide assurance to the Board that the CCDC has an effective and competitive People and Pay Strategy in place that supports the delivery of the Strategy, promoting an effective, high-performing, and diverse workforce, and to oversee issues relating to the remuneration of staff, with specific responsibility for making recommendations to the Board regarding the Remuneration Policy and the Executive's remuneration.

Risk Committee

The purpose of the Risk Committee is primarily to ensure that:

- risks to the organisation (including its subsidiaries), assets, and reputation of CCDC are identified, assessed, and monitored;
- a risk management framework is created and implemented;
- a register of risks is maintained; and
- a disaster response strategy and business continuity plan is in place.

The CCDC also has two wholly owned subsidiaries, CCDC Inc. and CCDC Services Limited with each holding one Board meeting per year with their Directors in April and May, respectively.

Management and Staffing

The day-to-day management of the CCDC is delegated by the Board of Trustees to the CEO and operational management is supported by the ELT and other managers who, in 2021, were:

Dr Jürgen Harter
Chief Executive Officer

Miss Suzanna Ward
Head of Data and Community

Dr Susan Reutzel-Edens
Head of Science (joined 1 March 2021)

Dr Jonathan Betts
Head of Commercial

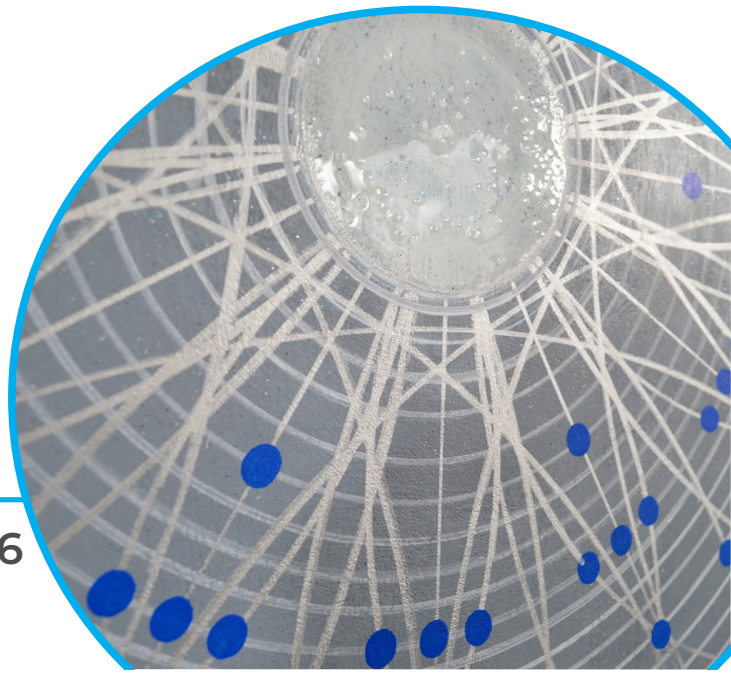
Dr James Ellis
Head of Operations (joined 1 September 2021)

Mrs Bing-Bing Waterman
Head of Finance

Ms Maggie Brown
Head of Human Resources and Organisational Design

Ms Carmen Nitsche
General Manager, CCDC Inc.

These individuals are the key management personnel. They provide reports for the Board of Trustees in support of governance of the Charity and attend Board of Trustees meetings to present operational reports, to position papers on topics of interest, and to regularly cover the centre's strategy.



Diffraction detail by Clare Crouchman.

Remuneration Policy

The Board of Trustees give their time freely and no trustee received remuneration in the year. Details of Trustees' expenses are disclosed in Note 8 to the accounts. The Board of Trustees entrust the directing, controlling, running, and operation of the Charity to the Chief Executive Officer who is supported by key management personnel. The pay of the senior staff is reviewed annually and increased in accordance with the company pay policy, which is applicable to all CCDC staff and approved by the Board of Trustees as part of the Budget approval process. Furthermore, the Remuneration Committee oversees any of the recommended salary changes, or any other changes to the organisations pay policy and discusses trends in line with up-to-date benchmarking data provided by HR.

Risk Management

The CCDC maintains a register of key risks to the organisation, which covers the following areas:

- Business: Staffing, External Dependencies, External Threats, Reputation
- Finance: Revenue, Expenditure, Financial Fraud
- Compliance: Health and Safety, Governance, GDPR
- Data and IT: Scientific Fraud, Protection of Data Assets, IT Infrastructure
- Building: Infrastructure, Fire, Lease

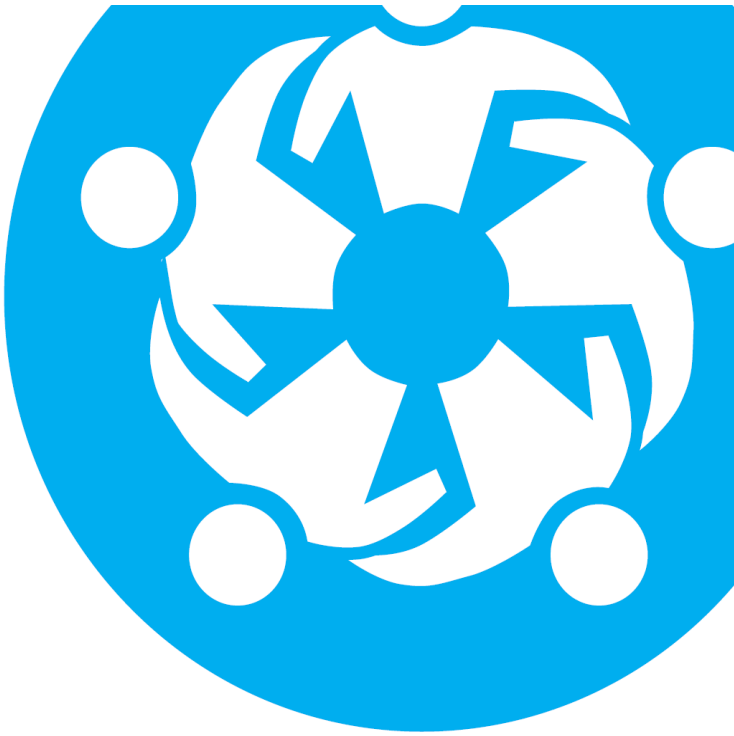
The Risk register entries detail the likelihood and impact of risks occurring, the steps the organisation takes to mitigate these and areas where further action is required.

The Trustees have oversight of risks facing the organisation through the Board Risk Committee, which reviews the Risk Register at least once a year. The Senior Leadership and Management Team at the CCDC undertook a comprehensive review of the organisation's risks towards the end of 2020—with further reviews of risks taking place over 2021. As a result of this review process, we identified additional risks relating to continuity. These are now managed at the Functional level, reported at XMT and form part of individuals objectives where appropriate.
Key risks and mitigation measures are summarised in the table below:

Table: key risks and mitigation measures.

Threat Type	Measures In Place
Inadequate staffing	Succession planning; salaries are reviewed and benchmarked annually; overall attractive benefit package; staff development opportunities
Reputational damage	Our good standing within the crystallography community rests on the quality of our data, its accessibility and our outreach activities. We continue to invest in the scale and quality of our scientific data and services.
University of Cambridge relationship	We have a formal relationship with the University and are known as a University Partner Institute; this agreement was renewed for 5 years in 2021.
Artificial Intelligence (AI) as competitive threat	We monitor machine access to our data and work with customers to ensure appropriate licences are in place for any party wishing to use AI/Machine Learning on the CSD.

Revenue below budget	Revenues are reviewed monthly along with the sales pipeline and historical data to give a clear and early insight into financial performance.
Financial fraud	Internal and external fraud risks are countered by defined processes requiring dual authorisation (e.g. payments) and ongoing training (e.g. phishing message awareness) and insurance policies.
Changes in Foreign Exchange Rates	We operate foreign currency bank accounts and forward contracts to avoid using spot-rate currency conversions into pounds sterling. We also operate a US subsidiary that enables some US dollar costs to be managed alongside revenue in US dollars.
Increasing pension costs	Employee and employer contributions have increased in recent years to address deficits in valuations.
Insufficient funds from investment	Our income and expenditure are well matched. Further, our professional investment provider is reviewed every 5 years, with monthly reports on performance. The fund is designated in the same currency as the majority of our costs, with US$ holdings at a similar level to our US$ costs.
Inability to generate revenue from Intellectual Property	We aim to ensure that our data services offer unique value and comply with community expectations regarding data stewardship. We use licensing authentication software to reduce the impact of pirated software.
Governance and compliance	Trustee board meetings are quarterly, with sub-groups as required to focus on particular topics, plus a Scientific Advisory Board (SAB). We maintain appropriate knowledge and skills to ensure compliance with our obligations e.g. Charity Commission requirements, GDPR, health and safety etc.
Information technology	Continuous availability of IT systems is critical to our organisation. We have dedicated facilities for our servers, monitor access to our services and have implemented cyber security training and systems. We also use 3rd parties to assess our systems and identify improvements. We have increased our use of Cloud-based systems to avoid being solely dependent on our own facilities, and ensure that critical assets are appropriately backed up.
Buildings and core infrastructure	We have an active programme of building maintenance to ensure our facilities remain fit for purpose, with service contracts and out of hours monitoring.



Ongoing Impact of COVID-19

The ongoing nature of the COVID-19 world pandemic has had a profound impact on the global economy. All businesses have been affected in one way or another, whether directly or indirectly. CCDC is no exception to this. The CCDC's Board of Trustees and management team have been closely monitoring the situation since the beginning of the outbreak and have put numerous health and safety measures in place. CCDC's business model is diverse. Our users are spread across academic research institutions and large pharmaceutical companies. The database and its associated products are distributed globally, to over 80 countries worldwide.

