

Trustees' report and financial statements

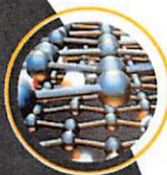
For year ending
31 December 2022

Registered in England No. 2155347 Registered Charity No. 800579

CCDC
advancing structural science



About the CCDC



Delivering our vision



Key product releases



Financial review



Structure and governance



Looking into the future



Administrative details



Independent auditors' report

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The Trustees present their annual report together with the audited financial statements of the group and the company for the year 1 January 2022 to 31 December 2022. 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).

About the CCDC



About the CCDC and its purpose

We shape the future of structural science

- With scientific software, high-quality data, and professional services that accelerate the discovery and development of new medicines, chemical products, and advanced/functional 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 scientists worldwide through outreach and education.

What we do

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

We specialise in the collation, curation, 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.



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 techniques and semantic rules) and through manual curation by our expert chemists and crystallographers. This means you can trust that the data within the CSD is accurate, consistent, and of highest quality.

Furthermore, we enrich 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 both scientists and machines (e.g. new AI-based algorithms) to interpret the structures in a chemically meaningful way.

Managing this data so that it is available and secure is a critical part how CCDC ensures the CSD remains an important global data repository. We continue to invest in multiple layers of cyber-security, work with 3rd parties to test our systems and software for vulnerabilities and run ongoing cyber-security training with staff.

Publication data

By collecting the crystallographic data from journal publications across the scientific enterprise, we provide a trusted repository to store the associated research data and make it easily available to readers. It also enables researchers who find crystallographic data in the CSD to link back to the original research article. This strengthens the scientific record, and is in keeping with emerging requirements of funding agencies worldwide.

Unique data

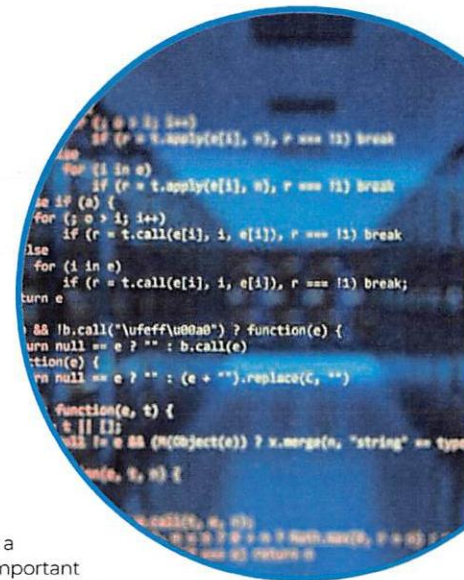
We enable researchers to publish data that otherwise would have remained unpublished, confidential, and unknown directly through the CSD. The CSD therefore contains data that isn't available anywhere else in the world.

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, visualise, 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 physiochemical properties within the CSD, we can extract new



About the CCDC and its purpose

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 users' 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, advanced searching, and visualisation to teaching, research, and analysis.

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 have 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 is based on a new, continuously 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 physiochemical data.

We endeavour to lead structural scientific research by working with all our in-house scientists, our research partners, commercial clients, 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.

Through our global education and outreach, we will 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.

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, neural nets, 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 customers and academic user bases.

About the CCDC and its purpose

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 2022 we have further embedded these values in the ways we work across all levels and functions of the organisation.



Community

We serve the global scientific communities for the public benefit.

Passion

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

Integrity

We act with integrity and communicate honestly and transparently.



Quality

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

Collaboration

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

Innovation

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



Agility

We are flexible and efficient without compromising quality.

Customer Centricity

We provide a quality service with a positive customer experience.

Diversity

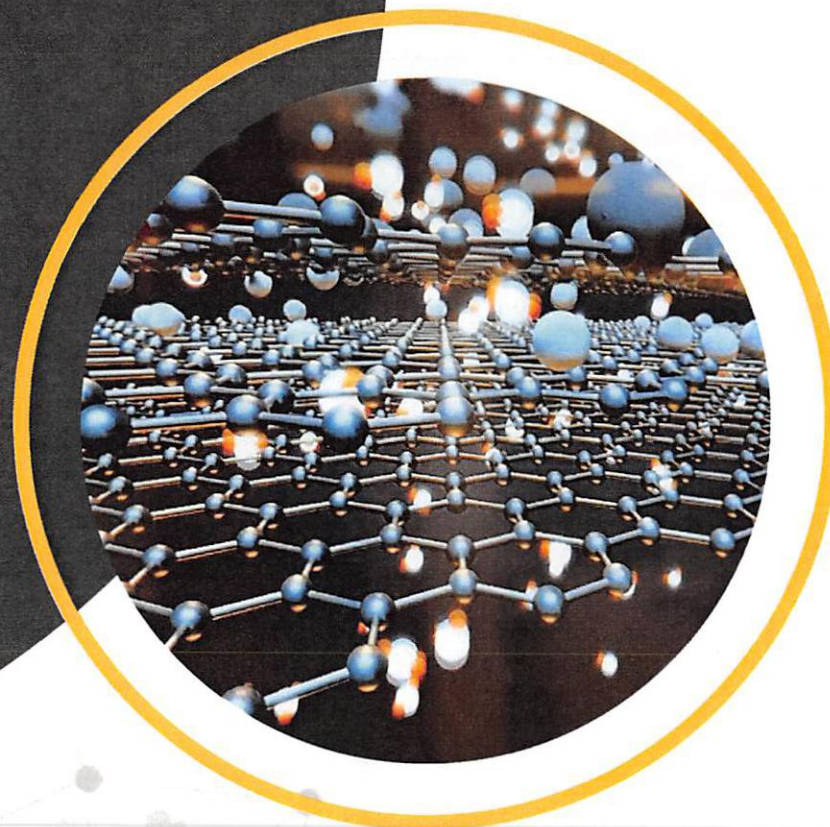
We believe in diversity and inclusion, and we work to create a culture of belonging, where everyone is welcome, valued and respected.

Public Benefits

The CCDC Board of Trustees holds in high regard the principle of public benefit and requires the CEO, the executive team, the 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 objectives. 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. The public benefit will be described in detail in the next section, Delivering our vision.



Delivering our vision



Delivering our vision

During 2022, the **Cambridge Structural Database (CSD)** grew by 5% to over 1.2 million entries. 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**.

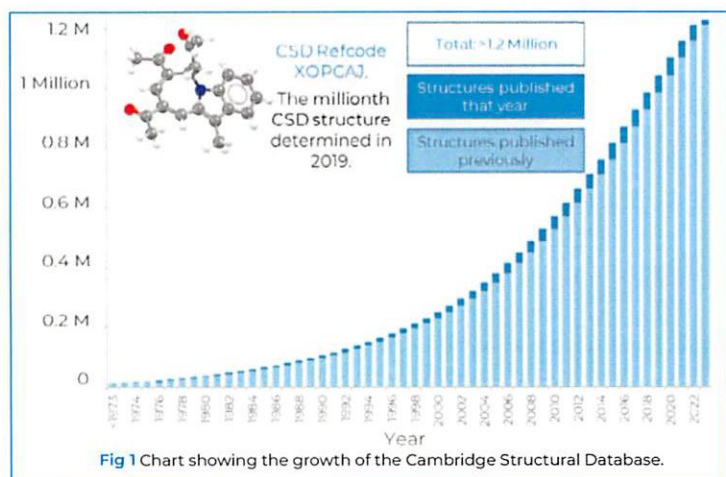
The CSD continues to be a global community resource, and in 2022 alone deposited structures were determined by over 15,000 different crystallographers from over 95 different countries. The ability for researchers to publish directly through the CSD for free as CSD Communications helped support the amount of new crystal structures shared with the community.

CSD Communications continued to be the number one way to share structural data, accounting for roughly 10% of the new structures added during the year. In total over 5K additional structures were shared in this way during the year and they now account for over 50K of the entries in the CSD.

The CCDC also supported researchers worldwide to help convert historical entries into the CSD from hard copy, printed information. With the continued growth of the database, the CCDC expanded our portfolio of targeted collections of data. 2022 saw the

launch of five new collections, namely three subsets that define the dimensionality of Metal-Organic Frameworks (MOFs) and two based on the disorder exhibited in a structure. These targeted datasets help to provide easy access to highly relevant structures that can be hard to locate with simple searches and 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.

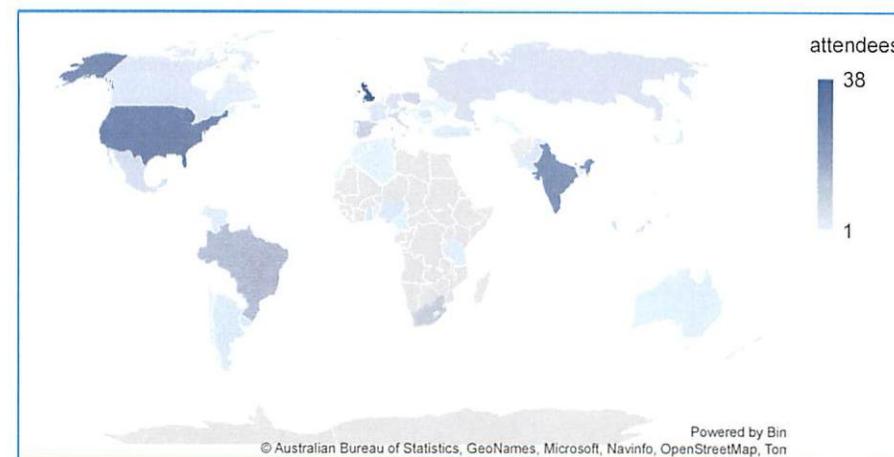
The value of one million plus crystal structures continued to be the subject of hundreds of articles worldwide, including 9 that were showcased through our Tools in Action series. In 2022, approximately one thousand peer-reviewed articles by researchers in academia and industry cited the CSD reference paper which equates to nearly 3 new citations a day. This highlights the breadth of applications made possible with this data.



During the year, the CCDC continued to support our global scientific community. We participated in many international conferences, including the British Crystallographic Association (BCA) meeting, the American Crystallographic Association (ACA) meeting, BioIT Word conference, both the Spring and Fall American Chemical Society (ACS) meetings, the Asian Crystallographic Association meeting (AsCA), the International Conference on the Chemistry of the Organic Solid State (ICCOSS), the European Crystallographic Meeting (ECM), the International Conference on Chemical Structures (ICCS), the Crystal Engineering Gordon Research Conference, the International Conference on Crystal Growth of Organic Materials, BioTechX and the Annual Inorganic Discussion Weekend (IDW).

Alongside participating in international conferences, the CCDC delivered over twenty workshops at crystallographic schools and training events worldwide (either in-person or virtually) including the Tunisian Powder Diffraction School, USNC/Cr Workshop Series, Mid-Atlantic Regional Meeting of the ACS, ACA Summer School, European Crystallography School, the ECM, the Slovenian-Croatian Crystallographic Meeting, AsCA, the X-TechLab training session in Benin, and the Latin American Crystallographic Association (LACA) school.

During 2022, the CCDC also hosted six free virtual workshops. The virtual workshops sessions were well attended from all over the world, with attendees from over 55 countries represented throughout the year. These sessions each had around 300 registrations and 100 attendees.



