

Series Outline

1. Correspondence and Non-Dunitz Publications, 1932-2009 undated
2. Biographical Materials and Photographs, 1967-2008 undated
3. Publications by Jack Dunitz, 1947-2004
4. Manuscripts and Lecture Materials, 1946-2006 undated
5. Research Notes and Notebooks, 1941-1989
6. Subject Files, 1927-2008

Detailed Description of the Collection

Box

1. Correspondence and Non-Dunitz Publications, 1932-2009 undated (26 boxes)

The folders in this series contain correspondence and publications by specific authors, as maintained by Dunitz. The correspondence materials include traditional letters as well as a large volume of emails and word processing files printed out over time by Dunitz. Highlights of the series include lengthy exchanges with a number of notable scientists including Carleton Gajdusek, Dorothy Hodgkin and Kenneth Trueblood. The activities of the Cambridge Crystallographic Data Centre are also well-documented in this series, as is Dunitz's work in preparing his *Biographical Memoirs of the Royal Society* article on Linus Pauling.

Access to the Cambridge Crystallographic Data Centre and the Royal Society correspondence in Series 1 is restricted due to the presence of confidential information. All requests for access to this material should be directed to the University Archivist.

1.001 Correspondence: A, 1976-2008 undated (16 folders)

Folder

- 1.1 Abir-Am, Pnina, 2001
- 1.2 Abrahams, Sidney C., 1982 2000
- 1.3 Academia Europaea, 1989 1991 1994-1995
- 1.4 *Accounts of Chemical Research*, 1994-1995 undated
- 1.5 *Acta Crystallographica*, 1976 1986 1989-1995 undated
- 1.6 Allinger, Norman L., 1992 1997 1999
- 1.7 American Academy of Arts and Sciences, 1997
- 1.8 American Chemical Society, 1989 1992 1996-1997
- 1.9 American Crystallographic Association, 1989-1991 1994
- 1.10 American Philosophical Society, 1997-1998
- 1.11 *Angewandte Chemie*, 1990-1992 1994-1996 undated
- 1.12 Anwar, Jamshed, 2005
- 1.13 Arrhenius, Gustav, 1992 2008
- 1.14 Auf der Hyde, Thomas, 1990-1994
- 1.15 Avnir, David, 1992-1996
- 1.16 A: General Correspondence,

1.002 Correspondence: Ba, 1982-2009 (3 folders)

- 2.1 Bader, Richard, 1982-2009 [Includes extensive correspondence with Vladimir Tsirelson regarding Richard Bader.]
- 2.2 Barron, Laurence D., 1988-1989 1993-1996 2001-2002 2004
- 2.3 Baur, Werner, 1997-1998

1.003 Correspondence: Be - Bo, 1960-2004 (10 folders)

- 3.1 Benner, Steven, 2004
- 3.2 Bent, Henry A., 1960-1968 [Publications only.]
- 3.3 Bijvoet, Johannes Martin, 1967-2001 [Includes portrait of Bijvoet, dated 1961.]
- 3.4 *Biopolymers*, 1997
- 3.5 Blow, David M., 2002
- 3.6 Boese, Roland, 1990-1991 1999 2001
- 3.7 Boldyreva, Elena, 1991-1993
- 3.8 Boll-Dornberger, Kate, 1963-1967
- 3.9 Bombicz, Petra, 2001-2002
- 3.10 Boorstin, Daniel, 1999

1.004 Correspondence: Br - Bu, 1954-2004 (9 folders)

- 4.1 Braga, Dario, 2001
- 4.2 Bragg, W. L., 1954-1955 1957-1958
- 4.3 Breau, Josef, 1998-1999
- 4.4 Brenner, Sydney, 1994 2000
- 4.5 Britton, Doyle, 1965 1973-1982 1990 1998
- 4.6 Brock, Carol, 1984-2000