We rely primarily on renewal income (approximately 90%) from a core of subscribers who have continued to access the database over the long term (for decades). As this is needed for their research, they are likely to continue to renew year-over-year. The database has become an integral part of research and business operations for such users, and, as it is digital, it can be remotely operated on and used. Because of this, its continued use is not necessarily dependent on people getting into their labs or research institutions.

In the last couple of years, we have invested heavily into more digital transformation and IT infrastructure that have enabled working remotely to become as efficient as working from the office. Additionally, the products and services we provide can be delivered electronically. Consequently, the nationwide lockdowns have had relatively little impact on our productivity and how we deliver our digital products and services.

Over 2021, CCDC staff grew accustomed to working from home. The centre has supported this transition through cooperation platforms, such as MSTeams, and Miro (for whiteboarding and other ideation). Plus, we are operating Slack for instant messaging to enable swift communications across teams, functions, geographies, and time zones.

We are committed to do all we can to support our staff. We provided necessary equipment for the further optimization of home working, allowing reduced and flexible working hours to support staff with personal commitments. Managers frequently checked in with staff for their wellbeing and mental health. The CCDC has not furloughed any staff, nor taken advantage of any of the government support schemes.

At the date of writing, we have visibility of almost 90% of the budget target in revenue. This is a fortunate position to be in at this point in the year. Most of the licensees have already renewed their licences for this calendar year. Moreover, ongoing multi-year agreements with large industrial partners will further contribute to achieving the revenue target for the year. Academic institutions account for about 25% of CCDC's revenue. It remains to be seen what impact COVID-19 will have on universities worldwide and their budgets; however, a negative impact on the academic community may result in pressures on CCDC's revenue from that segment. So far, this has not occurred.

We have budgeted to expand the workforce and further advance our charitable goals. However, these costs are not committed and can be scaled back if necessary. We are closely monitoring our financial position by continuous review and timely reforecasting.

The CCDC has a healthy cash balance in the bank, which is easily accessible. We do not anticipate needing to withdraw from the investment fund this year.

We maintain confidence in the sustainability of the CCDC's business operations for the long term. Given the nature of CCDC's business model, revenues for the year appear to remain robust. Continued productivity driven by improved operational efficiencies and CCDC's secure liquid asset holdings makes us confident that CCDC will overcome the hardships brought on by challenges like rising inflation, the cost-of-living crisis, and new geopolitical tensions.

Heightened pressure to find novel therapeutics faster than ever in fields like in silico drug design, pharmaceutical manufacturing, and data-based structural research may lead to increase demand for CCDC's products. This is especially true for the field of artificial intelligence, where new advances mean companies are eager to leverage high-quality data—like the CSD—in their algorithms and models.

Similarly, students and teachers of structural chemistry seeking at-home, online education solutions present new opportunities for CCDC's education and outreach efforts. Even as research professors return to their labs, it is likely they'll continue to appreciate flexible educational materials. Between our online educational resources and digital-first software offerings, we're ready to meet the evolving needs of the academic community.

Looking into the future

Looking into the mid-term future (two to three years), the CCDC will endeavour to launch a modern, more user-friendly, and adaptive website (including an eCommerce platform and revamped knowledge portal). This new website will underpin all the interactions with the end users and community, along with appropriate calls to action. This effort will help deliver and categorize any of the information and materials created from the last decades, plus host the new information in an organized, easily navigable, and searchable way for the next 10 years. This is important for future-proofing CCDC's online experience and to meet CCDC's goals around automation and optimization. Over 2021, we have already achieved the discovery phase for this new website. Expert project management from our new Project Management Office (PMO) has given us the project discipline to deliver effectively. As we work on other large projects (e.g., CRM changes) we will seek to expand the PMO with more staff.

The CCDC is fortunate to have an excellent scientific advisory board (SAB). The constituency of the SAB was drawn from our existing user base with scientists who have demonstrated track records in their respective fields along with an interest in applying crystallographic knowledge. Over 2022, our internal scientists and new Head of Science will continue to work with and further optimize the membership and operational running of the SAB. The SAB members are tasked with recommending, evaluating, and reviewing scientific choices and proposals as to areas to target for future development at CCDC—thereby influencing and driving our scientific strategy.

Photograph of the CCDC building entrance.

CCDC value poster - Agility

The addition of an Operations function has enabled us to define and start delivering against objectives that will improve the effectiveness of our systems/processes for staff and end-users. Initially, we are working on three business transformation programmes: HR Business Processes, CRM, and website. These programmes are defining the status quo, implementing immediate changes to add value in the short term, and helping to define longer-term programmes of work that will support the efficient scaling of our organisation in a way that maximises value to customers. A key theme to support our processes will be Quality. As we expand our organisation, we need a Quality Management System (QMS) that will help us define what we do and how we do it, to support training and value delivery to customers. Process definition within a QMS context will help us identify the most appropriate software solutions to facilitate the scale of our business (e.g., CRM ERP, e-commerce). As these initiatives require dedicated project management, we have started to build a Project Management Office to define and demonstrate best practices, and to ultimately deliver the required results to time, cost, and quality.

We will continue to run the CCDC in growth mode in order to achieve more of our charitable aims faster, turning the CCDC into a more agile organization with improved branding and raising awareness of our unique selling points and value proposition: a winning combination of high-quality data, excellent science, cutting-edge software, and vast expertise. We will go from £7.8m top-line revenue and 97 employees in 2021 to £8.5m revenue and 100 employees in 2022 and on to ~£10m revenue and 120+ employees by the end of 2023, if not sooner. We will focus on delivering excellent value with a sense of urgency to a growing set of existing and new customers in the biopharmaceutical, chemistry, and biotech sectors, as well as other industries such as agrochemical, petrochemical, and advanced materials. We will have a new drive to get into functional and advanced materials, which have good potential to open new markets for the CCDC.

We will widen our reach, increase customer engagement and centricity, and enable this growth by further growing the commercial function, including marketing, product management, channel management, partnerships and alliances, and service delivery.

Any generated surplus from the resulting growth will be reinvested in advancing science, data accessibility, and utility; improving our products and services experiences (UX/UI); growing education and outreach efforts; and optimizing and scaling up through our skilled people, systems, and processes. This is done with the goal of serving our end users and the wider international scientific community in the best and most sustainable way over the coming years.

It remains clear from recent world events (including the COVID-19 pandemic and growing focus on health research), that structural chemistry has a crucial role to play in battling diseases. As a community, we need to be versatile in our approaches to ensure rapid response. In silico drug design and manufacturing methods as well as digitally advanced materials design will have an important role to play. We believe a digital-first approach that saves time and resources on the experimental phase will become increasingly important in the coming years.

This will drive a need for intuitive and user-friendly solutions that use trusted data and methods to provide quick and accurate results. CCDC is the "go-to" partner for structural science innovation, and we look forward to providing those solutions to identify and mitigate risks—from early-phase drug discovery through manufacturing.

We continue to expect that the world will evolve towards more remote working or a mixed model, with regular hybrid ways of working. This is a great opportunity for the CCDC to push more digital ways of working since our teams have already adapted to the model. We intend to further pioneer a digital experience by leading the way with data and software that is accessible from anywhere in the world via the cloud. These new practices and methods will underpin future ways of working for the research community, academia (e.g., remote teaching and virtual education at scale), the biopharmaceutical industry, and other domains that have a clear and ongoing need for structural chemistry. CCDC will help to shape this future while staying true to our vision and mission to globally advance structural science based on high-quality, trusted big data and software—reaching an ever-growing end-user community.

The investment made throughout 2021 and into 2022 has been necessary to address years of under-investment. With these improvements to the building and the hybrid ways of working developed during the pandemic, we have a unique opportunity to leverage our building, location, and expertise.

Historically the building has hosted various scientifl c events, but we also have interests in associated disciplines, such as cyber security for large datasets. We will seek to develop events at CCDC that improve our network and access to ideas beyond science.

Reference and administration details of the charity, its trustees and advisers

Trustees

Dr David Martinsen, Chair
Professor Alessia Bacchi, Vice Chair
Ms Judith N Currano
Professor Jonathan M Goodman
Dr John Overington
Dr Nigel Pitchford
Professor Susan Bourne
Dr Ola Engkvist (Appointed 13 May 2021)

Company registered number 02155347

Charity registered number 800579

Registered office

12 Union Road
Cambridge
CB2 1EZ

Chief Executive Officer

Dr J Harter

Independent auditors

Peters Elworthy & Moore
Chartered Accountants
Salisbury House
Station Road
Cambridge
CB1 2LA

Bankers

Barclays Bank Plc
Cambridge
CB2 3AA

Solicitors

HCR Hewitsons
50-60 Station RoadCambridge
CB1 2JH5

Investment Advisers

Newton Investment Management Limited
160 Queen Victoria Street
London
EC4V 4LA

STATEMENT OF TRUSTEES' RESPONSIBILITIES FOR THE YEAR ENDED 31 DECEMBER 2021

The Trustees (who are also the directors of the Charity for the purposes of company law) are responsible for preparing the Trustees' Report including the Strategic Report and the financial statements in accordance with applicable law and United Kingdom Accounting Standards (United Kingdom Generally Accepted Accounting Practice).