Delivering our vision

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. New online training courses were added to CSDU, a new collection of free on-demand modules, with content comparable to that of live workshops and with a completion certificate to be earned at the end. These on-demand courses go beyond our existing platform of self-guided workshops with focused 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.

In addition to the CCDC activities and resources 2022 saw the launch of our CCDC Engagement Grants to support others to produce resources or activities to increase schools and public engagement in crystallography and structural science. In total six projects were funded and the outputs from the projects are due for delivery in 2023. CCDC also partnered with the RCSB Protein Data Bank (RCSB PDB) to create Bound! A new protein-drug matching card game to provide a fun way to learn about the importance of chemical and biological structures.

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. In 2022, thirteen new institutions were awarded a campus-wide CSD license under the FAIRE programme, nearly doubling the total number of FAIRE holders from 2021. In total the initiative has supported researchers to publish over 100 scientific publications in primary research journals since its launch.

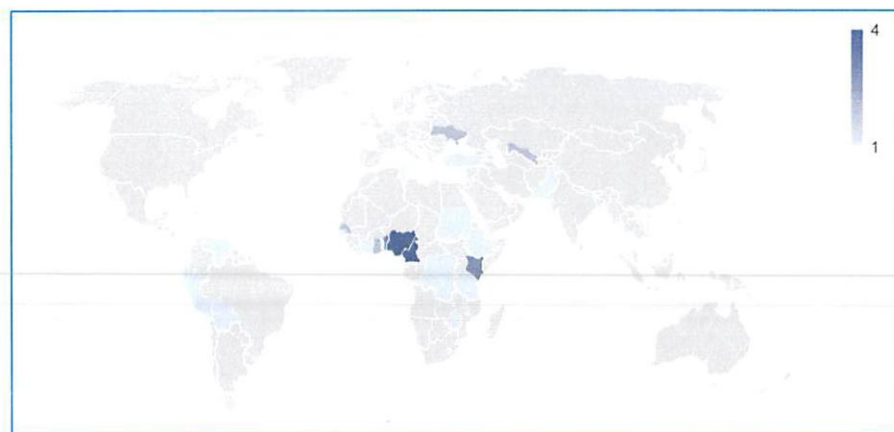


Fig 3 Map showing where our FAIRE programme is being used. Lighter to darker shades of blue represent a growing number of FAIRE holders ranging from one to four.

Scientific innovation

During the past year, CCDC has continued to innovate to develop new scientific methods. We have built a new group to explore the application of theoretical methods in consort with our data for crystal structure prediction and analysis. This team is now exploring new ways to make use of such information in impactful ways. We have prototyped using AI driven methodologies for both enhanced searching of the CSD and for prediction of co-crystal forms. Work in particle analysis has continued with better data-driven analytic methods for understanding crystal surface being developed. In discovery, we have been working to better understand the needs of our tools in a large-scale computational environment. We have developed new prototypes to intelligently augment protein structures to make them more modelling ready. We are also looking at how scientifically we can be more impactful in functional materials going forwards.

Impact of the CCDC in worldwide research

The CCDC's software and services continue to have impact in research across the world. In 2022, some 2,444 papers were published that cite at least one of the key reference papers that CCDC has published. Most of these papers are examples of use of the software or data in academic and industrial research. In these papers, at least one author was affiliated with an institution from 106 different countries according to Web of Science.

It is worth highlighting that nearly a quarter of these publications come from FAIRE-eligible countries.

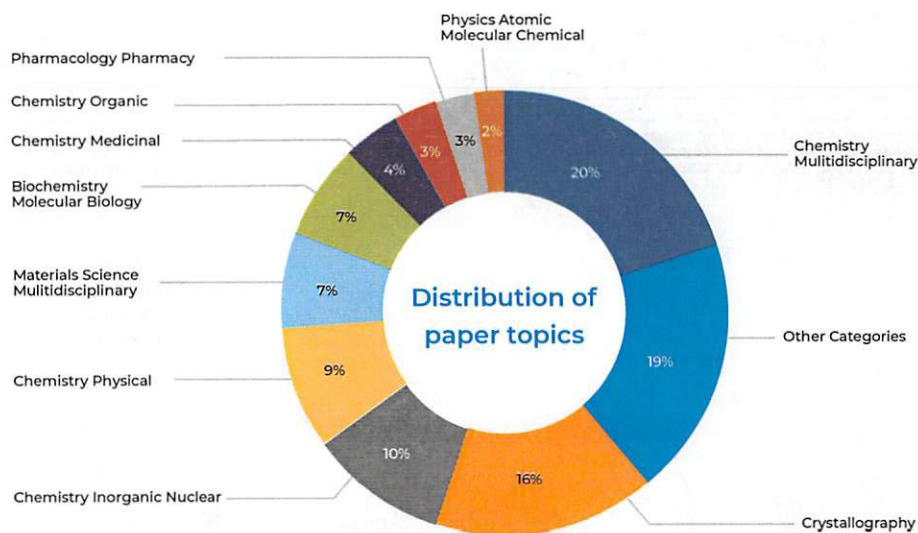
While the vast majority of citing publications in Web of Science fall into the Web of Science category of 'Chemistry Multidisciplinary' or 'Crystallography', 55 publication categories were featured in this year's set of published papers. The data, software and services continue to have broad impact across a diverse range of subject areas.



Fig 4 Map to show where 2022 publications citing at least one of the key reference papers that CCDC is from, countries outlined in red are FAIRE countries.

Delivering our vision

Fig 5 Chart showing the distribution of topics (according to Web of Science) for papers citing at least one of the key reference papers that CCDC has published.



CCDC publications & studentships

CCDC has a vibrant studentship program. We are associated with 4 doctoral training centres across the United Kingdom, and sponsor students in projects across a broad range of scientific domains. We currently sponsor 13 students. 12 papers were published in 2022 in collaboration with 50 different co-authors in a wide range of subject areas. In 2022, we have broadened our horizons and started a new studentship in collaboration with the Politecnico di Torino in Italy.

The 7th Crystal Structure Prediction Blind Test

A key focus in 2022 was the culmination of the 7th Crystal Structure Prediction Blind Test. The Crystal Structure Prediction Blind Test is a rigorous test of methods for predicting small molecule organic (and now metal-organic) crystal structures without prior knowledge of crystallographic information. Being able to reliably predict crystal structures before molecular synthesis would be highly valuable, as it would allow communities to use prediction to design new compounds with crystallographic properties in-silico. By conducting this test, CCDC ensures that methods development in this space is held to a high degree of scrutiny and provides a strong benchmark for external parties to use to evaluate state of the art methods in this scientific field.

The molecules used ranged in complexity as can be seen in the illustration below.

The challenges faced by participants were increased in this test, with the test being made more real-world oriented. For system XXX groups were asked to predict the stoichiometry of observed structures. For systems where more than one polymorph was observed, groups were asked to predict relative stabilities.

The test was broken into 2 stages: a landscape prediction stage and a landscape ranking stage.

We received 99 submissions from 22 groups to the first phase of the test and 78 submissions from 21 groups in the second phase. This represented work from over 150 researchers world-wide. To undertake the research over 80,000,000 CPU hours were used which shows the future challenge for such computational methodologies.

The test will be written up in the coming months as a pair of scientific publications which will highlight the successes and challenges faced in this scientific area.

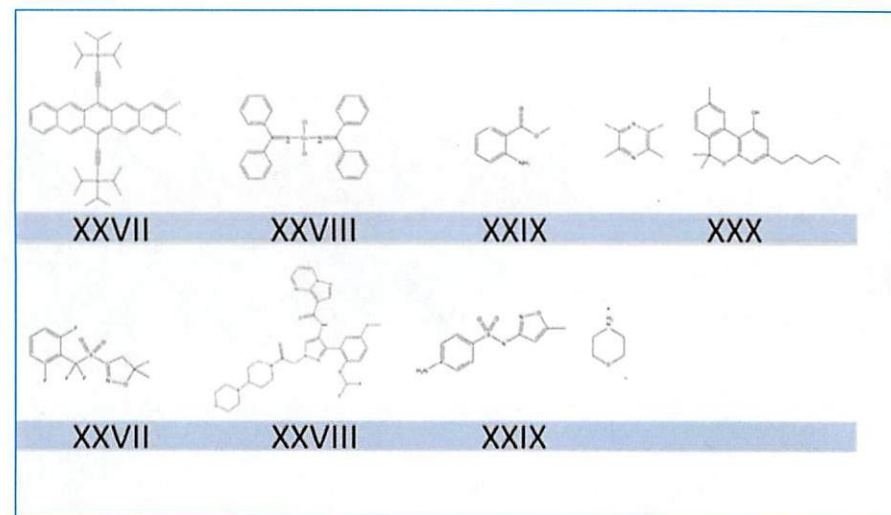
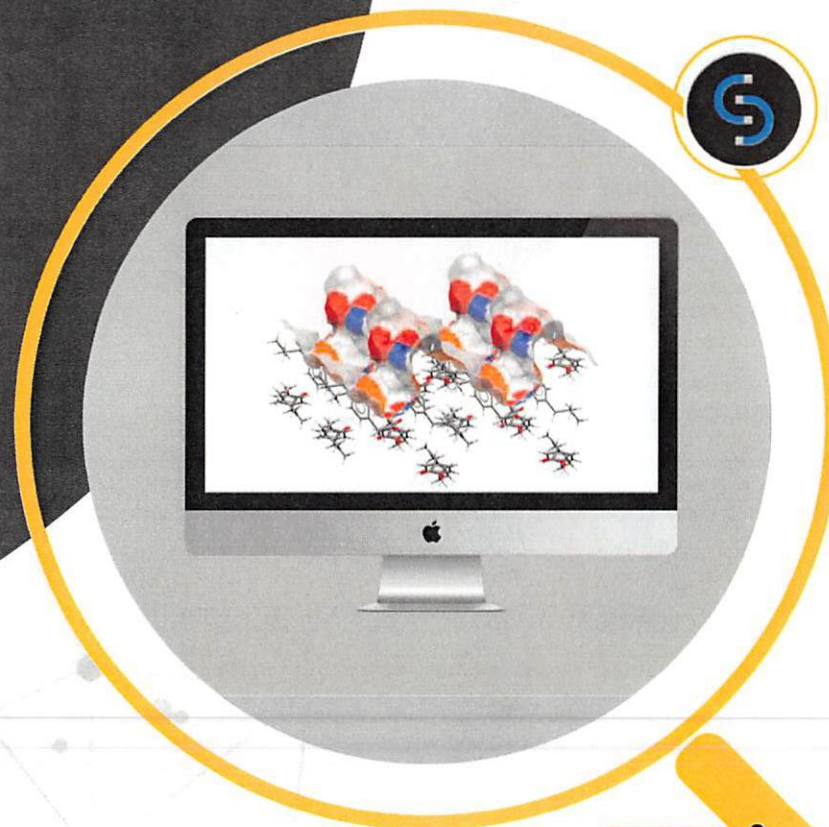


Fig 6 The molecules used ranged in complexity as can be seen in the illustration above

Key product releases



Key product releases

2022 saw **six major product launches** across the desktop and web platforms, plus five minor launches covering data updates and smaller improvements on our web platforms. Advances have been made across all the major areas of our portfolio, with prioritisation supported by active user engagement. A major highlight for 2022 was the first launch of the new product suite – **CSD-Particle**.

