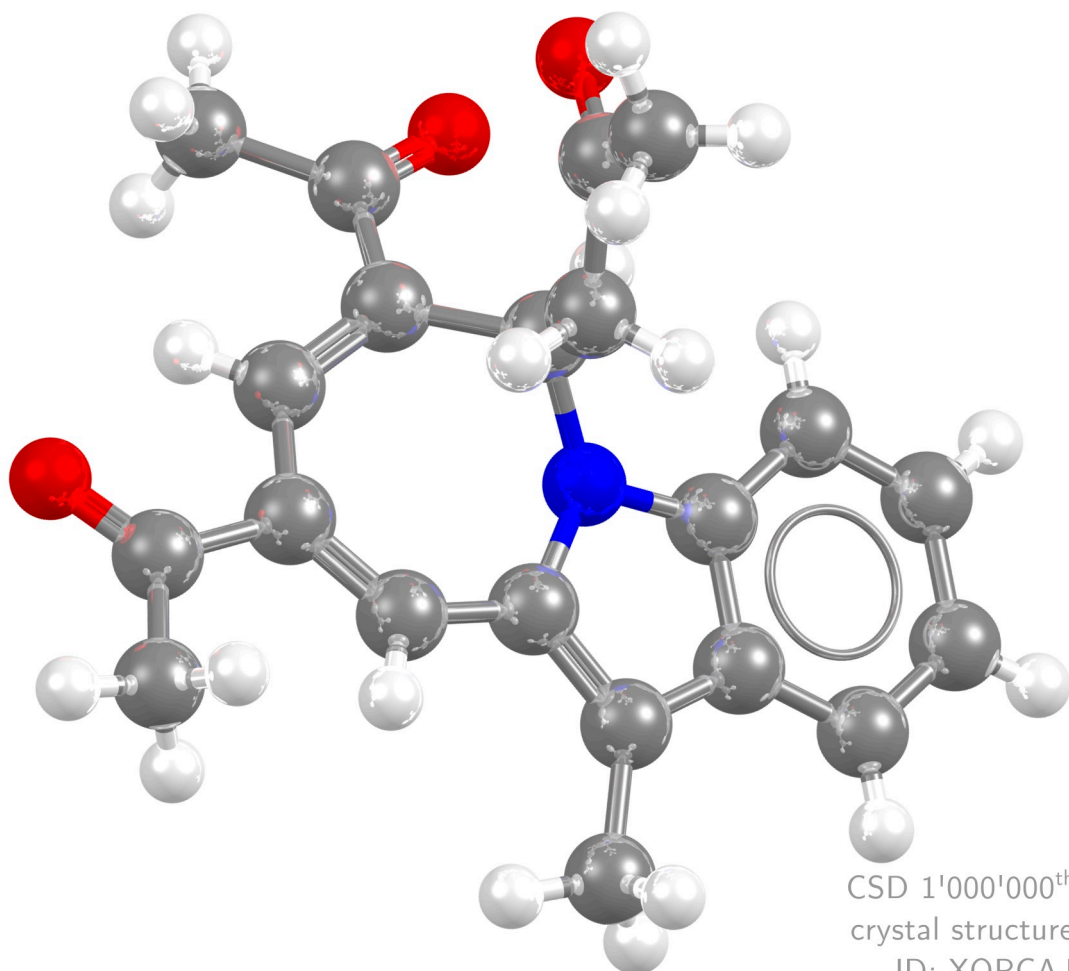




50th annual conference of the
British Association of Crystal Growth

BACG2019



CSD 1'000'000th
crystal structure
ID: XOPCAJ
(DOI 10.5517/ccdc.csd.cc20vdhs)

9-11 July **London**

CRYSTAL
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& DESIGN

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Welcome to the BACG 50th Annual Conference.