Company law requires the Trustees to prepare financial statements for each financial . Under company law, the Trustees must not approve the financial statements unless they are satisfied that they give a true and fair view of the state of affairs of the Group and the Charity and of their incoming resources and application of resources, including their income and expenditure, for that period. In preparing these financial statements, the Trustees are required to:

- select suitable accounting policies and then apply them consistently
- observe the methods and principles of the Charities SORP (FRS 102);
- make judgements and accounting estimates that are reasonable and prudent;
- state whether applicable UK Accounting Standards (FRS 102) have been followed, subject to any material departures disclosed and explained in the financial statements;
- prepare the financial statements on the going concern basis unless it is inappropriate to presume that the

The Trustees are responsible for keeping adequate accounting records that are sufficient to show and explain the Group and the Charity's transactions and disclose with reasonable accuracy at any time the financial position of the Group and the Charity and enable them to ensure that the financial statements comply with the Companies Act 2006. They are also responsible for safeguarding the assets of the Group and the Charity and hence for taking reasonable steps for the prevention and detection of fraud and other irregularities.

Jonathan Goodman

Approved by order of the members of the board of Trustees and signed on its behalf by:

Professor J M Goodman
Trustee
Date: 23 August 2022

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE

(A Company Limited by Guarantee)

INDEPENDENT AUDITORS' REPORT TO THE MEMBERS OF THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE

OPINION

We have audited the financial statements of The Cambridge Crystallographic Data Centre (the 'parent charitable company') and its subsidiaries (the 'group') for the year ended 31 December 2021 which comprise the Consolidated Statement of Financial Activities, the Consolidated Balance Sheet, the Charity Balance Sheet, the Consolidated Statement of Cash Flows and the related notes, including a summary of significant accounting policies. The financial reporting framework that has been applied in their preparation is applicable law and United Kingdom Accounting Standards, including Financial Reporting Standard 102 'The Financial Reporting Standard applicable in the UK and Republic of Ireland' (United Kingdom Generally Accepted Accounting Practice).

In our opinion the financial statements:

- give a true and fair view of the state of the Group's and of the parent charitable company's affairs as at 31 December 2021 and of the Group's incoming resources and application of resources, including its income and expenditure for the year then ended;
- have been properly prepared in accordance with United Kingdom Generally Accepted Accounting Practice; and
- have been prepared in accordance with the requirements of the Companies Act 2006.

BASIS FOR OPINION

We conducted our audit in accordance with International Standards on Auditing (UK) (ISAs (UK)) and applicable law. Our responsibilities under those standards are further described in the Auditors' responsibilities for the audit of the financial statements section of our report. We are independent of the Group in accordance with the ethical requirements that are relevant to our audit of the financial statements in the United Kingdom, including the Financial Reporting Council's Ethical Standard, and we have fulfilled our other ethical responsibilities in accordance with these requirements. We believe that the audit evidence we have obtained is sufficient and appropriate to provide a basis for our opinion.

CONCLUSIONS RELATING TO GOING CONCERN

In auditing the financial statements, we have concluded that the Trustees' use of the going concern basis of accounting in the preparation of the financial statements is appropriate.

Based on the work we have performed, we have not identified any material uncertainties relating to events or conditions that, individually or collectively, may cast significant doubt on the Group's or the parent charitable company's ability to continue as a going concern for a period of at least twelve months from when the financial statements are authorised for issue.

Our responsibilities and the responsibilities of the Trustees with respect to going concern are described in the relevant sections of this report.

OTHER INFORMATION

The other information comprises the information included in the Annual Report other than the financial statements and our Auditors' Report thereon. The Trustees are responsible for the other information contained within the Annual Report. Our opinion on the financial statements does not cover the other information and, except to the extent otherwise explicitly stated in our report, we do not express any form of assurance conclusion thereon. Our responsibility is to read the other information and, in doing so, consider whether the other information is materially inconsistent with the financial statements or our knowledge obtained in the course of the audit, or otherwise appears to be materially misstated. If we identify such material inconsistencies or apparent material misstatements, we are required to determine whether this gives rise to a material misstatement in the financial statements themselves. If, based on the work we have performed, we conclude that there is a material misstatement of this other information, we are required to report that fact.

We have nothing to report in this regard.

OPINION ON OTHER MATTERS PRESCRIBED BY THE COMPANIES ACT 2006

In our opinion, based on the work undertaken in the course of the audit:

- the information given in the Trustees' Report including the Strategic Report for the financial year for which the financial statements are prepared is consistent with the financial statements.
- the Trustees' Report and the Strategic Report have been prepared in accordance with applicable legal requirements.

MATTERS ON WHICH WE ARE REQUIRED TO REPORT BY EXCEPTION

In the light of our knowledge and understanding of the charitable company and its environment obtained in the course of the audit, we have not identified material misstatements in the Trustees' Report including the Strategic Report.

We have nothing to report in respect of the following matters in relation to which Companies Act 2006 requires us to report to you if, in our opinion:

- the parent charitable company has not kept adequate and sufficient accounting records, or returns adequate for our audit have not been received from branches not visited by us; or
- the parent charitable company financial statements are not in agreement with the accounting records and returns; or
- certain disclosures of Trustees' remuneration specified by law are not made; or
- we have not received all the information and explanations we require for our audit.

RESPONSIBILITIES OF TRUSTEES

As explained more fully in the Trustees' Responsibilities Statement, the Trustees (who are also the directors of the charitable company for the purposes of company law) are responsible for the preparation of the financial statements and for being satisfied that they give a true and fair view, and for such internal control as the Trustees determine is necessary to enable the preparation of financial statements that are free from material misstatement, whether due to fraud or error.

In preparing the financial statements, the Trustees are responsible for assessing the Group's and the parent charitable company's ability to continue as a going concern, disclosing, as applicable, matters related to going concern and using the going concern basis of accounting unless the Trustees either intend to liquidate the Group or the parent charitable company or to cease operations, or have no realistic alternative but to do so.

AUDITORS' RESPONSIBILITIES FOR THE AUDIT OF THE FINANCIAL STATEMENTS

Our objectives are to obtain reasonable assurance about whether the financial statements as a whole are free from material misstatement, whether due to fraud or error, and to issue an Auditors' Report that includes our opinion. Reasonable assurance is a high level of assurance, but is not a guarantee that an audit conducted in accordance with ISAs (UK) will always detect a material misstatement when it exists. Misstatements can arise from fraud or error and are considered material if, individually or in the aggregate, they could reasonably be expected to influence the economic decisions of users taken on the basis of these financial statements.

Irregularities, including fraud, are instances of non-compliance with laws and regulations. We design procedures in line with our responsibilities, outlined above, to detect material misstatements in respect of irregularities, including fraud. The extent to which our procedures are capable of detecting irregularities, including fraud is detailed below:
Our approach to identifying and assessing the risks of material misstatement in respect of irregularities, including fraud and non-compliance with laws and regulations, was as follows:

- the engagement partner ensured that the engagement team collectively had the appropriate competence, capabilities and skills to identify or recognise non-compliance with applicable laws and regulations;
- we identified the laws and regulations applicable to the charitable company through discussions with trustees and other management, and from our charitable sector knowledge and experience;
- we focused on specific laws and regulations which we considered may have a direct material effect on the financial statements or the operations of the charitable company, including the Companies Act 2006, Charities Act 2011, taxation legislation and data protection, anti-bribery and employment legislation and health and safety legislation;
- we assessed the extent of compliance with the laws and regulations identified above through making enquiries of management and inspecting legal correspondence;
- identified laws and regulations were communicated within the audit team regularly and the team remained alert to instances of non-compliance throughout the audit; and
- we reviewed the minutes of Trustees' meetings to identify and references to non-compliances with laws and regulations.

We assessed the susceptibility of the charitable company’s financial statements to material misstatement, including obtaining an understanding of how fraud might occur, by:

- making enquiries of management as to where they considered there was susceptibility to fraud, their knowledge of actual, suspected and alleged fraud; and
- considering the internal controls in place to mitigate risks of fraud and non-compliance with laws and regulations.

To address the risk of fraud through management bias and override of controls, we;

- performed analytical procedures to identify any unusual or unexpected relationships;
- tested journal entries to identify unusual transactions;
- evaluated the assumptions and judgements used by management within significant accounting

estimates and assessed whether these indicated evidence of management bias; and

- performed audit work over the risk of management override of controls, including testing of journal entries and other adjustments for appropriateness, evaluating the business rationale of significant transactions outside the normal course of business and reviewing accounting estimates for bias.

In response to the risk of irregularities and non-compliance with laws and regulations, we designed procedures which included, but were not limited to:

- agreeing financial statement disclosures to underlying supporting documentation;
- reading the minutes of meetings of those charged with governance;
- enquiring of management as to actual and potential litigation and claims; and
- reviewing correspondence with relevant regulators such as the Charity Commission.

There are inherent limitations in our audit procedures described above. The more removed that laws and regulations are from financial transactions, the less likely it is that we would become aware of non-compliance. Auditing standards also limit the audit procedures required to identify non-compliance with laws and regulations to enquiry of the directors and other management and the inspection of regulatory and legal correspondence, if any.

Material misstatements that arise due to fraud can be harder to detect than those that arise from error as they may involve deliberate concealment or collusion.

A further description of our responsibilities for the audit of the financial statements is located on the Financial Reporting Council's website at: www.frc.org.uk/auditorsresponsibilities. This description forms part of our Auditors' Report.

USE OF OUR REPORT

This report is made solely to the charitable company's members, as a body, in accordance with Chapter 3 of Part 16 of the Companies Act 2006. Our audit work has been undertaken so that we might state to the charitable company's members those matters we are required to state to them in an Auditors' Report and for no other purpose. To the fullest extent permitted by law, we do not accept or assume responsibility to anyone other than the charitable company and its members, as a body, for our audit work, for this report, or for the opinions we have formed.