Foundational area

Over 2022 we have been investing in the core visualisation and search capabilities in our web platform, with a new, more effective **3D visualiser** being introduced to our Public and On-Site web platform, plus the introduction of full 3D searching capabilities, which is something that our users have been asking about for several years.

Further improvements have been made specifically in the **On-Site WebCSD** platform over 2022, including improving the installation and update experience for the system for industrial users. In addition, On-Site WebCSD has been extended to provide the ability to control access to structures at a per-user, per-database level.

Both the Public and On-Site versions of WebCSD are now also underpinned by our new database technology which will be the foundation for all our future web functionality and will start to be used to also drive our desktop capabilities in future years.

Discovery & integrations area

In the Discovery & Integrations area, we have made significant updates in our handling of **SMARTS** (SMILES Arbitrary Target Specification) – a language for specifying substructural patterns in molecules, allowing the use of recursive and dot-disconnect SMARTS in the **CSD Python API**, **Mercury**, and **Hermes**. There is also now full implementation of atom conditionals, and variable bond conditions are supported. These changes allow for the automation of large numbers of queries, as well as making it possible to do more complex searches not currently possible in ConQuest.

We have also made significant improvements to the installation of the **CSD Python API**, making this simpler and more accessible for both Python beginners and Python experts. Support is also now provided for the CSD Python API on both **Python 3.7** and **Python 3.9**.

Solid form area

CCDC continues to host the **Crystal Form Consortium (CFC)**. The CFC brings together solid form scientists from 12 leading pharmaceutical companies to develop informatics-based approaches to solid form challenges. The CFC has been running successfully for 14 years providing pharmaceutical scientists with a pre-competitive environment within which to share common drug development challenges, exchange best practice and develop new solutions.

CSD-Materials suite

The most well-established product suite in the Solid Form area of our portfolio is **CSD-Materials**, having first launched in 2008. Over 2022, improvements have been made across the **CSD-Materials suite**, but in particular the performance of Full Interaction Maps has been significantly improved (now on average two times faster), and major usability improvements have been made to our Hydrogen Bond Propensity component, allowing users to assess more complex systems, obtain new more advanced results, and customise the results view.

CSD-Theory suite

The **CSD-Theory product suite**, which was first launched in 2021, continued to evolve over 2022 with new capabilities introduced over two web launches including improved crystal structure prediction (CSP) landscape visualisation capabilities, automated synchronisation between experimental databases and CSP landscapes, similarity analysis across all low energy predicted structures, and further structure-matching capabilities to assess CSP landscapes and compare experimental PXRD patterns against CSP landscapes.

CSD-Particle suite

Also in the Solid Form area, 2022 saw the first launch of a brand-new product suite for the CCDC called **CSD-Particle**. This is a new product suite to analyse the mechanical and chemical properties of crystalline particles. With this, formulation decisions can be guided, and manufacturing bottlenecks caused by issues in tabletability, wettability, flow, or sticking can be identified. In CSD-Particle you can predict particle facets, visualize surface chemistry, charge, topology, and interactions, identify potential slip planes, determine H-bond dimensionality, quantify surface chemistry and topology, and more.

Key product releases

Looking forward

We expect to see continued growth in the value that we are delivering to our users over 2023, particularly investing more in the CSD-Discovery product suite over the next year. **Strong focus areas in 2023 across the portfolio will include improving the installation and update experience, plus improvements in user experience in general.**

We will continue to engage with the market to uncover evolving challenges and develop data-driven products and services to address these challenges. Our professional services offering helps increase adoption of CSD-based tools within companies, understand new areas of application, as well as generating revenue that is reinvested in the charity.

Financial review



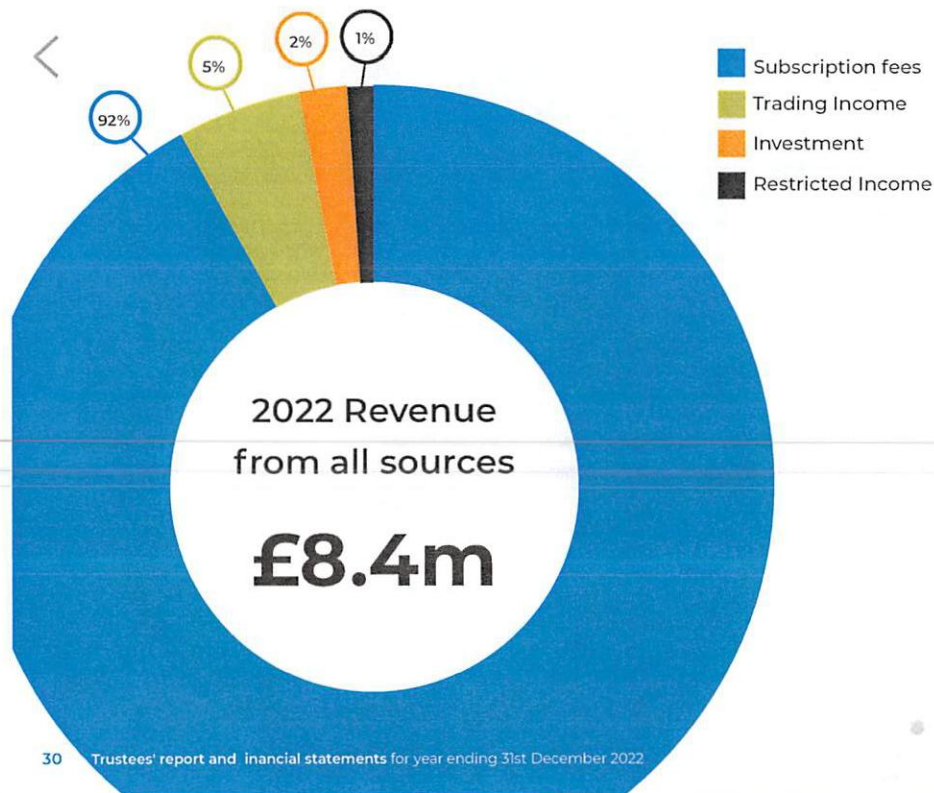
Financial review

Principle funding

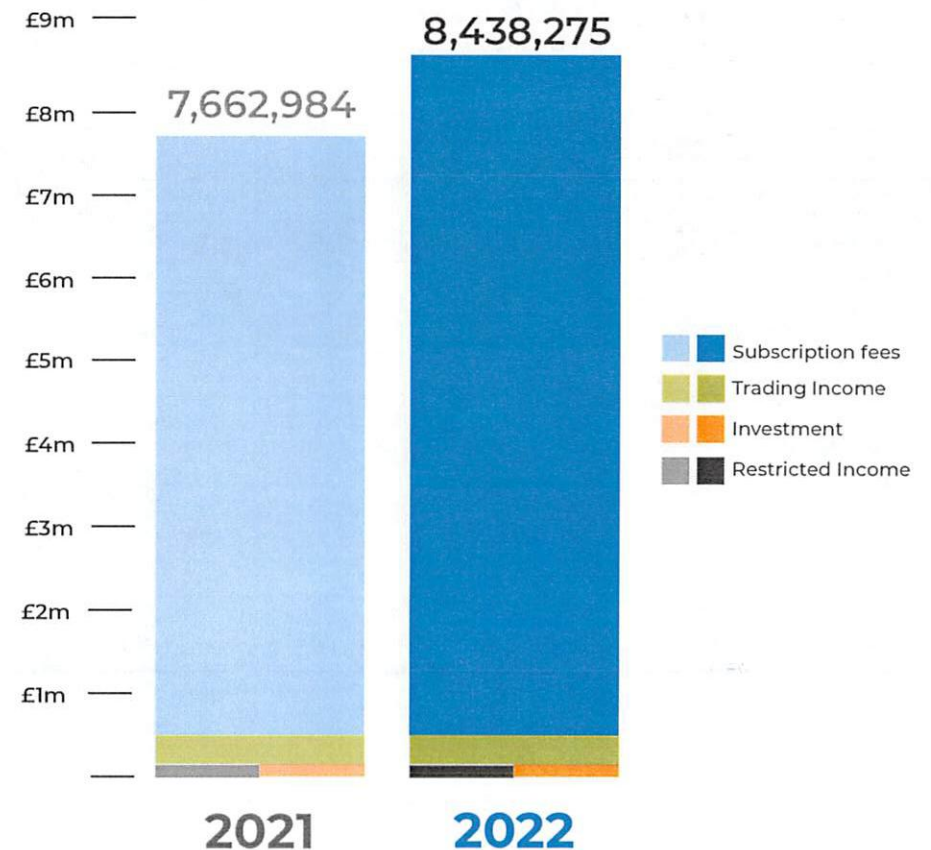
The CCDC's principal funds arise from the subscription fee to the CSD and its associated scientific software. Its subscribers are academic research institutions from around the globe and industrial companies, mainly within the pharmaceutical and biotech sectors and growing into other sectors such as agrochemistry and the chemical industry. The annual contributions requested from the worldwide academic community are significantly discounted as compared to the contributions requested from industrial subscribers, 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. It enables the CCDC to invest in relevant scientific methods and applications' research and development. The CCDC received government grants for specific projects (Restricted income) during 2022. 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.

A breakdown of the revenue can be seen below:



Total Revenue



Revenue continued to grow in 2022. User retention rate remains high. Coupled with new subscribers, 2022 saw a 10% growth compared to the year before. The total revenue was £8,438,275 (2022 restated: £7,662,984). The growth is primarily gained from subscriptions fees, as shown from the chart above, while the other revenue streams remained at a similar level as 2021.

The accounting policy for the recognition of free subventions and subsidies as a gift in kind has been reviewed during the year.

It was concluded that they did not meet the definition of a gift-in-kind and therefore, a prior year adjustment has been made to reduce income and expenditure by the value of the free subventions and subsidies provided. In 2022, we continued to promote the FAIRE program that provides free access to the CSD to users who may not otherwise have access; heavy subsidies are also provided to users who have limited funds. The total monetary value amounted to £359,433 (2021: £163,475).