Welcome to the 50th meeting of the British Association of Crystal Growth (BACG). We can look back on how much the world has changed since the society was founded, and the role that crystalline materials have played in shaping our society. But the main purpose of our meeting is to look forward and discuss today's new insights into the materials that we have been studying, which will help shape tomorrow's world.

Our venues, in two of London's many Learned Society buildings, emphasises how scientists of like interests have come together to exchange ideas and uphold the best practices of the past in supporting the development of their fields. The Royal College of Obstetricians and Gynaecologists was established in 1929 in Manchester, with a Royal Charter in 1947 and moved to these premises in 1960. It had been considered a minor component of the Royal College of Surgeons, whose origins go back to the fourteenth century with the foundation of the Guild of Surgeons Within the City of London. The oldest national science society emerged from a dining club. The Royal Society, formally The Royal Society of London for Improving Natural Knowledge had its Royal Charter granted in 1660 by King Charles II, and moved to its current location in 1967. The research done by the members of the BACG and being presented at this meeting draws on many traditional disciplines.

The BACG at 50 is still maturing, and we can be agile and modern in our development. The annual meeting is the means when we can come together to exchange ideas, with the discussions of our wide range of lectures and posters, improving the science and disseminating best practice.

So thank you for coming to London to participate in this 50th meeting. I hope that you enjoy the conference, have scientifically worthwhile discussions and meet new people as well as catching up with friends.

Best Wishes
Sally Price

Local Organising Committee

Sally Price, UCL (Co-Chair)	Linda Seton, Liverpool John Moores
Matteo Savalaglio, UCL (Co-chair)	Joop ter Horst, Strathclyde
Ghazala Sadiq, CCDC	Bill Jones, Cambridge University

Scientific committee

Sally Price, UCL (Co-Chair)	Matteo Savalaglio, UCL (Co-chair)	Bill Jones, Cambridge University
Devis Di Tommaso, QMUL	Jerry Heng, ICL	Kreso Bucar, UCL
Christoph Salzmann, UCL	Luca Mazzei, UCL	Asterios Gavrilidis, UCL

Timetable

Tuesday 9th July

08:30 Registration Opens / Morning Coffee

Plenary Session: Crystal Nucleation and Growth

Chair: Devis Di Tommaso (QMUL)

Room: Lecture Theatre

09:15 Introductory Remarks: Prof Sally Price (UCL, UK)

09:30 Plenary: Michael Doherty

University of California at Santa Barbara, US

Towards Digital Drug Product Design for Polymorph Selection and Crystal Growth

10:10 Invited: Nora de Leeuw

University of Cardiff, UK

Modelling the nucleation and growth of iron sulfides

10:40 Kevin Roberts

University of Leeds, UK

The Crystallisation Structural Pathway of Para amino Benzoic acid: From Solvated Molecule through Solute Clustering and Nucleation to the Growth of Facetted Crystals

11:10 Coffee Break

Crystal Nucleation and Growth

Chair: Elena Simone (University of Leeds)

Room: Lecture Theatre

11:30 Kieran Hodnett

University of Limerick, Ireland

Lifetimes of Adsorbed Active Pharmaceutical Ingredients on Heterosurfaces

11:50 David Mackechnie

University of Strathclyde, UK

Interfacial Supersaturation as the Driving Force for Heterogeneous Nucleation at Liquid-Liquid Interfaces

12:10 Sarah Wright

University of Manchester, UK

Unusual Conformations in Molecular Crystals

Experimental Techniques

Chair: Grahame Woollam (Novartis)

Room: U4/5 - The Collegiate Suite

Anuradha Pallipurath

National University of Ireland, Ireland

The effect of functional group terminations on organic crystal facets: A polarised Raman and computational study

Victoria Hamilton

University of Bristol, UK

In situ observation of organic crystal growth of a pharmaceutical using liquid cell electron microscopy

Elizabeth Willneff

University of Leeds, UK

Near-Ambient Pressure X-ray Photoelectron Spectroscopy: A New Laboratory Technique for Characterising Structure and Bonding at Surfaces of Molecular Crystals