Jayne Rowe

Jayne Rowe (Senior Statutory Auditor)
for and on behalf of
Peters Elworthy & Moore
Chartered Accountants
Statutory Auditors
Salisbury House
Station Road
Cambridge
CB1 2LA

Date: 25 August 2022

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE

(A Company Limited by Guarantee)

CONSOLIDATED STATEMENT OF FINANCIAL ACTIVITIES (INCORPORATING INCOME AND EXPENDITURE ACCOUNT) FOR THE YEAR ENDED 31 DECEMBER 2021

	Note	Unrestricted funds 2021 £	Restricted funds 2021 £	Total funds 2021 £	Total funds 2020 £
Income from:					
Charitable activities	2	**7,091,975**	**164,111**	**7,256,086**	6,563,179
Other trading activities	4	**430,176**	**-**	**430,176**	472,427
Investments	5	**140,197**	**-**	**140,197**	131,924
Total income		**7,662,348**	**164,111**	**7,826,459**	7,167,530
Expenditure on:					
Charitable activities	6	**10,967,936**	**207,808**	**11,175,744**	6,629,236
Total expenditure		**10,967,936**	**207,808**	**11,175,744**	6,629,236
Net (expenditure)/income before net gains/(losses) on investments		**(3,305,588)**	**(43,697)**	**(3,349,285)**	538,294
Net gains/(losses) on investments	13	**945,035**	**-**	**945,035**	(31,800)
Net (expenditure)/income		**(2,360,553)**	**(43,697)**	**(2,404,250)**	506,494
Transfers between funds	18	**(58,739)**	**58,739**	**-**	-
Net movement in funds		**(2,419,292)**	**15,042**	**(2,404,250)**	506,494
Reconciliation of funds:					
Total funds brought forward		**7,545,444**	**24,125**	**7,569,569**	7,063,075
Net movement in funds		**(2,419,292)**	**15,042**	**(2,404,250)**	506,494
Total funds carried forward		**5,126,152**	**39,167**	**5,165,319**	7,569,569

The Consolidated Statement of Financial Activities includes all gains and losses recognised in the year.

The notes on pages 44 to 74 form part of these financial statements.

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE

(A Company Limited by Guarantee)
REGISTERED NUMBER: 02155347

CONSOLIDATED BALANCE SHEET
AS AT 31 DECEMBER 2021

	Note		2021 £		2020 £
Fixed assets					
Tangible assets	12		**2,002,697**		2,024,755
Investments	13		**6,869,644**		5,924,609
			8,872,341		7,949,364
Current assets					
Debtors	14	**2,433,077**		2,349,740	
Cash at bank and in hand		**3,415,237**		3,199,162	
		5,848,314		5,548,902	
Creditors: amounts falling due within one year	15	**(4,131,653)**		(3,454,971)	
Net current assets			**1,716,661**		2,093,931
Total assets less current liabilities			**10,589,002**		10,043,295
Creditors: amounts falling due after more than one year	16		**(226,534)**		(508,265)
Provisions for liabilities	17		**(5,197,149)**		(1,965,461)
Total net assets			**5,165,319**		7,569,569
Charity funds					
Restricted funds	18		**39,167**		24,125
Unrestricted funds	18		**5,126,152**		7,545,444
Total funds			**5,165,319**		7,569,569

The Trustees acknowledge their responsibilities for complying with the requirements of the Act with respect to accounting records and preparation of financial statements.

The financial statements were approved and authorised for issue by the Trustees and signed on their behalf by:

Jonathon Goodman

Professor J M Goodman

Date: 23 August 2022

The notes on pages 44 to 74 form part of these financial statements.

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE

(A Company Limited by Guarantee)
REGISTERED NUMBER: 02155347

CHARITY BALANCE SHEET
AS AT 31 DECEMBER 2021

	Note		2021 £		2020 £
Fixed assets					
Tangible assets	12		**2,002,697**		2,023,868
Investments	13		**7,033,133**		6,088,098
			9,035,830		8,111,966
Current assets					
Debtors	14	**2,882,309**		2,761,044	
Cash at bank and in hand		**2,613,738**		2,565,605	
		5,496,047		5,326,649	
Creditors: amounts falling due within one year	15	**(4,090,917)**		(3,524,587)	
Net current assets			**1,405,130**		1,802,062
Total assets less current liabilities			**10,440,960**		9,914,028
Creditors: amounts falling due after more than one year	16		**(226,534)**		(508,265)
Provisions for liabilities	17		**(5,197,149)**		(1,965,461)
Total net assets			**5,017,277**		7,440,302
Charity funds					
Restricted funds	18		**39,167**		24,125
Unrestricted funds	18		**4,978,110**		7,416,177
Total funds			**5,017,277**		7,440,302

The Charity's net movement in funds for the year was £(2,423,025) (2020 - £514,122).

The Trustees acknowledge their responsibilities for complying with the requirements of the Act with respect to accounting records and preparation of financial statements.

The financial statements were approved and authorised for issue by the Trustees and signed on their behalf by:

Jonathan Goodman

Professor J M Goodman

Date: 23 August 2022

The notes on pages 44 to 74 form part of these financial statements.

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
(A Company Limited by Guarantee)

CONSOLIDATED STATEMENT OF CASH FLOWS FOR THE YEAR ENDED 31 DECEMBER 2021

	Note	2021 £	2020 £
Cash flows from operating activities			
Net cash used in operating activities	20	**180,254**	1,071,413
Cash flows from investing activities			
Dividends, interests and rents from investments		**140,197**	131,924
Purchase of tangible fixed assets		**(105,263)**	(42,486)
Foreign exchange on fixed assets		**887**	-
Net cash provided by investing activities		**35,821**	**89,438**
Change in cash and cash equivalents in the year		**216,075**	**1,160,851**
Cash and cash equivalents at the beginning of the year		**3,199,162**	2,038,311
Cash and cash equivalents at the end of the year	21	**3,415,237**	3,199,162

The notes on pages 44 to 74 form part of these financial statements

1. ACCOUNTING POLICIES

1.1 BASIS OF PREPARATION OF FINANCIAL STATEMENTS

The financial statements have been prepared in accordance with the Charities SORP (FRS 102) - Accounting and Reporting by Charities: Statement of Recommended Practice applicable to charities preparing their accounts in accordance with the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) (effective 1 January 2019), the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) and the Companies Act 2006.

The Cambridge Crystallographic Data Centre meets the definition of a public benefit entity under FRS 102. Assets and liabilities are initially recognised at historical cost or transaction value unless otherwise stated in the relevant accounting policy.

The Consolidated Statement of Financial Activities (SOFA) and Consolidated Balance Sheet consolidate the financial statements of the Charity and its subsidiary undertaking. The results of the subsidiary are consolidated on a line by line basis.

1.2 COMPANY STATUS

The company is a company limited by guarantee. The members of the company are the Trustees named on page 1. In the event of the company being wound up, the liability in respect of the guarantee is limited to £1 per member of the company.

1.3 FUND ACCOUNTING

General funds are unrestricted funds which are available for use at the discretion of the Trustees in furtherance of the general objectives of the Group and which have not been designated for other purposes.

Designated funds comprise unrestricted funds that have been set aside by the Trustees for particular purposes. The aim and use of each designated fund is set out in the notes to the financial statements.

Restricted funds are funds which are to be used in accordance with specific restrictions imposed by donors or which have been raised by the Group for particular purposes. The costs of raising and administering such funds are charged against the specific fund. The aim and use of each restricted fund is set out in the notes to the financial statements.

Investment income, gains and losses are allocated to the appropriate fund.

1.4 BASIS OF CONSOLIDATION

The financial statements consolidate the accounts of The Cambridge Crystallographic Data Centre and all of its subsidiary undertakings ('subsidiaries'). The results of the subsidiaries are consolidated on a line by line basis.

The Company has taken advantage of the exemption allowed under section 408 of the Companies Act 2006 and has not presented its own Statement of Financial Activities in these financial statements, however, note 18 of the accounts provides the funds movement of the company only.

1. ACCOUNTING POLICIES (CONTINUED)

1.5 GOING CONCERN

The Cambridge Crystallographic Data Centre meets its day to day working capital requirements through the cash it holds and generates. The charity undertakes a regular process of reviewing forecasts and projections to ensure that it has adequate resources for its continued operations and can draw on its investment portfolio to support its planned activities if required.

Management have reviewed the impact to date of the global COVID-19 pandemic on the operations of the charity and having considered a number of scenarios and mitigating actions in relation to the potential impact of the virus such that the Trustees have a reasonable expectation that the charity has adequate resources to continue in operational existence for at least 12 months. For this reason, the charity continues to adopt the going concern basis in preparing its financial statements.

1.6 INCOME

All income is recognised once the Charity has entitlement to the income, it is probable that the income will be received and the amount of income receivable can be measured reliably.

Subscription income is recognised over the period to which it relates, with income being received in advance deferred.

Trading income, consisting of software and consultancy advice is recognised as supplied while maintenance and support services are recognised over the period to which they relate.

Interest on funds held on deposit is included when receivable and the amount can be measured reliably by the company; this is normally upon notification of the interest paid or payable by the Bank. Dividends are recognised once the dividend had been declared and notification has been received of the dividend due.

1.7 EXPENDITURE

Expenditure is recognised once there is a legal or constructive obligation to transfer economic benefit to a third party, it is probable that a transfer of economic benefits will be required in settlement and the amount of the obligation can be measured reliably.

Support costs are those costs incurred directly in support of expenditure on the objects of the company and include project management carried out at Headquarters. Governance costs are those incurred in connection with administration of the company and compliance with constitutional and statutory requirements.