- 4.7 Buck, Henk M., 1999-2000
- 4.8 Bürgi, Hans-Beat, 1969-2004
- 4.9 B: General Correspondence,
- 1.005 RESTRICTED: Cambridge Crystallographic Data Centre, 1988-2004 undated (4 folders)
- 5.1 RESTRICTED: Cambridge Crystallographic Data Centre, 1988-1995
- 5.2 RESTRICTED: Cambridge Crystallographic Data Centre, 1996
- 5.3 RESTRICTED: Cambridge Crystallographic Data Centre, 1997
- 5.4 RESTRICTED: Cambridge Crystallographic Data Centre, 1998-2004 undated
- 1.006 Correspondence: C, 1944-2007 undated (13 folders)
- 6.1 California Institute of Technology, 1948-1950 1952 1954 2007 [Folder contains audio files, transcripts and correspondence related to the "C. I. T. Cabaret" - stage productions and song parodies created for Christmas Party celebrations from 1948-1950, as well as "The Road to Stockholm" production performed in honor of Linus Pauling's receipt of the Nobel Chemistry Prize.]
- 6.2 Cambridge, University of, 1951
- 6.3 Cameron, T. Stanley, 1991 1996 1999-2000
- 6.4 Carnegie Trust, 1944 1946 1948
- 6.5 Castellano, Ronald K., 2002
- 6.6 Chakrabarti, Pinakpani, 1989 1993-1998 2000
- 6.7 *Chemical Physics Letters*, 1995-1998 undated
- 6.8 Cornell University Press, 1993-1994
- 6.9 Cotton, F. Albert, 2000
- 6.10 Coulson, Charles A., 1949 1951 1963 1968 1971
- 6.11 Crick, Francis, 1956
- 6.12 Cruickshank, D. W. J., 1977 1991 1996-1997 2001
- 6.13 C: General Correspondence,
- 1.007 Correspondence: D, 1946-2008 (11 folders)
- 7.1 Dougherty, Dennis A., 1993 1997
- 7.2 Delbrück, Max, 1967 1969 1990
- 7.3 Dervan, Peter, 1992-1999
- 7.4 Desiraju, Guatam, 1992-2005
- 7.5 Deutsche Akademie der Naturforscher Leopoldina, 1980-2008
- 7.6 Diederich, François, 1991-1998
- 7.7 Dobler, Max, 1983
- 7.8 Donohue, Jerry, 1956 1967-1983
- 7.9 Dunitz, Marguerite, 1998
- 7.10 Dunlop, W. R., 1946-1947 [Contains materials related to Dunitz's participation in Dunlop's "Correspondence Course on Analysis and Language."]
- 7.11 D: General Correspondence,
- 1.008 Correspondence: E, 1966-2006 (9 folders)
- 8.1 Egli, Martin, 1988-2006
- 8.2 Eijck, Boucke van, 1996 1999-2000 2002
- 8.3 Elguero, Jose, 1991-1998 2005
- 8.4 Eliel, Ernest L., 1973-1998
- 8.5 Ermer, Otto, 1966-1993
- 8.6 Eschenmoser, Albert, 1988-1989 2005
- 8.7 European Academy of Sciences and Arts, 1991-1992 1999 2004
- 8.8 European Science Foundation, 1999-2003
- 8.9 E: General Correspondence,
- 1.009 Correspondence: F, 1957-1999 (6 folders)
- 9.1 Flack, Howard, 1998-1999
- 9.2 Forrest, Hugh S., 1994 1997
- 9.3 Freeman, Hans C., 1957 1988-1989
- 9.4 French, Alfred D., 1999
- 9.5 Fundacion BBV, 1991-1992 1997-1998