12:30 Lunch & poster session

Executive committee meeting

13:00 **Poster Session & Sponsors Exhibition**

Plenary Session: Characterising, Modelling, and Controlling Polymorphism

Chair: Thomas Vetter (University of Manchester)

Room: Lecture Theatre

14:00 **Plenary: Allan Myerson**

Massachusetts Institute of Technology, US

Nucleation of Organic Molecular Crystals on Surfaces and in Confinement

14:40 **Invited: Aurora Cruz Cabeza**

University of Manchester, UK

Joel Bernstein, polymorphism and I

15:10 **Invited: Doris Braun**

University of Innsbruck, Austria

Unravelling complexity in the solid form landscapes of pharmaceuticals

15:40 *Coffee Break*

Polymorphism

Chair: Linda Seton (Liverpool John Moores)

Room: Lecture Theatre

16:00 **Riccardo Montis**

University of Manchester, UK

Combining Crystal Structure Prediction and Structural Comparison with Experimental Screening: a Potential Route to More Polymorphs, Including a 2-for-the-price-of-1 Special.

16:20 **Jason Potticary**

University of Bristol, UK

Control of polymorphism in the three organic systems through the application of strong magnetic fields during crystal growth

16:40 **Martin Ward**

University of Strathclyde, UK

Recovery of high-pressure solid forms to ambient pressures

Experimental Techniques

Chair: Burak Eral (TU Delft)

Room: U4/5 - The Collegiate Suite

Ian McPherson

University of Warwick, UK

Surface Charge Analysis of Calcite Using Scanning Ion Conductance Microscopy

Simon Clevers

Université de Rouen, France

In situ X-ray for monitoring crystallization in solution : In-situX®

Maxime Charpentier

University of Strathclyde, UK

Phase diagram screening of chiral compounds with UV/CD spectroscopy

17:00 **AGM**

17:30

-

19:30

Poster Session with drinks and BACG birthday cake

Wednesday 10th July

09:00 Morning Coffee

Plenary Session: Bio-inspired Crystallization

Chair: Joop Ter Horst (Strathclyde)

Room: Lecture Theatre

09:30 **Plenary: Fiona Meldrum**

University of Leeds, UK

A Crystallisation Approach to Nanocomposite Crystals

10:10 **Invited: Wim Noorduyn**

AMOLF, Netherlands

Shaping up bio-inspired functional materials

10:40 **Invited: Dominique Maes**

Vrije Universiteit Brussel, Belgium

Do protein crystals and aggregates go with the flow?

11:10 Coffee Break

Bio-inspired Crystallization

Chair: Jan Sefcik (Strathclyde)

Room: Lecture Theatre

11:30 **Fatima Ibis**

Delft University of Technology, Netherlands

Understanding Kidney Stone Formation: A microfluidic approach

11:50 **Ian Rosbottom**

Imperial College London, UK

A Novel Platform for Continuous Protein Crystallisation

12:10 **Alice Fayter**

University of Warwick, UK

Characterisation of the Effects on Ice Nucleation, Morphology and Growth upon Addition of Ice-active Compounds; a Biophysical Study

12:30 **Noushine Shahidzadeh**

University of Amsterdam, UK

The hopper growth of NaCl crystals

Co-Crystals and Formulation

Chair: Kreso Bucar (UCL)

Room: U4/5 - The Collegiate Suite

Huaiyu Yang

Loughborough University, UK

Jumping into Metastable 1:1 Urea-Succinic Acid Cocrystal Zones by Freeze-Drying

Marvah Aljohani

Galway University, Ireland

Influence of excipients on the stability of pharmaceutical cocrystals

Leila Keshavarz

University of Limerick, Ireland

Influence of Impurities on the Solubility, Nucleation, Crystallization and Compressibility of Paracetamol

Rafel Prohens

Universitat de Barcelona, Spain

Revisiting the Solid-State landscape of Sildenafil: New insights from an old drug