Financial review

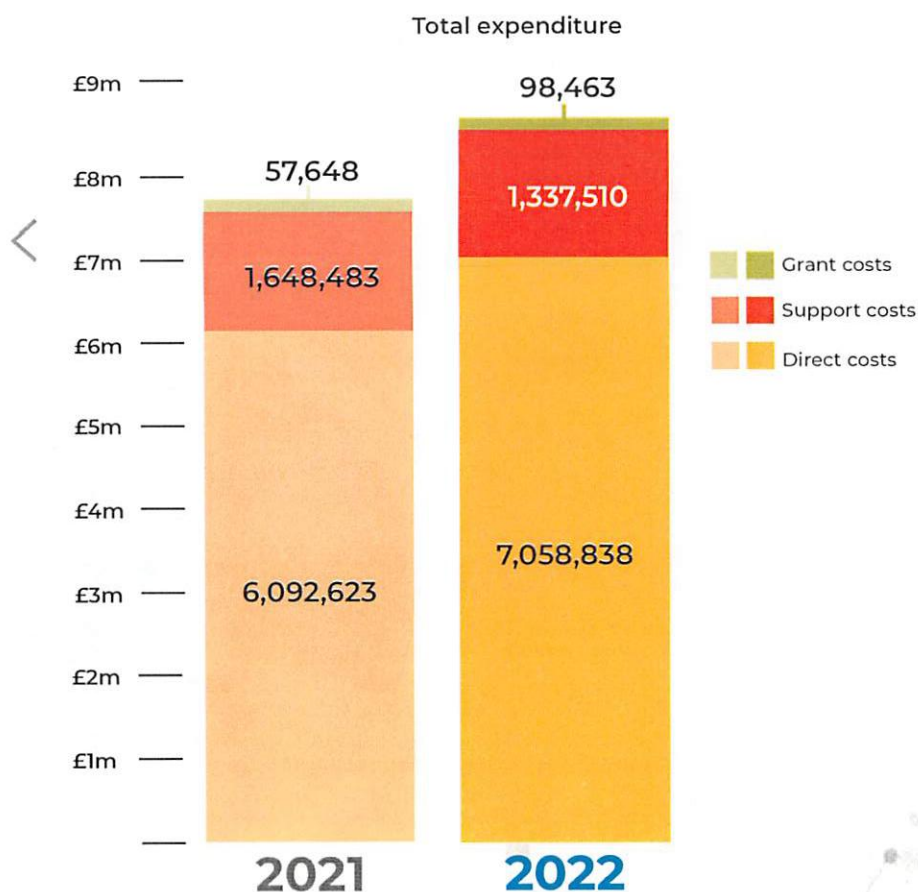
Expenditure

The activities undertaken in the year were carried out within the budget approved by the Trustees. All the expenditures were spent for CCDC's charitable purpose.

The total expenditure before pension adjustment in 2022 was **£8,494,811**, an increase of 9% on 2021 (£7,798,754).

A breakdown of the expenditure is shown below:

Direct costs are the costs resulted directly from undertaking the charitable activities, while support costs are the costs incurred to facilitate the activity. Direct Costs increased 16% in 2022 from £6.1m to £7.1m. It was largely due to increases in headcount, costs related to attending scientific conferences and software development outsourcing. Support costs decreased in 2022, despite increase to staff wages and salaries. This is due to a large gain in foreign exchange difference.



Staff Costs

Staff costs remain the largest expenditure for the CCDC. The total staff number increased from 97 to 102, between 1 January and 31 December 2022. Total staff costs in 2022 were **£6,900,740** (2021: £6,143,834), an increase of 12%. By the end of the year, we had filled most of the open positions in the Science Function, added one extra headcount to the Education and Outreach department and two new Product Managers. This enables us to focus on the science strategy in the coming years, improve our products in meeting user requirements and to reach out to a wider scientific community.

Staff costs remain the largest expenditure for the CCDC.

Other operating costs

The costs in maintenance of scientific equipment, including software and hardware, was **£342,139** in 2022, at a slight lower level to last year (2021: £362,116). The way of working has changed since 2020. CCDC adopted a hybrid working model, supporting staff to continue working remotely. We invested heavily into a new database architecture, collaborative working tools, cyber security, hardware and software. Costs for software have seen a higher than inflation increases lately. 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.

Pension Costs

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 recognise a liability for the contributions payable and the resulting expense in the income statement. Due to the change in USS membership at the CCDC and the higher interest rate (discount rate) used for the modeller, 2022 saw a favourable adjustment to the account, reducing pension liability provision by £2,351,229 (2021: increased liability £3,217,340). It significantly impacted the income statement, reducing staff costs by the same amount. Due to the significant variances this year, the movement has been split out from expenditure from charitable activities and is therefore not included in the totals above.

Costs in Attendance at scientific meetings have bounced back to pre-covid level. We spent £215,795 in 2021 attending relevant scientific conferences, providing workshops and visiting users. This enables us to support and engage with the user community more widely and easily. The grants for sponsoring research students were £98,463 this year (2021: £57,648). We sponsored two new students during 2022, two fewer than anticipated due to a delay in start date. They are due to join in 2023. We are currently co-sponsoring 13 students from 8 UK universities and 1 Italian university.

The CCDC holds an investment portfolio that is managed by Newton Investment Management. It produced an unrealised loss of £499,017 (2021: gain £945,035). This brought the overall financial performance of the CCDC to a surplus of £1,833,270 in 2022 (2021: deficit £2,404,250).

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

Financial review

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.

Fund performance calendar years %

| | 2022 | 2021 | 2020 | 2019 | 2018 |
|---|-------|-------|------|-------|-------|
| Newton Growth and Income Fund for Charities - Net | -5.27 | 18.54 | 1.55 | 18.34 | 1.08 |
| Newton Growth and Income Fund for Charities - Gross | -4.70 | 19.24 | 2.16 | 19.05 | -0.49 |
| Performance Benchmark* | -6.69 | 13.34 | 1.06 | 16.72 | -5.06 |

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.

2022 saw the most challenging time for investors since the outbreak of Covid-19 in 2020. The Russian invasion of Ukraine on 24th February 2022 was an obvious catalyst for market volatility. Global markets made respectable gains in Q4 after three consecutive quarters of declines. Although the Fund produced a negative return this year, it outperformed its performance benchmark. At the end of the year, the value of the portfolio was £6,370,627, representing an unrealised loss of £499,017. CCDC's investment strategy is investing for the long term. During the year, we received £142,968 investment income (2021: £139,470), which was not reinvested.

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 2022, CCDC's free reserve was **£3,453k (2021: £1,824k)**.

This is equivalent to almost 4 months of operating costs, lower than 50% of 2023 budgeted costs.

Our present position is:

| 31 Dec 2022 | |
|-------------------------------|---------|
| Unrestricted Reserves | £6,978k |
| Designated Funds | |
| Fixed Asset Fund | £2,324k |
| Research and Development Fund | £173k |
| Sponsorship and Outreach Fund | £20k |
| Pension provision Fund | £908k |
| Sustainability Fund | £100k |
| Free Reserves | £3,453k |



Structure and governance



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 2023).

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.

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 28th 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 9th 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), and the new Project Management Office (PMO). Other cross-functional teams or groups, such as the Wellbeing Committee and Culture Team, also exist.

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 the May and November 2022 Board meetings were hybrid meetings with people attending both in person and via video conference call. 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 financial performance, the investment performance and cash balances. The opportunity for all staff to interact with the Trustees is always encouraged and was specifically addressed as part of the on-site meetings. 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 2022, meetings of the Board Committees, Nomination, Audit, Risk, and Remuneration were held in accordance with their terms of reference.

Structure, management, and governance

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, productive, 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 are 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.

Management and staffing

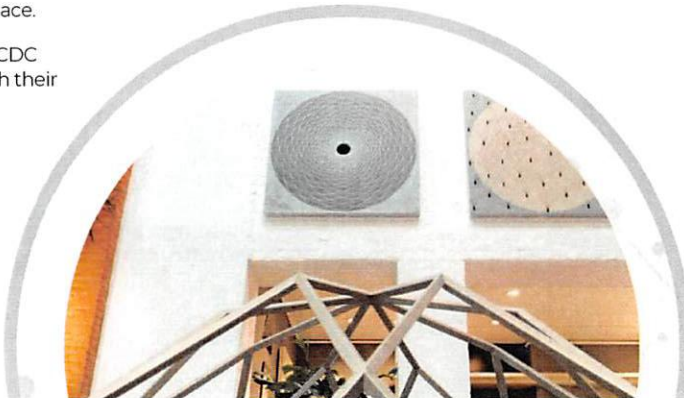
The day-to-day management of the CCDC is delegated by the Board of Trustees to the CEO and operational management is supported by the ELT and other managers who, in 2022, were:

| | |
|---------------------|---|
| Juergen Harter | Chief Executive Officer |
| Suzanna Ward | Head of Data and Community |
| Susan Reutzel-Edens | Head of Science |
| Jonathan Betts | Head of Commercial |
| James Ellis | Head of Operations |
| Bing-Bing Waterman | Head of Finance |
| Maggie Brown | Head of Human Resources and Organisational Design |

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.

Remuneration Policy

The Board of Trustees give their time freely and no Trustees received remuneration in the year. Details of Trustees' expenses are disclosed in Note 10 to the accounts. The Board of Trustees entrust the directing, controlling, running, and operation of the Charity to the CEO 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 organisation's pay policy and discusses trends in line with up-to-date benchmarking data provided by HR.



Structure, management, and governance

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 (hardware, software, and network) and cyber security
- Building: Infrastructure, Fire, Lease

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. Membership of the committee is kept under review. Day to day management of the risk register resides with the Head of Operations.

Key risks and mitigation measures are summarised in the table below:

| Threat type | Measure in place |
|--|---|
| Inadequate Staffing | Succession planning; salaries are reviewed and benchmarked annually; overall attractive benefit package; staff development opportunities. Supplementary staff payments were made in 2022 in order to address inflationary economic pressures. Such payments are kept under review by the leadership team. |
| 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, software products, and professional services. Additional community communications were used in 2022 to address risks arising from attempts at systematic data fraud. |
| University of Cambridge Relationship | We have a formal relationship with the University of Cambridge 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 users to ensure appropriate licences are in place for any party wishing to use AI/Machine Learning on the CSD. Mathematical models are already part of our software products. |

| Threat type | Measure in place |
|--|--|
| 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. We continue to invest in our Commercial team as we seek to increase revenues. In 2023, we aim to diversify our income through grant income. |
| Financial Fraud | Internal and external fraud risks are countered by defined processes requiring dual authorisation (e.g. payments), ongoing training (e.g. phishing message awareness) and insurance policies. |
| Changes in Foreign Exchange Rates | We operate foreign currency bank accounts 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 committee meetings 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. We received a positive review of our organisation by the Charity Commission in 2022. |
| Information Technology | Continuous availability of IT systems is critical to our global 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. We have various incident response plans to help re-establish services and benchmark ourselves against independent standards. |
| 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. |

Structure, management, and governance

Going concern

The COVID-19 world pandemic as well as more recent geopolitical events have 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 executive management team have been working hard to ensure CCDC as a global data repository and world-class research institute, is run in good sustainable fashion as a UK-based not-for-profit charity. CCDC's business model is diverse. Our users are spread across academic research institutions and large pharmaceutical companies as well as more recently, many new biotech. The database and its associated software products and services are distributed and digitally delivered globally, to over 80 countries worldwide and growing. 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-on-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. Our products and services we provide can be delivered electronically. We have built up excellent hybrid/flexible/remote working

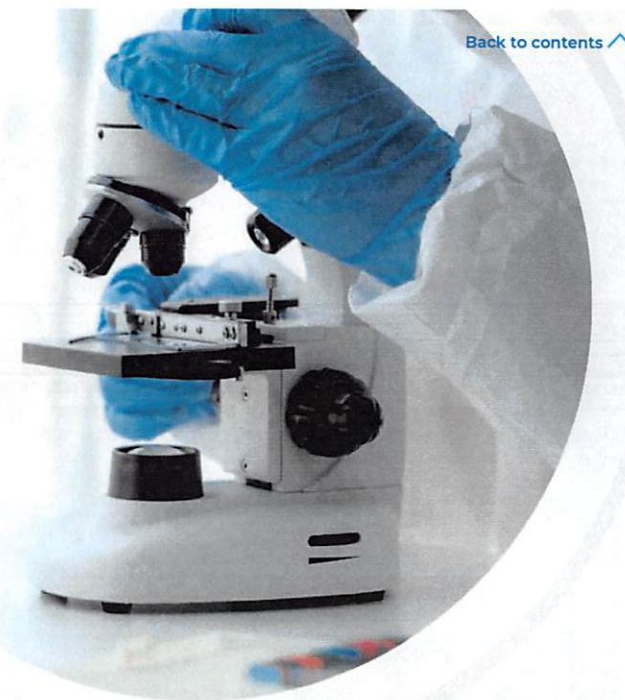
At the date of writing, we have visibility of almost 88% of the 2023 budget target in revenue.

capabilities accompanied by a good work environment, and we are global in nature as an organisation. CCDC's productivity remains high and we are very agile and dynamic in how we deliver our digital products and services, to all geographies and time zones.