- 9.6 F: General Correspondence,
- 1.010 Correspondence: Ga, 1989-2008 (3 folders)
- 10.1 Gajdusek, D. Carleton, 1994-2008 [Includes images of Caltech graduate student colleagues, including Jack Dunitz, on camping trips circa 1948. Also includes two photographs of Gajdusek at his own eightieth birthday party.]
- 10.2 Gatti, Carlo, 2003-2004
- 10.3 Gavezzotti, Angelo, 1989 1994 1996-2006
- 1.011 Correspondence: Gi - Gu, 1971-2000 (6 folders)
- 11.1 Gillespie, Ron, 1990-1994
- 11.2 Ginsburg, David, 1971-1990
- 11.3 Glusker, Jenny, 1994-1995 1999-2000
- 11.4 Gould, Stephen Jay, 1998
- 11.5 Gunsteren, Wilfred van, 1995 [Publications only.]
- 11.6 G: General Correspondence,
- 1.012 Correspondence: H, 1934-2007 undated (12 folders)
- 12.1 Hager, Tom, 1995-1996 2006
- 12.2 Hargittai, Istvan and Magdolna, 1991-1992 1995-1999
- 12.3 Harris, Kenneth D. M., 1996 1999 2002 2006
- 12.4 Harvard University, 1993-1995
- 12.5 Heilbronner, Edgar, 1956-1957 1973-1998
- 12.6 *Helvetica Chimica Acta*, 1990-1991 2003 undated
- 12.7 Herbstein, Frank H., 1974-2007
- 12.8 Hirshfeld, Fred L., 1982-1986
- 12.9 Hodgkin, Dorothy, 1934 1939-1940 1950-1951 1956-1999 [Includes color negative of oil portrait of Dorothy Hodgkin.]
- 12.10 Hoffman, Roald, 1993 1996 2006
- 12.11 Huber-Buser, Effi, 1962-1970
- 12.12 H: General Correspondence,
- 1.013 Correspondence: I - K, 1958-2008 undated (21 folders)
- 13.1 Ibers, James, 1972-1991 2008
- 13.2 *Inorganic Chemistry*, 1991 undated
- 13.3 Irwin, John Joseph, 1987-1995 [Includes a copy of Irwin's Ph. D. thesis, "The Cambridge Structural Database as a New Scientific Tool."]
- 13.4 I: General Correspondence,
- 13.5 Jortner, Joshua, 1994
- 13.6 *Journal of the American Chemical Society*, 1990-1991 1994-1995 undated
- 13.7 *Journal of Physical Chemistry*, 1989
- 13.8 *Journal of Physical Organic Chemistry*, 1991 1994 undated
- 13.9 J: General Correspondence,
- 13.10 Kalman, Alajos, 1990 1992 2000-2003
- 13.11 Kamb, Linda Pauling, 1993 1995-1997
- 13.12 Karplus, Martin, 1988 1994-1995
- 13.13 Kendrew, John, 1958
- 13.14 Kennard, Olga, 1967 1982 1992 1995-1996 2006
- 13.15 Kirby, Anthony J., 1984 1991 1993-1994
- 13.16 Klebe, Gerhard, 1993 1996
- 13.17 Koshland, Daniel E., Jr., 1993-1994
- 13.18 Kresinski, Roman, 1997
- 13.19 Kroon, Jan, 1980 1996-1997 1999-2000
- 13.20 Kuhn, Hans, 1962-1963
- 13.21 K: General Correspondence,
- 1.014 Laboratory Research Assistant Applicants - Post-Doctoral and Sabbatical, (22 folders)
- 14.1 Laboratory Research Assistant Applicants: A,
- 14.2 Laboratory Research Assistant Applicants: B,

- 14.3 Laboratory Research Assistant Applicants: C,
- 14.4 Laboratory Research Assistant Applicants: D,
- 14.5 Laboratory Research Assistant Applicants: E,
- 14.6 Laboratory Research Assistant Applicants: F,
- 14.7 Laboratory Research Assistant Applicants: G,
- 14.8 Laboratory Research Assistant Applicants: H,
- 14.9 Laboratory Research Assistant Applicants: I - J,
- 14.10 Laboratory Research Assistant Applicants: K,
- 14.11 Laboratory Research Assistant Applicants: L,
- 14.12 Laboratory Research Assistant Applicants: M,
- 14.13 Laboratory Research Assistant Applicants: N,
- 14.14 Laboratory Research Assistant Applicants: O,
- 14.15 Laboratory Research Assistant Applicants: P - Q,
- 14.16 Laboratory Research Assistant Applicants: R,
- 14.17 Laboratory Research Assistant Applicants: S,
- 14.18 Laboratory Research Assistant Applicants: T,
- 14.19 Laboratory Research Assistant Applicants: U,
- 14.20 Laboratory Research Assistant Applicants: V,
- 14.21 Laboratory Research Assistant Applicants: W,
- 14.22 Laboratory Research Assistant Applicants: X - Z,
- 1.015 Correspondence: L, 1950-2004 (9 folders)
- 15.1 Lahav, Meir and Leslie Leiserowitz, 1993-1995 2002-2004
- 15.2 Laube, Thomas, 1988 1995-1996
- 15.3 Leonard, Nelson J., 1960 1974 1996
- 15.4 Lerner, Richard, 1994-1998
- 15.5 Lifson, Shneoir, 1999
- 15.6 Linden, Anthony, 2000
- 15.7 Lipscomb, William, 1951-1952
- 15.8 Lonsdale, Kathleen, 1950-1951 1998
- 15.9 L: General Correspondence,
- 1.016 Correspondence: M, 1956-2004 undated (12 folders)
- 16.1 Mackay, Alan L., 1973-1975 1984-1990
- 16.2 MacKinnon, Roderick, 1998
- 16.3 Maddox, Brenda, 1999 2002
- 16.4 Mandel, George, 1956-1957 [Folder includes series of x-ray crystallographic photographs of Guanine and Azoguanine taken by Mandel.]
- 16.5 Mason, Stephen, 1978-1991 1996
- 16.6 McBride, J. Michael, 1991-1992 1998 2002
- 16.7 McGrayne, Sharon, 1991
- 16.8 Mislow, Kurt, 1991 1995-1996
- 16.9 Mnyukh, Yuri, 2002-2003
- 16.10 *Molecular Physics*, 1994 undated
- 16.11 Murray-Rust, Peter, 1975-1976 2004
- 16.12 M: General Correspondence,
- 1.017 Correspondence: N, 1954-1999 undated (6 folders)
- 17.1 National Academy of Sciences, 1988 1993 1998-1999
- 17.2 National Institutes of Health, 1954-1955
- 17.3 *Nature*, 1963-1964 1991 1993 undated
- 17.4 Novotny-Bregger, Elisabeth, 1991-1994
- 17.5 Nyholm, Ronald S., 1957-1960
- 17.6 N: General Correspondence,
- 1.018 Correspondence: O, 1949-2002 (6 folders)
- 18.1 Olovsson, Ivar, 1990-1993 2001-2002
- 18.2 Orgel, Leslie, 1952-1958 1964 1995-1998