13:00 Lunch & poster session

13:30 **Poster Session & Sponsors Exhibition**

Awards Session

Chair: Bill Jones (Cambridge),

Room: Lecture Theatre

14:30 **BACG Young Investigator Award: Mark Holden**

University of Central Lancashire, UK

The role of active sites in heterogeneous ice nucleation

15:00 **BACG Annual Lecture: Leslie Leiserowitz**

Weizmann Institute of Science, Rehovot, Israel

Mode of action of quinoline antimalarial drugs in red blood cells infected by *Plasmodium falciparum*, revealed in-vivo

15:45 *Break: preparation for the evening dinner at the Royal Society*

Reception and Dinner at the Royal Society

18:00 Royal Society opens

18:30 Reception starts

19:00 **Conference Dinner, Awards presentation and Evening talk by Roger Davey**

Thursday 11th July

09:00 Morning Coffee

Plenary Session: Engineering Crystallization

Chair: Aurora Cruz-Cabeza (Manchester)

Room: Lecture Theatre

09:30 **Plenary talk: Marco Mazzotti**

ETH Zurich, Switzerland

On the Manipulation of the Size and Shape of Needle-like Crystals

10:10 **Thomas Vetter**

University of Manchester, UK

Design and optimization of isothermal and non-isothermal deracemization

10:40 **Yuri Abramov**

XtalPi, US

Modeling Support of Finite Pharmaceutical Crystal Growth

11:10 Coffee Break

Engineering Crystallization

Chair: Huaiyu Yang (Loughborough)

Room: Lecture Theatre

11:30 **Jose Capdevila Echeverria**

University of Strathclyde, UK

pH and Temperature Dependent Solubilities and Eutectic Points for the Continuous Chiral Resolution by Integration of Membrane and Crystallisation Technologies

11:50 **Johannes Hoffmann**

University of Strathclyde, UK

Serial Separation and Resolution in Eutectic Solutions

12:10 **Brigitta Bodák**

ETH Zurich, Switzerland

Model-based analysis of solid-state deracemization via temperature cycles

Nucleation and Growth

Chair: Virginia Burger (XtalPi)

Room: U4/5 - The Collegiate Suite

Yumin Liu

University of Manchester, UK

When crystals don't grow – the growth dead zone

Torsten Jensen

University of Bristol, UK

A Planar Aromatic Molecule that Cannot Crystallise: A Combined Computational and Experimental Study of 2nd Generation Sulflower

Ilaria Gimondi

University College London, UK

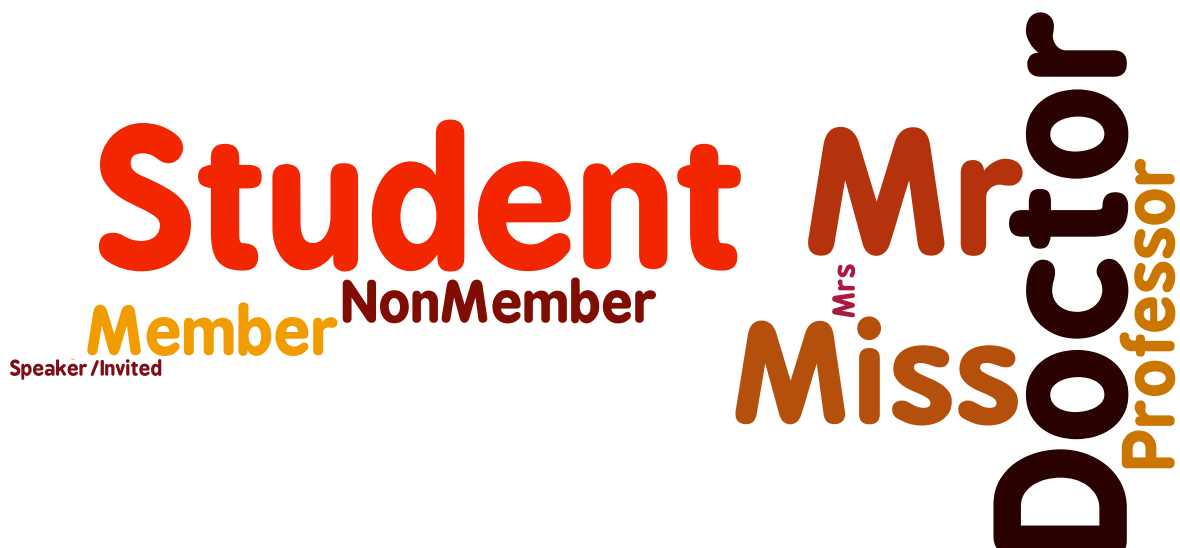
Conformational complexity limitations to the simulation of the nucleation of succinic acid polymorphs