We are committed to do all we can to support our staff and ensure they are adequately trained and up-skilled. We provided necessary equipment for the further optimisation 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. In 2022 we have built a new workplace well-being framework, along with the establishment of workplace well-being champions. We will continue to deploy helpful and supportive activities, touching eight key dimensions of wellbeing.

At the date of writing, we have visibility of almost 88% of the 2023 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. 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.



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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 & discovery, pharmaceutical development & manufacturing, and data-based structural research may lead to increased demand for CCDC's products and services. This is especially true for the field of artificial intelligence, where new advances

mean companies are eager to leverage high-quality data—like the Cambridge Structural Database (CSD)—in their algorithms and models (e.g. machine learning and deep learning / neural nets).

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 have returned to their labs at universities, it is likely they will continue to appreciate flexible educational materials and being able to run and access information from their homes. Between our online educational resources and digital-first software offerings, we are ready to meet the evolving needs of the academic scientific community.

Looking to the future



Looking into the future

Looking into the mid-term future (two to three years), the CCDC will endeavour to grow our modern, more user-friendly, and adaptive website (with a view to eventually establish an eCommerce platform and revamped knowledge portal to serve the scientific community even better).

Over 2022, we worked with an agency to design, build, and launch our new website. Expert project management from our new Project Management Office (PMO) has given us the project discipline to deliver effectively. CCDC's new website will underpin all the interactions with the end users and community, along with appropriate calls to action. We are deploying ongoing effort to help deliver and categorize any of the information and materials created from the last decades, in modern and fresh ways, plus host the new information in an organised, easily navigable, and searchable way for the coming years. This is important for future-proofing CCDC's online experience and to meet CCDC's goals around automation and optimisation. 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, we reflected what else will be needed to continue to work with and further optimise the membership and operational running of the SAB. Usually 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. We are evolving this setup to see how we can make this more interactive, and ensuring that all our diverse scientific areas are regularly and adequately covered by world experts, from both industry and academic, commercial and non-commercial backgrounds.

Over 2022, we worked with an agency to design, build, and launch our **new website**.

Our Operations function has a clear purpose to enable us to define and start delivering against objectives that will improve the effectiveness of our systems/processes for staff and end-users. Operations will continue to drive operational efficiencies, and help us reach higher levels of automation over time in all of CCDC's functions. We are working on several business transformation programmes: for example HR Business Processes, CRM/Hubspot, and more improvements to the website, as well as all our social media platforms. These programmes are challenging 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 better creates and maximises value to users. A key theme to support our processes will be boosting quality even further. 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 users. Process definition within a QMS context will help us identify the most appropriate software and platform solutions to facilitate the scale of our organisation, for example Enterprise Resource Planning (ERP) solution to span all functions, CRM/HubSpot, e-commerce, and others. As these bigger initiatives require dedicated project management, the growing Project Management Office is there to define and demonstrate best practices, and to ultimately deliver the required results to time, cost, and quality.

Operations will also continue to adopt best-practice agile software development, investing in new roles to allow this approach to be better realised, keeping our architectural approach under review and utilising 3rd parties where it is most efficient to do so. For example, we will use a 3rd party to improve the User Experience and User Interface of our customer-facing software. Such approaches are intended to help scale our not-for-profit charity.

We will continue to run the CCDC in growth and value creation mode in order to achieve more of our charitable aims faster, turning the CCDC into a more agile organisation 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 £8.4m top-line revenue and average 98 employees in 2022 to £10m revenue and 111 employees in 2023 and on to ~£15m revenue and 140+ employees by the end of 2024. We will focus on delivering excellent value to all our stakeholders with a sense of urgency to a growing set of existing and new users in the biopharmaceutical, chemistry, and biotech sectors, as well as other industries such as agrochemical, petrochemical, and advanced & functional 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.

Looking into the future

We will widen our reach, increase user engagement and customer centricity, and enable this growth by further growing the commercial function, the science and data functions. New initiatives in marketing, product & services management, channel management, partnerships and alliances, and service delivery will all play a role to create more value.

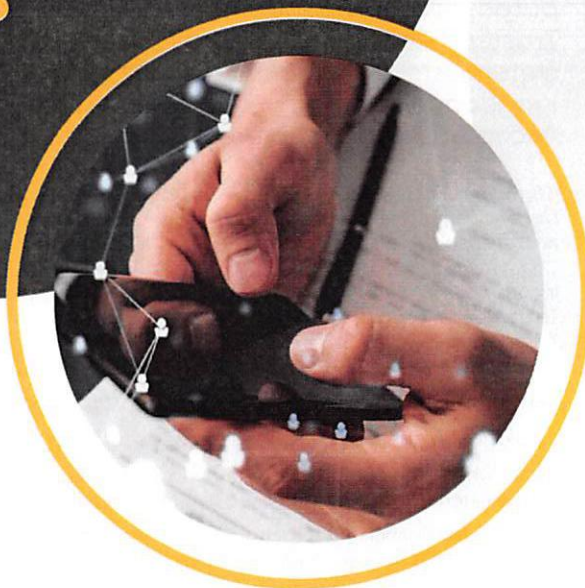
Any generated surplus from the resulting growth will be reinvested in advancing science, data accessibility, and utility; improving our products and services experiences (UX/UI); growing education and outreach efforts globally; and optimising and scaling up through our skilled people, systems, and processes. 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.

Structural science (structural chemistry and biology) has a crucial role to play in battling human and animal diseases. As a community, we need to be versatile and innovative in our approaches to ensure rapid response, and new scientific progress based on knowledge/data driven insights. 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 development and manufacturing.

The world post Covid-19 has evolved 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 adapted to the model very well. We intend to further pioneer a digital experience by leading the way with high-quality data and scientific software that is accessible from anywhere in the world via the cloud, and a stronger and more seamless end user experience. 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.

We believe
a digital-first approach that saves time and resources on the experimental phase will become increasingly important in the coming years.

Administrative details



Trustees

Dr David Martinsen, Chair to May 2022

Professor Alessia Bacchi, Vice Chair to May 2022

Ms Judith N Currano (Retired May 2022)

Professor Jonathan M Goodman, Appointed Chair May 2022

Professor John P Overington

Dr Nigel Pitchford

Professor Susan Bourne, Appointed Vice Chair May 2022

Professor Ola Engkvist

Dr Ye Li (Appointed May 2022)

Chief Executive Officer

Dr Juergen Harter

Company & Charity Registration

Company registered number **02155347**

Charity registered number **800579**

Registered office **12 Union Road, Cambridge CB2 1EZ**

Auditors, Bank, Solicitors and Investment advisers

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 Road
Cambridge
CB1 2JHS

Investment Advisers

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

Statement of Trustees' responsibilities

Statement of Trustees' responsibilities

For the year ended 31 December 2022

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 year. 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 judgments 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 Group will continue in business.

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.

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

Professor J M Goodman

Trustee

Date:

29 September 2023

DocuSigned by:

Jonathan Goodman

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Independent auditors' report

The logo for Peters Elworthy & Moore, consisting of the lowercase letters 'pem' in a white, sans-serif font, centered within a large orange circle.

Peters Elworthy & Moore
Chartered Accountants



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 2022 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 2022 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 Trustee's 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 Trustee 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

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

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

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 Trustee's Report including the Strategic Report for the financial year for which the financial statements are prepared is consistent with the financial statements.
- the Trustee's 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 Trustee's 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 Trustee's 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 Trustee's 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

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
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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 Responsible Individual 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 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 and taxation legislation, as well as laws and regulations relating to operations such as data protection and employment 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.

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.

We discussed among the engagement team the opportunities and incentives that may exist within the organisation for fraud and how and where fraud might occur in the financial statements.

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

- tested the appropriateness of journal entries and other adjustments.
- designed procedures to identify unexpected and unusual journal entries and performed testing to confirm the validity of such postings.
- assessed whether the accounting judgements and estimates made in the financial statements, as detailed in Note 1.17, were indicative of potential bias.
- evaluated the business rationale of any significant transactions that were unusual or outside the normal course of business.

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

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

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

- 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.

DocuSigned by:

Kathryn Hebden

C8E87A7C9189472

Kathryn Hebden (Senior Statutory Auditor)

for and on behalf of
Peters Elworthy & Moore
Chartered Accountants
Statutory Auditors
Salisbury House
Station Road
Cambridge
CB1 2LA

Date: 29 September 2023

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 2022

| | Note | Unrestricted funds 2022 £ | Restricted funds 2022 £ | Total funds 2022 £ | As restated Total funds 2021 £ |
|--|------|---------------------------------|-------------------------------|--------------------------|---|
| INCOME FROM: | | | | | |
| Donations and legacies | 2 | 7,160 | - | 7,160 | - |
| Charitable activities | 3 | 7,767,674 | 111,866 | 7,879,430 | 7,092,611 |
| Other trading activities | 5 | 407,919 | - | 407,919 | 430,176 |
| Investments | 6 | 143,776 | - | 143,776 | 140,197 |
| TOTAL INCOME | | 8,326,419 | 111,866 | 8,438,275 | 7,662,984 |
| EXPENDITURE ON: | | | | | |
| Charitable activities | 8 | 8,300,834 | 193,977 | 8,494,811 | 7,798,754 |
| Other expenditure | 7 | (2,351,229) | - | (2,351,229) | 3,217,340 |
| TOTAL EXPENDITURE | | 5,949,605 | 193,977 | 6,143,582 | 11,016,094 |
| NET INCOME/(EXPENDITURE) BEFORE NET (LOSSES)/GAINS ON INVESTMENTS | | 2,376,814 | (82,121) | 2,294,693 | (3,353,110) |
| Net (losses)/gains on investments | 13 | (499,017) | - | (499,017) | 945,035 |
| NET INCOME/(EXPENDITURE) | | 1,877,797 | (82,121) | 1,795,676 | (2,408,075) |
| Transfers between funds | 19 | (63,864) | 63,864 | - | - |
| NET MOVEMENT IN FUNDS BEFORE OTHER RECOGNISED GAINS | | 1,813,943 | (18,267) | 1,795,676 | (2,408,075) |
| OTHER RECOGNISED GAINS: | | | | | |
| Other gains | | 37,694 | - | 37,694 | 3,825 |
| NET MOVEMENT IN FUNDS | | 1,851,537 | (18,267) | 1,833,270 | (2,404,250) |
| RECONCILIATION OF FUNDS: | | | | | |
| Total funds brought forward | | 5,126,152 | 39,167 | 5,165,319 | 7,569,569 |
| Net movement in funds | | 1,851,537 | (18,267) | 1,833,270 | (2,404,250) |
| TOTAL FUNDS CARRIED FORWARD | | 6,977,689 | 20,900 | 6,998,589 | 5,165,319 |

The Consolidated Statement of Financial Activities includes all gains and losses recognised in the year. The notes on pages 67 to 97 form part of these financial statements.