Charitable activities and governance costs are costs incurred on the company's operations, including support costs and costs relating to the governance of the company apportioned to charitable activities based on staff roles and time.

Grants payable are charged in the year when the offer is made except in those cases where the offer is conditional, such grants being recognised as expenditure when the conditions attaching are fulfilled. Grants offered subject to conditions which have not been met at the year end are noted as a commitment, but not accrued as expenditure.

1. ACCOUNTING POLICIES (CONTINUED)

1.8 TANGIBLE FIXED ASSETS AND DEPRECIATION

All assets costing more than £10,000 are capitalised.

A review for impairment of a fixed asset is carried out if events or changes in circumstances indicate that the carrying value of any fixed asset may not be recoverable. Shortfalls between the carrying value of fixed assets and their recoverable amounts are recognised as impairments. Impairment losses are recognised in the Statement of Financial Activities.

The cost of replacing and upgrading scientific computer equipment is written off as maintenance to scientific equipment in the income and expenditure account.

Assets in the course of construction are included at costs incurred to date. Depreciation on these assets is not charged until they are brought into use.

Tangible fixed assets are carried at cost, net of depreciation and any provision for impairment. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives on the following bases:

Long-term leasehold property	- 2% straight line
Fixtures and fittings	- 25% reducing balance
Computer equipment	- 3-5 years straight line

1.9 INVESTMENTS

Fixed asset investments are a form of financial instrument and are initially recognised at their transaction cost and subsequently measured at fair value at the Balance Sheet date, unless the value cannot be measured reliably in which case it is measured at cost less impairment. Investment gains and losses, whether realised or unrealised, are combined and presented as ‘Gains/(Losses) on investments’ in the Consolidated Statement of Financial Activities.

Investments in subsidiaries are valued at cost less provision for impairment.

1.10 DEBTORS

Trade and other debtors are recognised at the settlement amount after any trade discount offered. Prepayments are valued at the amount prepaid net of any trade discounts due.

1.11 CASH AT BANK AND IN HAND

Cash at bank and in hand includes cash and short-term highly liquid investments with a short maturity of three months or less from the date of acquisition or opening of the deposit or similar account.

1. ACCOUNTING POLICIES (CONTINUED)

1.12 LIABILITIES

Liabilities and provisions are recognised when there is an obligation at the Balance Sheet date as a result of a past event, it is probable that a transfer of economic benefit will be required in settlement, and the amount of the settlement can be estimated reliably.

Liabilities are recognised at the amount that the Charity anticipates it will pay to settle the debt or the amount it has received as advanced payments for the goods or services it must provide.

Provisions are measured at the best estimate of the amounts required to settle the obligation. Where the effect of the time value of money is material, the provision is based on the present value of those amounts, discounted at the pre-tax discount rate that reflects the risks specific to the liability. The unwinding of the discount is recognised within support costs.

1.13 FINANCIAL INSTRUMENTS

The Group only has financial assets and financial liabilities of a kind that qualify as basic financial instruments. Basic financial instruments are initially recognised at transaction value and subsequently measured at their settlement value with the exception of bank loans which are subsequently measured at amortised cost using the effective interest method.

1.14 FOREIGN CURRENCIES

Monetary assets and liabilities denominated in foreign currencies are translated into sterling at rates of exchange ruling at the balance sheet date.

Transactions in foreign currencies are translated into sterling at the rate ruling on the date of the transaction.

Exchange gains and losses are recognised in the Statement of Financial Activities.

1.15 PENSIONS

The Charity participates in the Universities Superannuation Scheme, a defined benefit scheme which is externally funded and contracted out of the State Earnings-related Pension Scheme. The fund is valued every three years by a professionally qualified independent actuary using the projected unit method, the rates of contribution payable being determined by the trustees on the advice of the actuary. In the intervening years, the actuary reviews the progress of the scheme. Pension costs are accounted for over the period during which the Charity benefits from the employees services.

The Charity also participates in the Cambridge University Assistants' Contributory Pension Scheme (CUACPS) which is a defined benefit scheme. The Charity's contributions are affected by a surplus or deficiency in the CUACPS but the Charity is unable to identify its share of the underlying assets and liabilities in the Scheme on a consistent and reasonable basis. The Charity therefore accounts for its contributions to the CUACPS as if it were a defined contribution scheme.

1. ACCOUNTING POLICIES (CONTINUED)

1.16 CRITICAL ACCOUNTING ESTIMATES AND AREAS OF JUDGEMENT

Estimates and judgements are continually evaluated and are based on historical experience and other factors, including expectations of future events that are believed to be reasonable under the circumstances.

Critical accounting estimates and assumptions:

The charity makes estimates and assumptions concerning the future. The resulting accounting estimates and assumptions will, by definition, seldom equal the related actual results. The estimates and assumptions that have a significant risk of causing a material adjustment to the carrying amounts of assets and liabilities within the next financial year are discussed below.

Critical areas of judgment:

FRS102 makes the distinction between a group pension plan and a multi-employer pension scheme. A group plan consists of a collection of entities under common control typically with a sponsoring employer. A multi-employer scheme is a scheme for entities not under common control and represents (typically) an industry-wide scheme such as that provided by USS. The accounting for a multi-employer scheme where the employer has entered into an agreement with the scheme that determines how the employer will fund a deficit results in the recognition of a liability for the contributions payable that arise from the agreement (to the extent that they relate to the deficit) and the resulting expense is recognised in profit or loss. The Executive Committee are satisfied that the scheme provided by USS meets the definition of a multi-employer scheme and has therefore recognised the discounted fair value of the contractual contributions under the funding plan in existence at the date of approving the financial statements.

2. INCOME FROM CHARITABLE ACTIVITIES

	Unrestricted funds 2021 £	**Restricted funds 2021 £**	**Total funds 2021 £**	Total funds 2020 £
Scientific Activity - Subscription Fees	7,091,975	164,111	**7,256,086**	6,563,179
TOTAL 2020	6,434,079	129,100	6,563,179	

Included within the above is a gift in kind, being free subventions amounting to £163,475 (2020 - £201,727).

3. TURNOVER

The whole of the turnover is attributable to the principal activites of the Charity.

A geographical split of turnover is disclosed as follows: United Kingdom 19% (2020 - 17%), Other EU 21% (2020 - 21%) and Rest of the World 60% (2020 - 62%)

4. INCOME FROM TRADING ACTIVITIES

Income from non charitable trading activities

	Unrestricted funds 2021 £	**Total funds 2021 £**	Total funds 2020 £
Trading subsidiary sales	430,176	**430,176**	472,427
TOTAL 2020	472,427	472,427	

The wholly owned trading subsidiary CCDC Services Limited is incorporated in the United Kingdom and pays all of its profits to the charity under a deed of covenant. The summary financial performance of the subsidiary is shown in note 27.

5. INVESTMENT INCOME

	Unrestricted funds 2021 £	**Total funds 2021 £**	Total funds 2020 £
Investment income	139,470	**139,470**	116,960
Bank & other interest receivable	727	**727**	14,964
	140,197	**140,197**	131,924
TOTAL 2020	131,924	131,924	

In 2021, all investment income was unrestricted.

6. ANALYSIS OF EXPENDITURE BY ACTIVITIES

	Activities undertaken directly 2021 £	Grant funding of activities 2021 £	Support costs 2021 £	Total funds 2021 £	Total funds 2020 £
Scientific Activities	6,256,098	57,648	4,861,998	**11,175,744**	6,629,236
TOTAL 2020	5,329,896	243,337	1,056,003	6,629,236	

In 2021, restricted expenditure amounted to £207,808 (2020: £182,347) and unrestricted expenditure was £10,967,936 (2020: £6,446,889).

7. DIRECT COSTS

Included within the above direct costs is a gift in kind, being free subventions amounting to £163,475 (2020 - £201,727) and £23,808 related to delivering grant funding activities (2020 - £11,493).

8. SUPPORT COSTS

	2021 £	2020 £
Audit and accountancy	**55,327**	36,738
Bad debt expense	**6,963**	491
Banking costs	**5,660**	2,759
Consultants	**57,001**	25,736
Depreciation	**126,434**	133,342
Difference on Foreign exchange - Support	**87,904**	(92,030)
Finance cost of unwinding of discounting	**14,348**	(111,338)
General expenses	**21,654**	37,918
Insurance	**52,553**	48,649
IT equipment, software and hardware	**16,721**	15,041
Legal and other professional fees	**119,961**	25,780
Recruitment costs	**132,503**	96,502
Premises costs	**200,518**	200,052
Staff development	**35,063**	13,510
Telephone and network costs	**14,381**	5,832
Wages and salaries	**3,915,007**	617,021
	4,861,998	1,056,003

During the year ended 31 December 2021, the company incurred the following Governance costs:

Board expenses £7,259 (2020 - £NIL) and audit fees £22,673 (2020 - £21,723).