12:30 Closing Remarks - Joop ter Horst

University of Strathclyde, UK

12:40 Lunch

BACG50 at a glance



Useful Information

Registration

The BACG registration desk will be open on Tuesday 9th July at 8.15 am in the lobby inside the Rooms on Regent's Park. Delegates will be provided with name badges, lanyards, WiFi password, poster voting form, Crystal in Art voting form and conference materials. The registration desk will be staffed each day during conference hours. Please do come along and see anyone on the registration desk to request any information.

Language

The official language of the conference is English.

Weather

June is a good month for weather in London with temperatures generally ranging between 16 – 23°C (64-80 F). However, this is the UK so please do be prepared for rain and much cooler temperatures. Pack an umbrella and a jacket.

Security

Please kindly wear your name badge and lanyards during the conference hours so people are aware that you are a conference participant.

Poster Sessions, voting, and prizes

The poster sessions will be held on Tuesday 9th and Wednesday 10th July. The main poster session will be on Tuesday evening following the conclusion of the afternoon session. Drinks and canapes will be provided including birthday cake to celebrate the 50th anniversary of the BACG.

There are five poster prizes which have been kindly sponsored by CGD, the Buckley Trust, and XtalPi Inc. The prizes are: 1st Prize is £100, 2nd Prize is £75 and 3rd Prize is £50. In addition to the top three overall posters there will be a fourth poster prize of £100 dedicated to novel experimental techniques, and a fifth poster prize of £100 dedicated to modelling contributions.

Each delegate is allowed two votes for their preferred poster. You will be given a voting form during registration. Votes will be collected in a ballot box at the registration desk. Poster prize winners will be announced at the conference dinner on Wednesday evening. Good luck!

The posters can be displayed throughout the duration of the conference. All materials required to display your poster will be provided and can be collected from the registration desk. Please display your poster on the poster board allocated with your number. Posters must be taken down at lunchtime on Thursday 11th July.

Crystals in Art and voting

There are three Crystals in Art prizes which have been kindly sponsored by CGD. The prizes are: 1st Prize is £100, 2nd Prize is £75 and 3rd Prize is £50.

Each delegate will vote for the Art submission they think should be recognised with a prize. You will be given a voting form during registration. Each delegate is allowed two votes. Votes will be collected in a dedicated ballot box at the registration desk. Crystals in Art prize winners will be announced at the conference dinner on Wednesday evening. Good luck!

The art work can be displayed throughout the duration of the conference. All materials required to display your work will be provided and can be collected from the registration desk. Please display your art work on the crystals in art poster board. Please make sure your art work is provided with a clear label including your name and art work title. Art work must be taken down at lunchtime on Thursday 11th July.

Eating

London has an overwhelming choice of places to eat. The nearest “pub with grub” is The Windsor Castle, which backs onto the conference centre. There are a variety of eating places nearby in Baker Street, past 221B (which is between 239 and 241 for reasons that may elude Watson). However a walk through Regents Park (café serves breakfast) can take you to the diverse eateries of Camden (Greek, Argentinian, Japanese, ...) and Drummond Street (Indian).