- 18.3 Oster, Gerald, 1949
- 18.4 Ovchinnikov, Yuri A., 1969
- 18.5 Oxford, University of, 1951-1953
- 18.6 O: General Correspondence,
- 1.019 Pauling, Linus, 1950-2001 (2 folders)
- 19.1 Pauling, Linus, 1950-1994
- 19.2 Materials re: *Biographical Memoirs of the Royal Society* article on Linus Pauling, written by Jack Dunitz, 1994-2001
- 1.020 Correspondence: P - Q, 1952-2007 (11 folders)
- 20.1 Patterson, A. Lindo, 1955
- 20.2 Pauling, Peter, 1966 1970 1998-2000
- 20.3 Perutz, Max, 1955-1956 1958 1994 1997 2002
- 20.4 Pepinsky, Ray, 1952 1957-1960
- 20.5 Petsko, Gregory, 1992
- 20.6 Phillips, David C., 1957-1958 1963-1964 1966 1977 1990-1999
- 20.7 Popelier, David, 2006-2007
- 20.8 Prelog, Vladimir, 1957 1987 1995
- 20.9 P: General Correspondence,
- 20.10 Quack, Martin, 1989 1992-2002
- 20.11 Q: General Correspondence,
- 1.021 Correspondence: R, 1932-2008 undated (9 folders)
- 21.1 Rich, Alexander, 1957 1974 1994-1995 2000
- 21.2 Roberts, Jack, 1995 undated
- 21.3 Robertson, J. Monteath, 1934-1959 [Publications only.]
- 21.4 Rollett, John S., 1954-1955
- 21.5 Royal Institution, 1955
- 21.6 RESTRICTED: Royal Society, 1974-2008
- 21.7 Rundle, R.E., 1950-1964
- 21.8 Ruzicka, Leopold, 1932 1934-1935 1956-1957 1973-1976 [Includes one letter written to Ruzicka by J. D. Bernal.]
- 21.9 R: General Correspondence,
- 1.022 Correspondence: Sa - Sp, 1948-2005 (15 folders)
- 22.1 Sanders, Jeremy K. M., 1995
- 22.2 Sands, Donald, 1976-1991
- 22.3 Sarma, J. A. R. P., 1986 1989-1991
- 22.4 Saunders, Martin, 1988-1989 1992-1993 2002
- 22.5 Schmidt, Gerhard, 1965-1966
- 22.6 Schmidtchen, Franz P., 2003
- 22.7 Schomaker, Verner, 1948 1970 1995-1996
- 22.8 Seebach, Dieter, 1988-2005
- 22.9 Seiler, Paul, 1976-2003
- 22.10 Shaik, Sason, 1993-1994
- 22.11 Shankland, Norman, 1998
- 22.12 Shearer, Harrison, 1957
- 22.13 Sim, George A., 1966
- 22.14 Somorjoi, Gabor, 1987 1993 2004
- 22.15 Spek, Anthony L., 1998-2000
- 1.023 Correspondence: St - Su, 1968-2004 (5 folders)
- 23.1 Steiner, Thomas, 1996-1997
- 23.2 Stent, Gunther, 1968-2004
- 23.3 Stølevik, Reidar, 1996
- 23.4 Sutherland, G. B. B. M., 1955
- 23.5 S: General Correspondence,
- 1.024 Correspondence: T - V, 1951-2006 (12 folders)