9. ANALYSIS OF GRANTS

	Grants to Institutions 2021 £	Total funds 2021 £	Total funds 2020 £
Grants	57,648	**57,648**	243,337
TOTAL 2020	243,337	243,337	

The Group has made the following material grants to institutions during the year:

9. ANALYSIS OF GRANTS (CONTINUED)

	2021 £	2020 £
NAME OF INSTITUTION		
University of Leeds	**16,000**	8,000
University of Cambridge	**-**	53,966
University of Liverpool	**-**	34,000
University of Strathclyde	**-**	30,000
University of Sheffield	**39,273**	30,000
University of Edinburgh	**-**	37,874
University of Durham	**-**	48,000
Other immaterial grant costs	**2,375**	1,497
	57,648	243,337
	57,648	243,337

10. NET INCOME/(EXPENDITURE)

	2021 £	2020 £
Auditors' remuneration - audit	**22,673**	21,723
Depreciation of tangible fixed assets:		
- owned by the charitable group	**126,434**	133,340

11. STAFF COSTS, KEY MANAGEMENT PERSONNEL AND TRUSTEES' REMUNERATION AND EXPENSES

Staff costs were as follows:

	Group 2021 £	Group 2020 £	Charity 2021 £	Charity 2020 £
Wages and salaries	**4,725,564**	3,943,208	**4,328,716**	3,612,868
Social security costs	**512,095**	448,381	**436,181**	377,358
Other pension costs	**4,123,515**	726,700	**4,083,216**	693,096
	9,361,174	5,118,289	**8,848,113**	4,683,322

11. STAFF COSTS, KEY MANAGEMENT PERSONNEL AND TRUSTEES' REMUNERATION AND EXPENSES (CONTINUED)

The average number of persons employed by the Charity during the year was as follows:

	Group 2021 No.	Group 2020 No.	**Charity 2021 No.**	Charity 2020 No.
Office and Administration	**9**	8	**8**	7
Technical	**80**	69	**74**	65
	89	77	**82**	72

The number of employees whose employee benefits (excluding employer pension costs) exceeded £60,000 was:

	Group 2021 No.	Group 2020 No.
In the band £60,001 - £70,000	**9**	9
In the band £70,001 - £80,000	**8**	8
In the band £80,001 - £90,000	**7**	4
In the band £90,001 - £100,000	**4**	-
In the band £100,001 - £110,000	**2**	-
In the band £110,001 - £120,000	**1**	1
In the band £120,001 - £130,000	**-**	-
In the band £130,001 - £140,000	**-**	1
In the band £140,001, - £150,000	**-**	-
In the band £150,001 - £160,000	**-**	-
In the band £160,001 - £170,000	**-**	-
In the band £170,001 - £180,000	**1**	-
In the band £180,001 - £190,000	**1**	-

The key management personnel of the charity comprise the trustees, the Chief Executive Officer and the Senior Leadership Management Team. No trustees received any remuneration or benefits in kind from the charity (2020 - £NIL). The total employee benefits of the key management personnel, including employers' NIC and employers pension of the charity were £1,039,750 (2020 - £990,426).

A total of £NIL (2020 - £NIL) was reimbursed or paid directly to 0 (2020 - 0) trustees in respect of travel and accommodation costs.

12. TANGIBLE FIXED ASSETS

GROUP

	Long-term leasehold property £	Fixtures and fittings £	Other fixed assets £	Total £
COST OR VALUATION				
At 1 January 2021	**3,966,255**	**732,597**	**-**	**4,698,852**
Additions	**-**	**-**	**105,263**	**105,263**
Foreign exchange movement	**-**	**(228)**	**-**	**(228)**
At 31 December 2021	**3,966,255**	**732,369**	**105,263**	**4,803,887**
DEPRECIATION				
At 1 January 2021	**2,075,671**	**598,426**	**-**	**2,674,097**
Charge for the year	**79,325**	**47,109**	**-**	**126,434**
Foreign exchange movement	**-**	**659**	**-**	**659**
At 31 December 2021	**2,154,996**	**646,194**	**-**	**2,801,190**
NET BOOK VALUE				
At 31 December 2021	**1,811,259**	**86,175**	**105,263**	**2,002,697**
At 31 December 2020	1,890,584	134,171	-	2,024,755

12. TANGIBLE FIXED ASSETS (CONTINUED)

CHARITY

	Long-term leasehold property £	Fixtures and fittings £	Assets under construction £	Total £
COST OR VALUATION				
At 1 January 2021	**3,966,255**	**728,545**	**-**	**4,694,800**
Additions	**-**	**-**	**105,263**	**105,263**
At 31 December 2021	**3,966,255**	**728,545**	**105,263**	**4,800,063**
DEPRECIATION				
At 1 January 2021	**2,075,671**	**595,261**	**-**	**2,670,932**
Charge for the year	**79,325**	**47,109**	**-**	**126,434**
At 31 December 2021	**2,154,996**	**642,370**	**-**	**2,797,366**
NET BOOK VALUE				
At 31 December 2021	**1,811,259**	**86,175**	**105,263**	**2,002,697**
At 31 December 2020	1,890,584	133,284	-	2,023,868

13. FIXED ASSET INVESTMENTS

GROUP	Listed investments £
COST OR VALUATION	
At 1 January 2021	**5,924,609**
Revaluations	**945,035**
AT 31 DECEMBER 2021	**6,869,644**

13. FIXED ASSET INVESTMENTS (CONTINUED)

All the listed fixed asset investments are held in the UK.

All investments are carried at their fair value. Investments in equities and fixed interest securities are all traded in quoted public markets, primarily the London Stock Exchange. Holdings in common investment funds, unit trusts and open-ended investment companies are at bid price. The basis of fair value for quoted investments is equivalent to the market value, using the bid price. Asset sales and purchases are recognised at the date of trade at cost (that is their transaction value).

The Charity does not make use of derivatives and similar complex financial instruments as it takes the view that investments are held for long term growth and annual income.

The Group has no material investment holdings in markets subject to exchange controls or trading restrictions.

CHARITY	**Investments in subsidiary companies £**	**Listed investments £**	**Total £**
COST OR VALUATION			
At 1 January 2021	**163,489**	**5,924,609**	**6,088,098**
Revaluations	**-**	**945,035**	**945,035**
AT 31 DECEMBER 2021	**163,489**	**6,869,644**	**7,033,133**

14. DEBTORS

	Group 2021 £	Group 2020 £	**Charity 2021 £**	Charity 2020 £
DUE WITHIN ONE YEAR				
Trade debtors	**2,093,902**	2,035,220	**1,966,206**	1,899,268
Amounts owed by group undertakings	**-**	-	**586,560**	582,851
Other debtors	**48,867**	56,244	**46,097**	51,210
Prepayments and accrued income	**290,308**	258,276	**283,446**	227,715
	2,433,077	2,349,740	**2,882,309**	2,761,044

15. CREDITORS: AMOUNTS FALLING DUE WITHIN ONE YEAR

	Group 2021 £	Group 2020 £	**Charity 2021 £**	Charity 2020 £
Trade creditors	**99,031**	57,564	**94,108**	56,839
Amounts owed to group undertakings	**-**	-	**58,177**	169,533
Other taxation and social security	**182,226**	218,251	**166,507**	175,767
Other creditors	**153,984**	160,252	**153,984**	160,252
Accruals and deferred income	**3,696,412**	3,018,904	**3,618,141**	2,962,196
	4,131,653	3,454,971	**4,090,917**	3,524,587

	Group 2021 £	Group 2020 £	**Charity 2021 £**	Charity 2020 £
Deferred income at 1 January	**2,938,109**	2,305,300	**2,888,318**	2,210,436
Resources deferred during the year	**3,549,573**	2,938,109	**3,492,679**	2,888,318
Amounts released from previous periods	**(2,938,109)**	(2,305,300)	**(2,888,318)**	(2,210,436)
Deferred income at 31 December	**3,549,573**	2,938,109	**3,492,679**	2,888,318

Deferred income relates to subscriptions received in advance.

16. CREDITORS: AMOUNTS FALLING DUE AFTER MORE THAN ONE YEAR

	Group 2021 £	Group 2020 £	**Charity 2021 £**	Charity 2020 £
Other creditors	**86,864**	194,500	**86,864**	194,500
Accruals and deferred income	**139,670**	313,765	**139,670**	313,765
	226,534	508,265	**226,534**	508,265

Other creditors relate to grant commitments due after more than one year.

17. PROVISIONS

GROUP AND CHARITY

	Pension deficit funding provision £
At 1 January 2021	**1,965,461**
Additions	**3,231,688**
	5,197,149

PENSION DEFICIT FUNDING PROVISION

The Charity participates in the University Superannuation Scheme (USS), a multi-employer defined benefit scheme. The charity is making additional contributions to address the funding deficit of the scheme and in accordance with FRS102 provision has been made for the future funding requirement. A discount factor of 0.97% (2020 - 0.73%) has been applied to future contributions and the liability represents the present value of the contributions payable. The provision has been valued using BUFDG – Guidance regarding discount rate for institutions participating in USS.