Exercise

Do explore Regents Park, which is right in front of the venue, and use it as a pleasanter route than walking along the Marylebone/Euston Road. The Rose Garden is particularly good at this time of year.

Travel

TFL can help with route planning around London on <https://tfl.gov.uk/plan-a-journey/>. Payments for underground or buses can be made with contactless cards on boarding a bus (flat fare), and entering and leaving underground or overground rail stations.

Conference Dinner

The conference dinner is organised at The Royal Society, 6-9 Carlton House Terrace, London SW1Y 5AG.

Online information on the venue can be found on:

<https://royalsociety.org/about-us/contact-us/carlton-house-terrace-london/>.

It starts with a reception with some light canapes at 6.30 pm in The City of London Rooms which overlook The Mall, with the meal at 7.00 pm. There will be a speech at the dinner after the main course. This will be followed by a prize giving ceremony after dessert over tea, coffee and petit fours. You will need your BACG conference badge to pass through the reception area.

Please allow at least 40 minutes for your journey, and consider allowing longer to enjoy the surrounding area. The official Transport for London fastest estimate from the conference venue is taking the 139 bus from Park Road/London Business School to Trafalgar Square and then walking is 35 minutes. Alternatives would be the underground from Baker Street to Piccadilly Circus and a short walk down Lower Regents Street. Going to Green Park allows a pleasant stroll through the parks via Buckingham Place, or to Oxford Street a chance to do some shopping as walking down Regents Street, but don't get lost in Hamleys toy shop.