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
(A Company Limited by Guarantee)
REGISTERED NUMBER: 02165347

CONSOLIDATED BALANCE SHEET
AS AT 31 DECEMBER 2022

| | Note | 2022 £ | 2021 £ |
|---|------|-------------------|-------------------|
| FIXED ASSETS | | | |
| Tangible assets | 12 | 2,324,407 | 2,002,697 |
| Investments | 13 | 6,370,627 | 6,869,644 |
| | | 8,695,034 | 8,872,341 |
| CURRENT ASSETS | | | |
| Debtors | 14 | 2,648,811 | 2,433,077 |
| Cash at bank and in hand | | 4,066,542 | 3,415,237 |
| | | 6,715,353 | 5,848,314 |
| Creditors: amounts falling due within one year | 15 | (5,323,915) | (4,131,653) |
| NET CURRENT ASSETS | | 1,391,438 | 1,716,661 |
| TOTAL ASSETS LESS CURRENT LIABILITIES | | 10,086,472 | 10,589,002 |
| Creditors: amounts falling due after more than one year | 16 | (191,651) | (226,534) |
| Provisions for liabilities | 17 | (2,896,332) | (5,197,149) |
| TOTAL NET ASSETS | | 6,998,589 | 5,165,319 |
| CHARITY FUNDS | | | |
| Restricted funds | 19 | 20,900 | 39,167 |
| Unrestricted funds | 19 | 6,977,689 | 5,126,152 |
| TOTAL FUNDS | | 6,998,589 | 5,165,319 |

The Trustee 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 Trustee and signed on their behalf by:

DocuSigned by:
Jonathan Goodman
2887775F937D4D5...
Professor J M Goodman

Date: 29 September 2023

The notes on pages 67 to 97 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 2022

| | Note | 2022 £ | 2021 £ |
|---|------|-------------------------|-------------------------|
| FIXED ASSETS | | | |
| Tangible assets | 12 | 2,324,407 | 2,002,697 |
| Investments | 13 | 6,534,116 | 7,033,133 |
| | | <u>8,858,523</u> | <u>9,035,830</u> |
| CURRENT ASSETS | | | |
| Debtors | 14 | 3,008,821 | 2,882,309 |
| Cash at bank and in hand | | 3,534,240 | 2,613,738 |
| | | <u>6,543,061</u> | <u>5,496,047</u> |
| Creditors: amounts falling due within one year | 15 | (5,515,135) | (4,090,917) |
| NET CURRENT ASSETS | | <u>1,027,926</u> | <u>1,405,130</u> |
| TOTAL ASSETS LESS CURRENT LIABILITIES | | <u>9,886,449</u> | <u>10,440,960</u> |
| Creditors: amounts falling due after more than one year | 16 | (191,551) | (226,534) |
| Provisions for liabilities | 17 | (2,896,332) | (5,197,149) |
| TOTAL NET ASSETS | | <u><u>6,798,566</u></u> | <u><u>5,017,277</u></u> |
| CHARITY FUNDS | | | |
| Restricted funds | 19 | 20,900 | 39,167 |
| Unrestricted funds | 19 | 6,777,666 | 4,978,110 |
| TOTAL FUNDS | | <u><u>6,798,566</u></u> | <u><u>5,017,277</u></u> |

The Charity's net movement in funds for the year was £1,781,289 (2021 - £(2,430,284)).

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

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
(A Company Limited by Guarantee)
REGISTERED NUMBER: 02155347

CHARITY BALANCE SHEET (CONTINUED)
AS AT 31 DECEMBER 2022

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

DocuSigned by:
Jonathan Goodman
2887775E9370AD5
Professor J M Goodman

Date: 29 September 2023

The notes on pages 67 to 97 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 2022

| | Note | 2022 £ | 2021 £ |
|--|------|------------------|------------------|
| CASH FLOWS FROM OPERATING ACTIVITIES | | | |
| Net cash used in operating activities | 21 | 944,270 | 180,254 |
| CASH FLOWS FROM INVESTING ACTIVITIES | | | |
| Dividends, interests and rents from investments | | 143,776 | 140,197 |
| Purchase of tangible fixed assets | | (436,741) | (105,263) |
| Foreign exchange on fixed assets | | - | 887 |
| NET CASH (USED IN)/PROVIDED BY INVESTING ACTIVITIES | | (292,965) | 35,821 |
| CHANGE IN CASH AND CASH EQUIVALENTS IN THE YEAR | | 651,305 | 216,075 |
| Cash and cash equivalents at the beginning of the year | 22 | 3,416,237 | 3,199,162 |
| CASH AND CASH EQUIVALENTS AT THE END OF THE YEAR | 22 | 4,066,542 | 3,415,237 |

The notes on pages 67 to 97 form part of these financial statements

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

NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022

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 undertakings. The results of the subsidiaries 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 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.

1.4 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 continuously review the trends in the biopharmaceutical market and wider growth trends in the technology and science fields. CCDC's data and scientific software offerings remain in good demand, and can furthermore help address new trends such as artificial intelligence, and the investments that are going into those efforts. The Trustees have a reasonable expectation that the charity has adequate resources to continue operational existence for at least 12 months. For this reason, the charity continues to adopt the going concern basis in preparing its financial statements.

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

**NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022**

1. ACCOUNTING POLICIES (CONTINUED)

1.5 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.

1.6 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 charity and compliance with constitutional and statutory requirements.

Charitable activities and governance costs are costs incurred on the charity'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.

1.7 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.

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

**NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022**

1. ACCOUNTING POLICIES (CONTINUED)

1.8 TAXATION

The Charity is considered to pass the tests set out in Paragraph 1 Schedule 6 of the Finance Act 2010 and therefore it meets the definition of a charitable company for UK corporation tax purposes. Accordingly, the Charity is potentially exempt from taxation in respect of income or capital gains received within categories covered by Chapter 3 Part 11 of the Corporation Tax Act 2010 or Section 256 of the Taxation of Chargeable Gains Act 1992, to the extent that such income or gains are applied exclusively to charitable purposes.

1.9 TANGIBLE FIXED ASSETS AND DEPRECIATION

Tangible fixed assets costing £10,000 or more are capitalised and recognised when future economic benefits are probable and the cost or value of the asset can be measured reliably.

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 |

1.10 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.

1.11 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.

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

**NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022**

1. ACCOUNTING POLICIES (CONTINUED)

1.12 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.

1.13 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 in the Consolidated Statement of Financial Activities as a finance cost.

1.14 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.

1.15 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.

The Charity operates a defined contribution plan for its employees. A defined contribution plan is a pension plan under which the Company pays fixed contributions into a separate entity. Once the contributions have been paid the Company has no further payment obligations.

The contributions are recognised as an expense in profit or loss when they fall due. Amounts not paid are shown in accruals as a liability in the Balance Sheet. The assets of the plan are held separately from the Company in independently administered funds.

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

**NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022**

1. ACCOUNTING POLICIES (CONTINUED)

1.16 FUND ACCOUNTING

General funds are unrestricted funds which are available for use at the discretion of the Trustee 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 Trustee 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.

1.17 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 judgement:

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 DONATIONS AND LEGACIES

| Unrestricted funds 2022 £ | Total funds 2022 £ | Total funds 2021 £ |
|------------------------------------|-----------------------------|-----------------------------|
|------------------------------------|-----------------------------|-----------------------------|

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

**NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022**

2. INCOME FROM DONATIONS AND LEGACIES

| | Unrestricted funds 2022 £ | Total funds 2022 £ | Total funds 2021 £ |
|-----------|------------------------------------|-----------------------------|-----------------------------|
| Donations | 7,150 | 7,150 | - |

3. INCOME FROM CHARITABLE ACTIVITIES

| | Unrestricted funds 2022 £ | Restricted funds 2022 £ | Total funds 2022 £ | As restated Total funds 2021 £ |
|---|------------------------------------|----------------------------------|-----------------------------|--|
| Scientific Activity - Subscription Fees | 7,767,574 | 111,856 | 7,879,430 | 7,092,611 |
| TOTAL 2021 AS RESTATED | 6,928,500 | 164,111 | 7,092,611 | |

4. TURNOVER

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

A geographical split of turnover is disclosed as follows: United Kingdom 21% (2021 - 19%), Other EU 26% (2021 - 21%) and Rest of the World 53% (2021 - 60%).

5. INCOME FROM TRADING ACTIVITIES

Income from non charitable trading activities

| | Unrestricted funds 2022 £ | Total funds 2022 £ | Total funds 2021 £ |
|-------------------|------------------------------------|-----------------------------|-----------------------------|
| Sales | 407,919 | 407,919 | 430,176 |
| TOTAL 2021 | 430,176 | 430,176 | |

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5. INCOME FROM TRADING ACTIVITIES (CONTINUED)

Income from non charitable trading activities (CONTINUED)

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 11.

6. INVESTMENT INCOME

| | Unrestricted funds 2022 £ | Total funds 2022 £ | Total funds 2021 £ |
|----------------------------------|------------------------------------|-----------------------------|-----------------------------|
| Investment income | 142,968 | 142,968 | 139,470 |
| Bank & other interest receivable | 808 | 808 | 727 |
| TOTAL 2021 | 140,197 | 140,197 | |

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NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022

7. OTHER EXPENDITURE

| | Unrestricted funds 2022 £ | Total funds 2022 £ | Total funds 2021 £ |
|--|------------------------------------|-----------------------------|-----------------------------|
| USS pension provision movement (note 25) | (2,351,229) | (2,351,229) | 3,217,340 |
| TOTAL 2021 | 3,217,340 | 3,217,340 | |

8. ANALYSIS OF EXPENDITURE BY ACTIVITIES

| | Activities undertaken directly 2022 £ | Grant funding of activities 2022 £ | Support costs 2022 £ | Total funds 2022 £ | Total funds 2021 £ |
|-----------------------|---|--|-------------------------------|-----------------------------|-----------------------------|
| Scientific Activities | 7,058,838 | 98,463 | 1,337,510 | 8,494,811 | 7,798,754 |
| TOTAL 2021 | 6,092,623 | 57,648 | 1,648,483 | 7,798,754 | |

In 2022, restricted expenditure amounted to £193,977 (2021: £207,808) and unrestricted expenditure was £8,300,834 (2021: £7,587,121).