18. STATEMENT OF FUNDS

STATEMENT OF FUNDS - CURRENT YEAR

	Balance at 1 January 2021 £	Income £	Expenditure £	Transfers in/out £	Gains/ (Losses) £	Balance at 31 December 2021 £
UNRESTRICTED FUNDS						
DESIGNATED FUNDS						
Fixed Asset Fund	**2,024,755**	**-**	**-**	**(22,058)**	**-**	**2,002,697**
Research and Development Fund	**173,406**	**-**	**-**	**-**	**-**	**173,406**
Sponsorship and Outreach Fund	**76,000**	**-**	**(57,648)**	**100,000**	**-**	**118,352**
CSD and Sustainability Fund	**100,086**	**-**	**-**	**-**	**-**	**100,086**
Pension Provision Fund	**744,000**	**-**	**-**	**164,000**	**-**	**908,000**
	3,118,247	**-**	**(57,648)**	**241,942**	**-**	**3,302,541**
GENERAL FUNDS						
General Funds - all funds	**4,427,197**	**7,662,348**	**(10,910,288)**	**(300,681)**	**945,035**	**1,823,611**
TOTAL UNRESTRICTED FUNDS	**7,545,444**	**7,662,348**	**(10,967,936)**	**(58,739)**	**945,035**	**5,126,152**

18. STATEMENT OF FUNDS (CONTINUED)

RESTRICTED FUNDS						
BBSRC Student grant fund	**24,125**	**(14,292)**	**-**	**(9,833)**	**-**	**-**
DDA Grant	**-**	**50,022**	**(83,372)**	**33,350**	**-**	**-**
DIDCOM Grant	**-**	**52,833**	**(88,055)**	**35,222**	**-**	**-**
BioChem GRAPH	**-**	**75,548**	**(36,381)**	**-**	**-**	**39,167**
	24,125	**164,111**	**(207,808)**	**58,739**	**-**	**39,167**
TOTAL OF FUNDS	**7,569,569**	**7,826,459**	**(11,175,744)**	**-**	**945,035**	**5,165,319**

18. STATEMENT OF FUNDS (CONTINUED)

STATEMENT OF FUNDS - PRIOR YEAR

	Balance at 1 January 2020 £	Income £	Expenditure £	Transfers in/out £	Gains/ (Losses) £	Balance at 31 December 2020 £
UNRESTRICTED FUNDS						
DESIGNATED FUNDS						
Fixed Asset Fund	2,115,609	-	-	(90,854)	-	2,024,755
Research and Development Fund	173,406	-	-	-	-	173,406
Scientific Travel Fund	16,011	-	-	(16,011)	-	-
Sponsorship and Outreach Fund	153,326	-	(243,337)	166,011	-	76,000
CSD and Sustainability Fund	100,086	-	-	-	-	100,086
Pension Provision Fund	-	-	-	744,000	-	744,000
	2,558,438	-	(243,337)	803,146	-	3,118,247
GENERAL FUNDS						
General Funds - all funds	4,490,718	7,038,430	(6,203,552)	(866,599)	(31,800)	4,427,197
TOTAL UNRESTRICTED FUNDS	7,049,156	7,038,430	(6,446,889)	(63,453)	(31,800)	7,545,444

18. STATEMENT OF FUNDS (CONTINUED)

RESTRICTED FUNDS						
BBSRC Student grant fund	13,919	29,049	(18,843)	-	-	24,125
DDA Grant	-	77,609	(129,349)	51,740	-	-
DIDCOM Grant	-	16,414	(27,356)	10,942	-	-
BioChem GRAPH	-	6,028	(6,799)	771	-	-
	13,919	129,100	(182,347)	63,453	-	24,125
TOTAL OF FUNDS	7,063,075	7,167,530	(6,629,236)	-	(31,800)	7,569,569

18. STATEMENT OF FUNDS (CONTINUED)

STATEMENT OF FUNDS - CHARITY ONLY

	Balance at 1 January 2021	Income	Expenditure	Transfers in/out	Gains/ (losses)	2021
	£	£	£	£	£	£
Designated funds (as detailed above)	3,119,221	-	(56,378)	241,942	-	3,304,785
General funds	4,296,956	7,653,759	(11,129,551)	(92,873)	945,035	1,673,326
Restricted funds (as detailed above)	24,125	164,111	(207,808)	58,739	-	39,167
Total	7,440,302	7,817,870	(11,393,737)	207,808	945,035	5,017,278

STATEMENT OF FUNDS - CHARITY ONLY - PRIOR YEAR

	Balance at 1 January 2020	Income	Expenditure	Transfers in/out	Gains/ (losses)	2020
	£	£	£	£	£	£
Designated funds (as detailed above)	2,558,438	-	(242,363)	803,146	-	3,119,221
General funds	4,353,823	7,029,381	(6,187,849)	(866,599)	(31,800)	4,296,956
Restricted funds (as detailed above)	13,919	129,100	(182,347)	63,453	-	24,125
Total	6,926,180	7,158,481	(6,612,559)	-	(31,800)	7,440,302

. **STATEMENT OF FUNDS (CONTINUED)**

The purpose of funds above are detailed as follows:

Fixed Asset Fund: This fund represents the balance of the groups' reserves held as fixed assets. The transfer represents movements to fixed assets in the year.

Research and Development Fund: This fund finances research activities and makes grants for research where general funds are not available for this purpose.

Sponsorship and Outreach Fund: This fund supports the cost of funding studentships worldwide.

CSD and Sustainability Fund: This fund is established to provide support in the event of unexpected legal, legislative or regulatory events which might have a negative effect on the Centre.

Scientific Travel Fund: This fund meets travel costs of non-staff members furthering the CCDC's objectives. The balance of this fund was transferred into Sponsorship and Outreach Fund to provide support to students worldwide.

Pension Provision Fund: a designated fund set up to provide provision to cover the deficit in the pension scheme.

RESTRICTED FUNDS:

BBSRC: This is a four year training grant funded by the BBSRC for research in global analysis of pharmacophoric space. It covers the period of 1 October 2016 to 30 September 2020 but was extended to 31 March 2021 due to the pandemic.

DDA Grant: The Digital Design Accelerator Platform is an InnovateUK funded project to develop digital risk assessments for pharmaceutical manufacturing processes. A collaboration between innovators, industry, and academia, this 24 month project is intended to build from recent advances in Digital Design methods. It provides us with industrial direction for research and development into Particle Informatics and the new CSD-Particle Suite. The project started on 1 March 2020.

BioChemGRAPH: The BioChemGRAPH project aims to establish a collaboration between PDBe, ChEMBL and CCDC to create an easily accessible resource that integrates structural, functional and biochemical annotations of small molecule data into one place. This project will promote interoperability between small molecule resources by implementing common data standards. The project also aims to improve the findability and accessibility of small molecule annotations via uniform data access mechanisms and develop intuitive web components to visualise these valuable data through web interfaces. It will significantly increase the synergies between structural and biochemical data and will lead to increased understanding of the role of small molecules in biological systems and translational

research in a number of areas, including synthetic biology, target validation, and drug development. The project started on 2 November 2020 and will last 36 months. BioChemGRAPH was 80% funded by BBSRC, 20% of the costs will be covered by the general fund.

DIDCOM: The Digital Design of Complex Materials for Formulated Products (DIDCOM-FP) grant was awarded through the UKRI's Industry Strategy Challenge Fund (ISCF) Manufacturing Made Smarter Challenge. It is a collaborative project with industrial partners, that started in July 2020, centred on materials modelling. Our involvement is focused on solid-liquid equilibria and aims to create a database to enable better solubility prediction and solvent selection tools. This project will last 24 months.

DDA, DIDCOM projects are funded by Innovate UK. However, the grant only covers 60% of the costs. 40% will be funded by the general fund.

19. ANALYSIS OF NET ASSETS BETWEEN FUNDS

ANALYSIS OF NET ASSETS BETWEEN FUNDS - CURRENT YEAR

	Unrestricted funds 2021 £	Restricted funds 2021 £	Total funds 2021 £
Tangible fixed assets	2,002,697	-	**2,002,697**
Fixed asset investments	6,869,644	-	**6,869,644**
Current assets	5,809,147	39,167	**5,848,314**
Creditors due within one year	(4,131,653)	-	**(4,131,653)**
Creditors due in more than one year	(226,534)	-	**(226,534)**
Provisions for liabilities and charges	(5,197,149)	-	**(5,197,149)**
TOTAL	5,126,152	39,167	**5,165,319**

ANALYSIS OF NET ASSETS BETWEEN FUNDS - PRIOR YEAR

	Unrestricted funds 2020 £	Restricted funds 2020 £	Total funds 2020 £
Tangible fixed assets	2,024,755	-	2,024,755
Fixed asset investments	5,924,609	-	5,924,609
Current assets	5,524,777	24,125	5,548,902
Creditors due within one year	(3,454,971)	-	(3,454,971)
Creditors due in more than one year	(508,265)	-	(508,265)
Provisions for liabilities and charges	(1,965,461)	-	(1,965,461)
TOTAL	7,545,444	24,125	7,569,569

ANALYSIS OF NET ASSETS BETWEEN FUNDS (CONTINUED)

ANALYSIS OF NET ASSETS BETWEEN FUNDS - CHARITY ONLY - CURRENT YEAR

	Unrestricted funds 2021 £	Restricted funds 2021 £	Total funds 2021 £
Tangible fixed assets	2,002,697	-	2,002,697
Fixed asset investments	7,033,133	-	7,033,133
Current assets	5,307,812	188,235	5,496,047
Creditors due within one year	(4,090,917)	-	(4,090,917)
Creditors due in more than one year	(226,534)	-	(226,534)
Provisions for liabilities and charges	(5,197,149)	-	(5,197,149)
Total	4,829,042	188,235	5,017,277

ANALYSIS OF NET ASSETS BETWEEN FUNDS - CHARITY ONLY - PRIOR YEAR

	Unrestricted funds 2020 £	Restricted funds 2020 £	Total funds 2020 £
Tangible fixed assets	2,023,868	-	2,023,868
Fixed asset investments	6,088,098	-	6,088,098
Current assets	5,302,524	24,125	5,326,649
Creditors due within one year	(3,524,587)	-	(3,524,587)
Creditors due in more than one year	(508,265)	-	(508,265)
Provisions for liabilities and charges	(1,965,461)	-	(1,965,461)
Total	7,416,177	24,125	7,440,302

20. RECONCILIATION OF NET MOVEMENT IN FUNDS TO NET CASH FLOW FROM OPERATING ACTIVITIES

	Group 2021 £	Group 2020 £
Net income/expenditure for the year (as per Statement of Financial Activities)	**(2,404,250)**	506,494
ADJUSTMENTS FOR:		
Depreciation charges	**126,434**	133,340
(Gains) / losses on investments	**(945,035)**	31,800
Dividends, interests and rents from investments	**(140,197)**	(131,924)
(Increase)/decrease in debtors	**(83,337)**	(562,833)
Increase in creditors	**394,951**	1,205,874
Movement in provisions	**3,231,688**	(111,338)
NET CASH PROVIDED BY OPERATING ACTIVITIES	**180,254**	1,071,413

21. ANALYSIS OF CASH AND CASH EQUIVALENTS

	Group 2021 £	Group 2020 £
Cash in hand	**3,415,237**	3,199,162
TOTAL CASH AND CASH EQUIVALENTS	**3,415,237**	3,199,162

22. ANALYSIS OF CHANGES IN NET DEBT

	At 1 January 2021 £	Cash flows £	At 31 December 2021 £
Cash at bank and in hand	**3,199,162**	**216,075**	**3,415,237**
	3,199,162	**216,075**	**3,415,237**

23. CAPITAL COMMITMENTS

	Group 2021 £	Group 2020 £	**Charity 2021 £**	Charity 2020 £
CONTRACTED FOR BUT NOT PROVIDED IN THESE FINANCIAL STATEMENTS				
Acquisition of tangible fixed assets	**144,400**	-	**144,400**	-

24. PENSION COMMITMENTS

The Group operates a defined benefit pension scheme.