Directions to the Rooms on Regent's Park

27 Sussex Place, Regent's Park


London

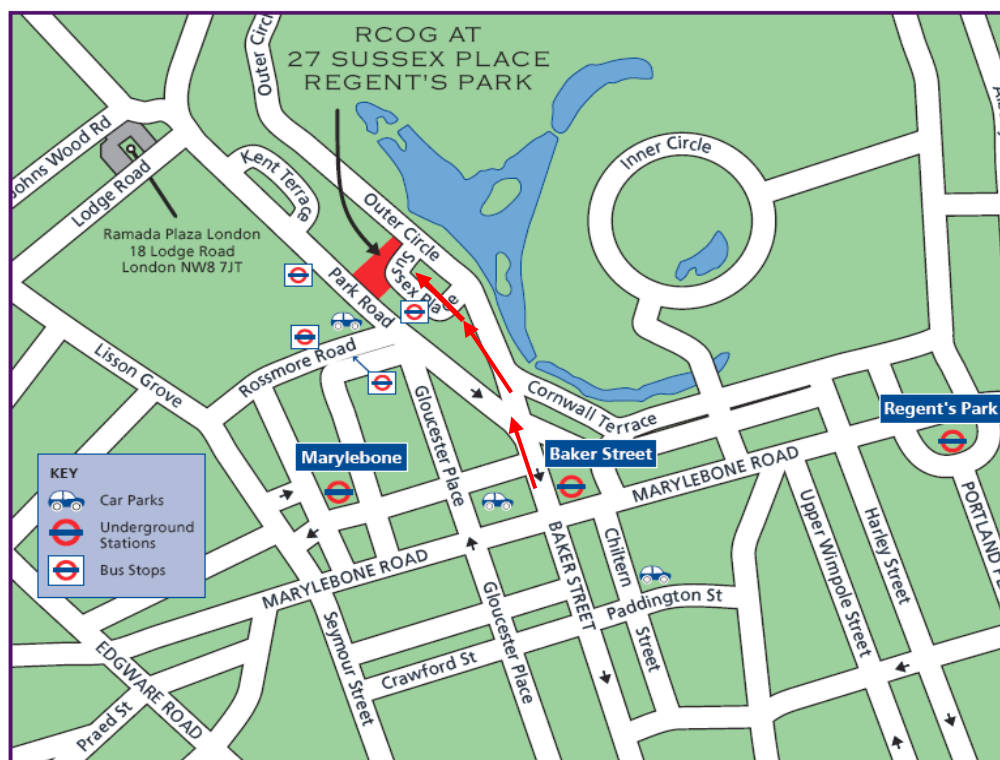
NW1 4RG

Tel: 0207 772 6-200

www.rcog.org.uk



- **By Train:** Marylebone mainline rail station is only a ten-minute walk Paddington, Euston; King's Cross and St Pancras are also close by.
- **By Tube:** The nearest Underground station is Baker Street (served by the Hammersmith & City, Bakerloo, Circle, Jubilee and Metropolitan lines). **Exit** Transport for London **Lost Property** office.
- **By Bus:** The area is also well served by a number of different buses, including the numbers: 13, 82, 113, 139, 189 and 274.
- **By Car:** Car parking facilities are available at the NCP Park Road (24-hour) and on the Regent's Park Outer Circle (short-stay metered parking). For directions and route planner please see http://www.theaa.com/travelwatch/planner_main.jsp
- **NCP Park Road information:**
www.londontown.com/LondonInformation/Travel/Park_Road_NCP/5341/
-  **From Baker Street Tube, walk down to the Outer Circle of Regent's Park, continue until you pass the London Business School (huge white building) and look out for the distinguish glass cones (see above picture)**





Chain Times of The Regent's Park

January	5:00pm
February	6:00pm
March (BST)	7:00pm
April (BST)	8:00pm
May	9:00pm
June	9:30pm
July	9:30pm
August	9:00pm
September	8:30pm
October (BST)	7:30pm
November	6:30pm
December	4:30pm

Underground station

Bus stop

Cycle hire

Cycle parking

Car parking

Disabled car parking

Information

Accessible toilets

Public toilets

Children's toilets and drinking fountain

Children's play area

Deckchair hire (seasonal)

Café

Seasonal Café

Restaurant

Drinking fountain

Viewing point

Road open to motor traffic and cyclists

Shared use pedestrian and cycle way

Park features

Public access sites (opening periods vary)

Non public access sites

Jubilee Greenway

Cycling Permitted

THE ROYAL PARKS
www.royalparks.org.uk

PARK MANAGEMENT
Nick Biddle
The Seward, Inner Circle
Regent's Park, London NW1 4NR
T: 020 601 2100
E: regent@royalparks.org.uk

CONTACTING POLICE
T: 999 for emergencies
T: 101 for other calls
www.met.police.uk
www.met.police.uk
The park is open from 5:00am to dusk 4 year round. The following park is open from dusk to dawn 7 year round:
Park Square East & West, York Gate, Lower & Upper Circus, Grosvenor Gardens, Grosvenor Square, Victoria Tower Gardens, St James's Park, Kensington Gardens, The Regent Park & Primrose Hill

THE ROYAL PARKS ARE
Bury Park
The Green Park
Greenwich Park
Hampton Court Palace
Kensington Gardens
Kew Gardens
St James's Park
The Regent Park & Primrose Hill
The Royal Parks

QUEEN MARY'S GARDENS
Queen Mary's Gardens was originally used as a plant nursery while the park was under development as a residential estate. It was the first garden to be planted in the Regent's Park. The gardens were designed by the architect John Lubbock, who was the first to introduce the concept of a public garden in London. The gardens were designed to be a place where people could enjoy the beauty of nature and the fresh air of the park. The gardens were designed to be a place where people could enjoy the beauty of nature and the fresh air of the park. The gardens were designed to be a place where people could enjoy the beauty of nature and the fresh air of the park.