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NOTES TO THE FINANCIAL STATEMENTS
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8. ANALYSIS OF EXPENDITURE BY ACTIVITIES (CONTINUED)

ANALYSIS OF DIRECT COSTS

| | Total funds 2022 £ | Total funds 2021 £ |
|-------------------------------------|-----------------------------|-----------------------------|
| Wages and salaries | 6,111,848 | 5,446,167 |
| Attendance at scientific meetings | 215,795 | 75,645 |
| Legal and other professional fees | 10,326 | - |
| Consultants | 320,545 | 123,176 |
| Maintenance of scientific equipment | 342,139 | 362,116 |
| Production and distribution costs | 74,390 | 85,411 |
| Difference on foreign exchange | (59,859) | (1,558) |
| Staff development | 43,654 | 1,666 |
| | 7,058,838 | 6,092,623 |

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8. ANALYSIS OF EXPENDITURE BY ACTIVITIES (CONTINUED)

ANALYSIS OF SUPPORT COSTS

| | Total funds 2022 £ | Total funds 2021 £ |
|--|-----------------------------|-----------------------------|
| Staff costs | 788,892 | 697,667 |
| Depreciation | 115,031 | 126,434 |
| Consultancy | 26,710 | 57,001 |
| Telephone and network costs | 14,762 | 14,381 |
| Recruitment | 127,787 | 132,503 |
| Legal and other professional fees | 88,552 | 119,961 |
| Audit and accountancy | 67,510 | 55,327 |
| Banking costs | 3,967 | 5,660 |
| Difference on foreign exchange | (311,650) | 91,729 |
| Insurance | 57,355 | 52,553 |
| Premises costs | 158,809 | 200,518 |
| Bad debt expense | 2,114 | 6,963 |
| IT equipment, software and hardware | 21,669 | 16,721 |
| General expenses | 40,329 | 21,654 |
| Staff development | 44,992 | 35,063 |
| Finance cost of unwinding of discounting | 50,412 | 14,348 |
| Board meeting costs | 40,269 | - |
| | <u>1,337,510</u> | <u>1,648,483</u> |

9. ANALYSIS OF GRANTS

| | Grants to Institutions 2022 £ | Total funds 2022 £ | Total funds 2021 £ |
|------------|--|-----------------------------|-----------------------------|
| Grants | <u>98,463</u> | <u>98,463</u> | <u>57,648</u> |
| TOTAL 2021 | <u>57,648</u> | <u>57,648</u> | |

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**NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022**

9. ANALYSIS OF GRANTS (CONTINUED)

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

| | 2022 £ | 2021 £ |
|---------------------------------|---------------|---------------|
| NAME OF INSTITUTION | | |
| University of Leeds | - | 16,000 |
| University of Southampton | 40,000 | - |
| Polytechnic University of Turin | 30,218 | - |
| University of Sheffield | - | 39,273 |
| Other immaterial grant costs | 500 | 2,375 |
| | <u>70,718</u> | <u>57,648</u> |
| Other grants to institutions | <u>27,745</u> | <u>-</u> |
| | <u>98,463</u> | <u>57,648</u> |

10. AUDITORS' REMUNERATION

| | 2022 £ | 2021 £ |
|--|--------------|--------------|
| Fees payable to the Charity's auditor in respect of: | | |
| Audit of the Charity's annual accounts | 30,494 | 22,673 |
| All taxation advisory services not included above | 3,037 | 7,545 |
| All non-audit services not included above | <u>9,035</u> | <u>9,490</u> |

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

Staff costs were as follows:

| | Group 2022 £ | Group 2021 £ | Charity 2022 £ | Charity 2021 £ |
|--|--------------------|--------------------|----------------------|----------------------|
| Wages and salaries | 5,316,818 | 4,725,564 | 4,779,605 | 4,328,716 |
| Social security costs | 592,600 | 512,095 | 503,724 | 436,181 |
| Other pension costs | 991,322 | 906,175 | 939,294 | 865,876 |
| USS pension provision movement (note 24) | (2,351,229) | 3,217,340 | (2,351,229) | 3,217,340 |
| | <u>4,649,511</u> | <u>9,361,174</u> | <u>3,871,294</u> | <u>8,848,113</u> |

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
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NOTES TO THE FINANCIAL STATEMENTS
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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 2022 No. | Group 2021 No. | Charity 2022 No. | Charity 2021 No. |
|---------------------------|----------------------|----------------------|------------------------|------------------------|
| Office and Administration | 9 | 9 | 8 | 8 |
| Technical | 89 | 80 | 82 | 74 |
| | <u>98</u> | <u>89</u> | <u>90</u> | <u>82</u> |

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

| | Group 2022 No. | Group 2021 No. |
|---------------------------------|----------------------|----------------------|
| In the band £60,001 - £70,000 | 7 | 7 |
| In the band £70,001 - £80,000 | 6 | 5 |
| In the band £80,001 - £90,000 | 5 | 7 |
| In the band £90,001 - £100,000 | - | 1 |
| In the band £100,001 - £110,000 | 1 | - |
| In the band £110,001 - £120,000 | 2 | - |
| In the band £130,001 - £140,000 | 1 | - |
| In the band £150,001 - £160,000 | - | 1 |
| In the band £160,001 - £170,000 | 1 | 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 (2021 - £NIL). The total employee benefits of the key management personnel, including employers' NIC and employers pension of the charity were £1,127,136 (2021 - £1,039,750).

A total of £9,371 (2021 - £NIL) was reimbursed or paid directly to 7 (2021 - 0) trustees in respect of travel and accommodation costs.

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NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022

12. TANGIBLE FIXED ASSETS

GROUP AND CHARITY

| | Long-term leasehold property £ | Fixtures and fittings £ | Other fixed assets £ | Total £ |
|---------------------------|---|-------------------------------|----------------------------|------------------|
| COST | | | | |
| At 1 January 2022 | 3,966,255 | 732,369 | 105,263 | 4,803,887 |
| Additions | - | - | 436,741 | 436,741 |
| Disposals | - | (5,708) | - | (5,708) |
| Foreign exchange movement | - | 457 | - | 457 |
| At 31 December 2022 | <u>3,966,255</u> | <u>727,118</u> | <u>542,004</u> | <u>5,235,377</u> |
| DEPRECIATION | | | | |
| At 1 January 2022 | 2,154,996 | 646,194 | - | 2,801,190 |
| Charge for the year | 79,325 | 35,706 | - | 115,031 |
| On disposals | - | (5,708) | - | (5,708) |
| Foreign exchange movement | - | 457 | - | 457 |
| At 31 December 2022 | <u>2,234,321</u> | <u>676,649</u> | <u>-</u> | <u>2,910,970</u> |
| NET BOOK VALUE | | | | |
| At 31 December 2022 | <u>1,731,934</u> | <u>50,469</u> | <u>542,004</u> | <u>2,324,407</u> |
| At 31 December 2021 | <u>1,811,259</u> | <u>86,175</u> | <u>105,263</u> | <u>2,002,697</u> |

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
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NOTES TO THE FINANCIAL STATEMENTS
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13. FIXED ASSET INVESTMENTS

| GROUP | Listed investments £ |
|----------------------------|----------------------------|
| COST OR VALUATION | |
| At 1 January 2022 | 6,869,644 |
| Revaluations | (499,017) |
| AT 31 DECEMBER 2022 | 6,370,627 |

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 2022 | 163,489 | 6,869,644 | 7,033,133 |
| Revaluations | - | (499,017) | (499,017) |
| AT 31 DECEMBER 2022 | 163,489 | 6,370,627 | 6,534,116 |

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NOTES TO THE FINANCIAL STATEMENTS
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13. FIXED ASSET INVESTMENTS (CONTINUED)

PRINCIPAL SUBSIDIARIES

The following were subsidiary undertakings of the Charity:

| Names | 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. |
| CCDC Inc | | One Boston Place, Suite 2600, Boston, MA 02108, United States | Provision of professional services for digital drug design and manufacture, and advanced training. |

| Class of shares | Holding | Included in consolidation |
|--------------------|---------|------------------------------|
| Ordinary | 100% | Yes |

| | | |
|---------|------|-----|
| Capital | 100% | Yes |
|---------|------|-----|

The financial results of the subsidiaries for the year were:

| Names | Income £ | Expenditure £ | Profit for the year £ | Net assets £ |
|-----------------------|-------------|------------------|-----------------------------|-----------------|
| CCDC Services Limited | 407,921 | (73,578) | 334,343 | 2,118 |
| CCDC Inc | 784,278 | (731,520) | 52,758 | (362,171) |

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NOTES TO THE FINANCIAL STATEMENTS
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14. DEBTORS

| | Group 2022 £ | Group 2021 £ | Charity 2022 £ | Charity 2021 £ |
|------------------------------------|--------------------|--------------------|----------------------|----------------------|
| DUE WITHIN ONE YEAR | | | | |
| Trade debtors | 2,165,037 | 2,092,430 | 2,038,805 | 1,986,206 |
| Amounts owed by group undertakings | - | - | 507,899 | 586,580 |
| Other debtors | 29,604 | 48,867 | 29,161 | 46,097 |
| Prepayments and accrued income | 454,170 | 291,780 | 432,956 | 283,446 |
| | <u>2,648,811</u> | <u>2,433,077</u> | <u>3,008,821</u> | <u>2,882,309</u> |

15. CREDITORS: AMOUNTS FALLING DUE WITHIN ONE YEAR

| | Group 2022 £ | Group 2021 £ | Charity 2022 £ | Charity 2021 £ |
|------------------------------------|--------------------|--------------------|----------------------|----------------------|
| Trade creditors | 126,695 | 99,031 | 122,283 | 94,108 |
| Amounts owed to group undertakings | - | - | 260,130 | 58,177 |
| Other taxation and social security | 229,828 | 182,226 | 211,356 | 166,507 |
| Other creditors | 127,760 | 153,984 | 127,760 | 153,984 |
| Accruals and deferred income | 4,839,632 | 3,696,412 | 4,793,606 | 3,618,141 |
| | <u>5,323,915</u> | <u>4,131,653</u> | <u>5,515,135</u> | <u>4,090,917</u> |

| | Group 2022 £ | Group 2021 £ | Charity 2022 £ | Charity 2021 £ |
|--|--------------------|--------------------|----------------------|----------------------|
| Deferred income at 1 January 2022 | 3,549,573 | 2,938,109 | 3,492,679 | 2,888,318 |
| Resources deferred during the year | 4,904,595 | 3,549,573 | 4,879,595 | 3,492,679 |
| Amounts released from previous periods | (3,549,573) | (2,938,109) | (3,492,679) | (2,888,318) |
| | <u>4,904,595</u> | <u>3,549,573</u> | <u>4,879,595</u> | <u>3,492,679</u> |

Deferred income relates to subscriptions received in advance.

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NOTES TO THE FINANCIAL STATEMENTS
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16. CREDITORS: AMOUNTS FALLING DUE AFTER MORE THAN ONE YEAR

| | Group 2022 £ | Group 2021 £ | Charity 2022 £ | Charity 2021 £ |
|------------------------------|--------------------|--------------------|----------------------|----------------------|
| Other creditors | 22,149 | 86,864 | 22,149 | 86,864 |
| Accruals and deferred income | 169,402 | 139,670 | 169,402 | 139,670 |
| | <u>191,551</u> | <u>226,534</u> | <u>191,551</u> | <u>226,534</u> |

17. PROVISIONS

GROUP AND CHARITY

| | Pension deficit funding provision £ |
|-------------------|---|
| At 1 January 2022 | 5,197,149 |
| Additions | (2,300,817) |
| | <u>2,896,332</u> |

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 3.33% (2021 - 0.97%) 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.

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18. PRIOR YEAR ADJUSTMENTS

The accounting policy for the recognition of free subventions as a gift in kind has been reviewed during the year. It was concluded that the free subventions did not meet the definition of a gift in kind and therefore a prior year adjustment has been made to reduce income and expenditure by the value of the free subventions.