The Charity's employees belong to two principal pension schemes, the Universities Superannuation Scheme (USS) and the Cambridge University Assistants' Contributory Pension Scheme (CUACPS). The total pension cost for the period was £906,175 (2020 - £726,700).

Universities Superannuation Scheme

The Charity participates in the Universities Superannuation Scheme (USS), a defined benefit scheme which is contracted out of the State Second Pension (S2P). The assets of the scheme are held in a separate fund administered by the trustee, Universities Superannuation Scheme Limited.

The latest available complete actuarial valuation of the Retirement Income Builder is at 31 March 2018 (the valuation date), which was carried out using the projected unit method. A valuation as at 31 March 2020 is underway but not yet complete.

Since the institution cannot identify its share of USS Retirement Income Builder (defined benefit) assets and liabilities, the following disclosures reflect those relevant for those assets and liabilities as a whole.
The 2018 valuation was the fifth valuation for the scheme under the scheme-specific funding regime introduced by the Pensions Act 2004, which requires schemes to adopt a statutory funding objective, which is to have sufficient and appropriate assets to cover their technical provisions. At the valuation date, the value of the assets of the scheme was £63.7 billion and the value of the scheme's technical provisions was £67.3 billion indicating a shortfall of £3.6 billion and a funding ratio of 95%.

The key financial assumptions used in the 2018 valuation are described below. More detail is set out in the Statement of Funding Principles.

Pension increases (CPI)	Term dependent rates in line with the difference between the Fixed Interest and Index Linked yield curves, less 1.3% p.a.
Discount rate (forward rates)	Years 1-10: CPI + 0.14% reducing linearly to CPI – 0.73% Years 11-20: CPI + 2.52% reducing linearly to CPI + 1.55% by year 21 Years 21 +: CPI + 1.55%

The main demographic assumption used relates to the mortality assumptions. These assumptions are based on analysis of the scheme's experience carried out as part of the 2018 actuarial valuation. The mortality assumptions used in these figures are as follows:

	2018 valuation
Mortality base table	Pre-retirement: 71% of AMC00 (duration 0) for males and 112% of AFC00 (duration 0) for females Post retirement: 97.6% of SAPS S1NMA "light" for males and 102.7% of RFV00 for females
Future improvements to mortality	CMI_2017 with a smoothing parameter of 8.5 and a long term improvement rate of 1.8% pa for males and 1.6% pa for females

24. PENSION COMMITMENTS (CONTINUED)

Principal actuarial assumptions at the Balance Sheet date (expressed as weighted averages):

	At 31 December 2021 %	At 31 December 2020 %
Discount rate	**2.59**	2.59
Pensionable salary growth	**n/a**	n/a
Pension increases (CPI)	**4.20**	4.20

The current life expectancies on retirement at age 65 are:

	At 31 December 2021 Years	At 31 December 2020 Years
Males currently aged 65 (years)	**24.4**	24.4
Males currently aged 45 (years)	**26.3**	26.3
Females currently aged 65 (years)	**25.9**	25.9
Females currently aged 45 (years)	**27.7**	27.7

24. PENSION COMMITMENTS (CONTINUED)

Cambridge University Assistants' Contributory Pension Scheme

The Charity also participates in the Cambridge University Assistants' Contributory Pension Scheme (CUACPS) which is a defined benefit scheme. The Charity's contributions are affected by a surplus or deficiency in the CUACPS but the Charity is unable to identify its share of the underlying assets and liabilities in the Scheme on a consistent and reasonable basis. The Charity therefore accounts for its contributions to the CUACPS as if it were a defined contribution scheme.

The most recent full actuarial valuation of the CUACPS was carried out as at 31 July 2018 by an independent actuary, Robert Sweet, who is a Fellow of the Institute of Actuaries. He is not an employee or officer of the Charity. The CUACPS is not a closed scheme nor one in which the age profile of the active membership is rising significantly.

The method used in the actuarial valuation as at 31 July 2018 was the Projected Unit funding method. The main assumptions were:

Economic	
Discount rate:	5.15%
Asset return for Recover Plan:	5.85%
Rate of Salary increases:	4.25%
Rate of increases in pensions in payment:	
- RPI max 12%, min 0%	3.25%
- RPI max 5%, min 0%	3.15%
- CPI max 5%, min 0%	2.25%
Rate of increases in pensions in deferment:	
- GMP	4.25%
- Pensions in escess of GMP:	
- RPI	3.25%
- CPI	2.25%
Assets & Expenses	
Valuation of assets:	Surrender value of the assets
Expenses:	
- Past service	1.0% of the liability excluding expenses
- Future service	0.9% of the Pensionable Salary
Pension Protection Fund levies:	Included in the future service cost expense
Demographic	
Rate of mortality:	121% of S2NMA pension mortaility tables for males and 90% of S2NFA pension mortality tables for females. Plus a projection based upon the CMI_2017 model with a long term 1.25% p.a. improvement.
Assumed Age at Retirement:	
UNI 1	
- Active members	Males 63, Females 62
- Deferred members	Males 61, Females 61
UNI 2 & UNI 3	Males 65, Females 65
Proportion married	85%
Age difference	Women 3 years younger than their partners

24. PENSION COMMITMENTS (CONTINUED)

Value of benefits in respect of service on or before 31 July 2018:

Technical Provisions	[a]	£742,670,000
Market Value of Scheme Assets	[b]	£708,068,000
Past Service Surplus/(Deficit)	[b-a]	£34,602,000
Level of Funding of Past Service Benefit	[b]/[a]	95%

The Trustee and the University have agreed that Employer contributions should continue at the current rates. The Trustee and the University have also agreed that the Employer will continue to pay additional contributions of £14,595,000 p.a. from 1 August 2018 to 31 July 2020, which will eliminate the funding shortfall.

The ongoing overall joint contribution rate for future service benefits, ignoring the past service position, is 12.2% of Pensionable Salaries. The split of this rate is shown below:

Pre 2013 Members paying additional contributions under Rule 45.6
- 21.2% pa of Pensionable Salaries (Salary Sacrifice Members); and
- 12.7% pa of Pensionable Salaries (Other Members).

Other pre 2013 Members paying
- 17.7% pa of Pensionable Salaries (Salary Sacrifice Members); and
- 12.7% pa of Pensionable Salaries (Other Members).

Post 2013 Members
- 8.2% pa of Pensionable Salaries (Salary Sacrifice Members); and
- 5.2% pa of Pensionable Salaries (Other Members).

25. RELATED PARTY TRANSACTIONS

In 2021 the following transactions took place between the Charity and its wholly owned subsidiary CCDC Services Limited:

The provision of management services by the Charity to the company of £92,287 (2020: £165,154).
The transfer under deed of covenant of the trading profits of CCDC Services Limited to the Charity of £329,300 (2020: £300,063).

In 2021 the following transactions took place between the Charity and its wholly owned subsidiary CCDC Inc:

The provision of a sales office and related services by the company to the Charity of £597,358 (2020: £511,211).

There were no other outstanding balances with related parties as at 31 December 2021 (2020 - £NIL)

26. INVESTMENT IN SUBSIDIARY COMPANIES

The Charity has a wholly owned subsidiary which is incorporated in the UK. CCDC Services Limited provides professional services in relation to digital drug design and manufacture, and advanced training. CCDC Services Limited transfers its taxable profits to The Cambridge Crystallographic Data Centre under a deed of covenant.

The Charity has a wholly owned subsidiary which is incorporated in the USA. CCDC Inc provides a sales office and administrative function for the charity within the US. All turnover in CCDC Inc arises from recharges to The Cambridge Crystallographic Data Centre. Therefore no amounts are disclosed within income from trading activites in the consolidated financial statements.

A summary of the results of CCDC Services Limited is shown in note 26.

27. PRINCIPAL SUBSIDIARIES

The following was a subsidiary undertaking of the Charity:

Name	Company number	Registered office or principal place of business	Principal activity
CCDC Services Limited	03483374	12 Union Road, Cambridge, CB2 1EZ	Provision of professional services for digital drug design and manufacture, and advanced training.

Class of shares	Holding	Included in consolidation
Ordinary	100%	Yes

The financial results of the subsidiary for the year were:

Name	Income £	Expenditure £	Profit/(Loss) / Surplus/ (Deficit) for the year £	Net assets £
CCDC Services Limited	**430,178**	**(100,878)**	**329,300**	**2,118**