THE BOATHOUSE CAFE
Best for hire for adults and children.
Open daily from 9:00am. Closing times vary seasonally. Between 10:00pm and 10:00pm. T: +44 (0)20 7274 4069

THE BROAD WALK CAFE
Open daily from 8:00am. Closing times vary seasonally. Between 10:00pm and 10:00pm. T: +44 (0)20 7274 4069

THE HUB CAFE
Open daily from 8:00am. Closing times vary seasonally. Between 10:00pm and 10:00pm. T: +44 (0)20 7274 4069

EATING & DRINKING
ESPRESSO BAR
Open daily from 8:00am. Closing times vary seasonally. Between 10:00pm and 10:00pm. T: +44 (0)20 7274 4069

THE REGENT'S BAR & KITCHEN
Open daily from 8:00am. Closing times vary seasonally. Between 10:00pm and 10:00pm. T: +44 (0)20 7274 4069

THE REGENT'S PARK TENNIS CENTRE
The Regent's Park Tennis Centre provides high quality tennis courts for hire for adults and children. The centre is open daily from 8:00am to 10:00pm. T: +44 (0)20 7274 4069

SPORT & LEISURE
A wide range of sports are available in The Regent's Park and Primrose Hill including: tennis, football, basketball, badminton, table tennis, and a range of other sports. The park is open daily from 8:00am to 10:00pm. T: +44 (0)20 7274 4069



Register for Royal Parks updates
www.royalparks.org.uk/registerupdates

WALKING DISTANCE (MINUTES)

A BRIEF HISTORY OF ST JAMES'S PARK

1531 Acquired by Henry VIII and Court of 50 years established residence of British sovereigns since 1837. Changing of the Guard ceremony every day in the summer and alternate days in the winter.

1660 Park laid out for James II with menagerie and duck, designs by John Vanbrugh.

1663 Horngates constructed.

1667 Equestrian bridge introduced including palaces.

1703 Buckingham House developed which later became the official Royal residence.

1827 John Nash agreed to carry out present landscape in the park.

1905 Queen Victoria Memorial Garden created.

FAMOUS LANDMARKS

BUCKINGHAM PALACE has served as the official London residence of British sovereigns since 1837. Changing of the Guard ceremony every day in the summer and alternate days in the winter.

CLARENCE HOUSE was designed by John Nash and built between 1825 and 1827 for the Duke of Clarence, later King George IV.

THE QUEEN VICTORIA MEMORIAL is a 25 metre (82 ft) high monument to Queen Victoria, designed by Sir Alfred Gilbert.

ST JAMES'S PALACE was built by Henry VIII along the River Thames.

ICA GALLERIES are home to the best new art and culture from Britain and around the world.

MALL GALLERIES a central London's focal point for new art and culture.

ST JAMES'S PARK LAND

ST JAMES'S PARK LAND is the largest of the park's three estates of land, covering 100 acres (40 hectares) and is home to the park's most famous landmarks including the famous palaces.

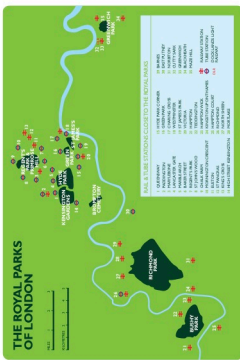
DUCK ISLAND is a nature reserve for the park's bird collection.

SWAN ISLAND is a nature reserve for the park's bird collection.

INN THE PARK RESTAURANT is where you can feast on the finest seasonal produce from small independent producers.

THE CHURCHILL MUSEUM & CABINET WAR ROOMS are dedicated to the life of the greatest Briton. The scene is set in the Churchill family home with the new centre of British war effort.

THE GUARDS MUSEUM contains a wealth of information and artefacts relating to the five regiments of Foot Guards.



PARK MANAGEMENT

St James's Park, Office
The Royal Parks, Office
St James's Park, London SW1A 2B
T: +44 (0) 20 7300 7393
F: +44 (0) 20 7300 7329
E: stjames@royalparks.gov.uk

METROPOLITAN POLICE

St James's Park, Office
The Royal Parks, Office
St James's Park, London SW1A 2B
T: +44 (0) 20 7300 7393
F: +44 (0) 20 7300 7329
E: stjames@royalparks.gov.uk

The park is open from 5am until midnight.

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