The effects on the Group are summarised below:

The retail value of the free subventions gifted in the prior year was £163,475

Total income for the year ended 31 December 2021 as previously reported: £7,826,459

Total income for the year ended 31 December 2021 following restatement: £7,662,984

Total expenditure for the year ended 31 December 2021 as previously reported: £11,175,744

Total expenditure for the year ended 31 December 2021 following restatement: £11,016,094

There is £nil impact on the net deficit and net assets in the year due to it being a gift in kind.

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19. STATEMENT OF FUNDS

STATEMENT OF FUNDS - CURRENT YEAR

| | Balance at 1 January 2022 £ | Income £ | Expenditure £ | Transfers in/out £ | Gains/ (Losses) £ | Balance at 31 December 2022 £ |
|---------------------------------|--------------------------------------|------------------|--------------------|--------------------------|-------------------------|---|
| UNRESTRICTED FUNDS | | | | | | |
| DESIGNATED FUNDS | | | | | | |
| Fixed Asset Fund | 2,002,697 | - | (115,031) | 436,741 | - | 2,324,407 |
| Research and Development Fund | 173,406 | - | - | - | - | 173,406 |
| Sponsorship and Outreach Fund | 118,352 | - | (98,230) | - | - | 20,122 |
| CSD and Sustainability Fund | 100,086 | - | - | - | - | 100,086 |
| Pension Provision Fund | 908,000 | - | - | - | - | 908,000 |
| | 3,302,541 | - | (213,261) | 436,741 | - | 3,526,021 |
| GENERAL FUNDS | | | | | | |
| General Funds | 1,823,611 | 8,326,419 | (5,736,344) | (500,595) | (461,423) | 3,451,668 |
| TOTAL UNRESTRICTED FUNDS | 5,126,152 | 8,326,419 | (5,949,605) | (63,854) | (461,423) | 6,977,689 |

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19. STATEMENT OF FUNDS (CONTINUED)

RESTRICTED
FUNDS

| | | | | | | |
|--------------------------|------------------|------------------|--------------------|---------------|------------------|------------------|
| BBSRC Student grant fund | - | - | - | - | - | - |
| DDA Grant | - | 44,137 | (73,562) | 29,425 | - | - |
| DIDCOM Grant | - | 51,644 | (86,073) | 34,429 | - | - |
| BioChem GRAPH | 39,167 | 16,075 | (34,342) | - | - | 20,900 |
| | <u>39,167</u> | <u>111,856</u> | <u>(193,977)</u> | <u>63,854</u> | <u>-</u> | <u>20,900</u> |
| TOTAL OF FUNDS | <u>5,165,319</u> | <u>8,438,275</u> | <u>(6,143,582)</u> | <u>-</u> | <u>(461,423)</u> | <u>6,998,589</u> |

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19. STATEMENT OF FUNDS (CONTINUED)

STATEMENT OF FUNDS - PRIOR 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 |
| | <u>3,118,247</u> | <u>-</u> | <u>(57,648)</u> | <u>241,942</u> | <u>-</u> | <u>3,302,541</u> |
| GENERAL FUNDS | | | | | | |
| General Funds | 4,427,197 | 7,662,348 | (10,910,288) | (300,681) | 945,035 | 1,823,611 |
| TOTAL UNRESTRICTED FUNDS | <u>7,545,444</u> | <u>7,662,348</u> | <u>(10,967,936)</u> | <u>(58,739)</u> | <u>945,035</u> | <u>5,126,152</u> |

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19. 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 |
| | <u>24,125</u> | <u>164,111</u> | <u>(207,808)</u> | <u>58,739</u> | <u>-</u> | <u>39,167</u> |

| | | | | | | |
|----------------|------------------|------------------|---------------------|----------|----------------|------------------|
| TOTAL OF FUNDS | <u>7,569,569</u> | <u>7,826,459</u> | <u>(11,175,744)</u> | <u>-</u> | <u>945,035</u> | <u>5,165,319</u> |
|----------------|------------------|------------------|---------------------|----------|----------------|------------------|

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. The project ended on 31 August 2022.

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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. The project ended on 30 June 2022.

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.

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.

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FOR THE YEAR ENDED 31 DECEMBER 2022

20. ANALYSIS OF NET ASSETS BETWEEN FUNDS

ANALYSIS OF NET ASSETS BETWEEN FUNDS - CURRENT YEAR

| | Unrestricted funds 2022 £ | Restricted funds 2022 £ | Total funds 2022 £ |
|--|------------------------------------|----------------------------------|-----------------------------|
| Tangible fixed assets | 2,324,407 | - | 2,324,407 |
| Fixed asset investments | 6,370,627 | - | 6,370,627 |
| Current assets | 6,694,453 | 20,900 | 6,715,353 |
| Creditors due within one year | (5,323,915) | - | (5,323,915) |
| Creditors due in more than one year | (191,551) | - | (191,551) |
| Provisions for liabilities and charges | (2,896,332) | - | (2,896,332) |
| TOTAL | 6,977,689 | 20,900 | 6,998,589 |

ANALYSIS OF NET ASSETS BETWEEN FUNDS - PRIOR 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 |

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

| | Unrestricted funds 2022 £ | Restricted funds 2022 £ | Total funds 2022 £ |
|--|------------------------------------|----------------------------------|-----------------------------|
| Tangible fixed assets | 2,324,407 | - | 2,324,407 |
| Fixed asset investments | 6,534,116 | - | 6,534,116 |
| Current assets | 6,522,161 | 20,900 | 6,543,061 |
| Creditors due within one year | (5,515,135) | - | (5,515,135) |
| Creditors due in more than one year | (191,551) | - | (191,551) |
| Provisions for liabilities and charges | (2,896,332) | - | (2,896,332) |
| | 6,777,666 | 20,900 | 6,798,566 |

ANALYSIS OF NET ASSETS BETWEEN FUNDS - CHARITY ONLY - PRIOR 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 | 5,456,880 | 39,167 | 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) |
| | 4,978,110 | 39,167 | 5,017,277 |

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
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NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2022

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

| | Group 2022 £ | Group 2021 £ |
|--|--------------------|--------------------|
| Net income/expenditure for the year (as per Statement of Financial Activities) | 1,795,676 | (2,408,075) |
| ADJUSTMENTS FOR: | | |
| Depreciation charges | 115,031 | 126,434 |
| Losses / (gains) on investments | 499,017 | (945,035) |
| Dividends, interests and rents from investments | (143,776) | (140,197) |
| Increase in debtors | (215,734) | (83,337) |
| Increase in creditors | 1,167,279 | 394,951 |
| Movement in provisions | (2,300,817) | 3,231,688 |
| Movement in foreign exchange reserve | 37,594 | 3,825 |
| NET CASH PROVIDED BY OPERATING ACTIVITIES | 944,270 | 180,254 |

22. ANALYSIS OF CASH AND CASH EQUIVALENTS

| | Group 2022 £ | Group 2021 £ |
|--|--------------------|--------------------|
| Cash in hand | 4,066,542 | 3,415,237 |
| TOTAL CASH AND CASH EQUIVALENTS | 4,066,542 | 3,415,237 |

23. ANALYSIS OF CHANGES IN NET DEBT

| | At 1 January 2022 £ | Cash flows £ | At 31 December 2022 £ |
|--------------------------|------------------------------|-----------------|--------------------------------|
| Cash at bank and in hand | 3,415,237 | 651,305 | 4,066,542 |
| | 3,415,237 | 651,305 | 4,066,542 |

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
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24. CAPITAL COMMITMENTS

| | Group 2022 £ | Group 2021 £ | Charity 2022 £ | Charity 2021 £ |
|--|--------------------|--------------------|----------------------|----------------------|
| CONTRACTED FOR BUT NOT PROVIDED IN THESE FINANCIAL STATEMENTS | | | | |
| Acquisition of tangible fixed assets | - | 144,400 | - | 144,400 |

25. 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 (2021 - £865,876).

During the year, the Charity added a third pension scheme, a defined contribution scheme. The assets of the scheme are held separately from those of the Company in an independently administered fund. The pension cost charge represents contributions payable by the Company to the fund.

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 as at 31 March 2020 (the valuation date), and was carried out using the projected unit method.

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 2020 valuation was the sixth valuation for the scheme under the scheme-specific funding regime introduced by the Pensions Act 2004, which requires schemes to have sufficient and appropriate assets to cover their technical provisions. At the valuation date, the value of the assets of the scheme was £66.5 billion and the value of the scheme's technical provisions was £80.6 billion indicating a shortfall of £14.1 billion and a funding ratio of 83%.

The key financial assumptions used in the 2020 valuation are described below. More detail is set out in the Statement of Funding Principles (uss.co.uk/about-us/valuation-and-funding/statement-of-funding-principles).

CPI assumption: Term dependent rates in line with the difference between the Fixed Interest and Index Linked yield curves less 1.1% p.a. to 2030, reducing linearly by 0.1% p.a. to a long term difference of 0.1% p.a. from 204

Pension increases (subject to a floor of 0%): CPI assumption plus 0.05%

Discount rate (forward rates): Fixed interest gilt yield curve plus: Pre-retirement: 2.75% p.a.; Post retirement: 1.00% p.a.

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25. PENSION COMMITMENTS (CONTINUED)

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 2020 actuarial valuation. The mortality assumptions used in these figures are as follows:

| | 2020 valuation |
|----------------------------------|---|
| Mortality base table | 101% of S2PMA "light" for males and 95% of S3PFA for females. |
| Future improvements to mortality | CMI 2019 with a smoothing parameter of 7.5, an initial addition of 0.5% p.a. and a long-term improvement rate of 1.8% pa for males and 1.6% pa for females. |

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

| | At 31 December 2022 % | At 31 December 2021 % |
|-------------------------|--|--|
| Discount rate | 3.33 | 0.97 |
| Pension increases (CPI) | 6 | 4.20 |

The current life expectancies on retirement at age 65 are:

| | At 31 December 2022 Years | At 31 December 2021 Years |
|-----------------------------------|--|--|
| MORTALITY RATES (IN YEARS) | | |
| Males currently aged 65 years | 23.9 | 24.7 |
| Males currently aged 45 years | 25.5 | 26.1 |
| Females currently aged 65 years | 25.9 | 26.7 |
| Females currently aged 45 years | 27.3 | 27.9 |

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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 excess 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 mortality 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 |

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

| | |
|----------------------|------------------|
| Technical Provisions | [a] £742,670,000 |
|----------------------|------------------|

THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE
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**NOTES TO THE FINANCIAL STATEMENTS
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| | | |
|--|---------|--------------|
| 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).

26. OPERATING LEASE COMMITMENTS

The Group and the Charity had no commitments under non-cancellable operating leases at 31 December 2022.

27. RELATED PARTY TRANSACTIONS

In 2022 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 £93,161 (2021: £92,287). The transfer under deed of covenant of the trading profits of CCDC Services Limited to the Charity of £334,343 (2021: £329,300).

At the year end a balance of £507,899 (2021: £586,560) was owed to the Charity by CCDC Services Limited.

In 2022 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 £786,506 (2021: £597,358).

At the year end a balance of £260,130 (2021: £58,177) was owed to CCDC Inc by the Charity.

There were no other outstanding balances with related parties as at 31 December 2022 (2021 - £NIL).



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