- 24.1 Tame, Jeremy, 2006
- 24.2 Tanaka, Jiro, 1972-1973 1987
- 24.3 Taylor, W. H., 1951
- 24.4 Third World Academy of Sciences, 1989-2002
- 24.5 Thomas, John Meurig, 1989-2002
- 24.6 Trueblood, Ken, 1956-1980
- 24.7 Trueblood, Ken, 1981-1998
- 24.8 T: General Correspondence,
- 24.9 U: General Correspondence,
- 24.10 Venkatesan, K., 1988-1992
- 24.11 Vincent, Beverly, 1987 1991 1995-1996
- 24.12 V: General Correspondence,
- 1.025 Correspondence: W, 1959-2004 (8 folders)
- 25.1 Waser, Jurg, 1971-1972
- 25.2 Watson, James, 1997
- 25.3 Weizmann Institute of Science, 1984-2004
- 25.4 Williams, Dudley, 1993 2004
- 25.5 Willis, B. T. M., 1959 1963-1964
- 25.6 Wilson, Chick C., 2002
- 25.7 Wüthrich, Kurt, 1998-2002 [Publications only.]
- 25.8 W: General Correspondence,
- 1.026 Correspondence: Y - Z, 1985-2007 (6 folders)
- 26.1 Yang Qing-Chuan, 1985-1991
- 26.2 Y: General Correspondence,
- 26.3 Zagrovic, Bojan, 2006-2007
- 26.4 Zahradník, Rudolf, 1995 1998-1999
- 26.5 Zewail, Ahmed, 1992-1999
- 26.6 Z: General Correspondence,

Box

2. Biographical Materials and Photographs, 1967-2008 undated (2 boxes)

A wide range of biographical data is contained in this small series. Of particular note is a collection of autobiographical typescripts written by Dunitz from 1988-1990. The handful of photographs found in series 2 are complemented by the Caltech graduate student images located in the Gajdusek correspondence file.

- 2.001 Assorted Dunitz Biographical Materials, 1967-2008 undated (12 folders)
 - 1.1 Magazine Article: "Return to Alma Mater," *Chemistry in Britain*, February 1978 [Article refers to Dunitz's delivery of a Centenary Lecture at Glasgow University.]
 - 1.2 Typescripts: autobiographical remembrances by Jack Dunitz, 1988-1990 [Typescripts are titled *La Primavera*, *Family Background, Pasadena (1948-51)*, *Donde está la carretera para Mexico?*, *Back to Oxford (1951-53)*, *Zurich* and *Notes on this and that.*]
 - 1.3 Magazine Article: "American Crystallographic Association to Meet in Toledo," *Physics Today*, June 1991 [Article contains reference to Dunitz's receipt of the Martin J. Buerger Award from the American Crystallographic Association.]
 - 1.4 Typescript: *Scientific Work of J. D. Dunitz*, by Jack Dunitz [?], March 1996
 - 1.5 Correspondence re: Dunitz family genealogy, December 1996
 - 1.6 Bound Volume: *Arthur C. Cope Scholar Award*, presented to Jack Dunitz at the 214th American Chemical Society National Meeting, September 1997 [Volume contains abstracts of 270 scientific papers authored by Dunitz.]
 - 1.7 Typescript: *Jack Dunitz*. Oral history interview conducted by Istvan Hargittai, September 6, 1999
 - 1.8 Typescript: untitled memorial address delivered at the funeral of Jack Dunitz's brother-in-law, Harold Sellyn. Address written and delivered by Sellyn's son, who is unnamed, November 2001

- 1.9 Typescript: *Personal Records of Fellows of the Royal Society*. Autobiographical data compiled by Jack Dunitz, ca. 2004
- 1.10 Typescripts: *Curriculum Vitae* and *List of Publications*, 2008
- 1.11 Typescript: *Why My Great Grandparents Left England*, by David J. Dunitz, ca. 2000s [David Dunitz is Jack Dunitz's second cousin.]
- 1.12 Assorted Correspondence re: details of and reflections on Jack Dunitz's life and work, 1967-1992 undated
- 2.002 Photographs, 1973-2003 undated (4 folders)
- 2.1 Jack Dunitz speaking with a colleague in a lecture hall at the Bürgenstock Conference, Switzerland. Photo courtesy of Jiro Tanaka, 1973
- 2.2 Jack Dunitz engaged in discussion with A. I. Kitaigorodskii and Olga Kennard at the International Congress of Crystallography, Amsterdam. Photo courtesy of Olga Kennard, 1973
- 2.3 Group photograph of participants, including Jack Dunitz, at a gathering in Wales. Photo by Grants Studio, Llanidloes, ca. 1970s
- 2.4 Jack Dunitz posing outside an office with a younger unidentified colleague, 2003

Box**3. Publications by Jack Dunitz, 1947-2004 (8 boxes)**

Series 3 is comprised of reprints of scientific publications authored or co-authored by Jack Dunitz, as collected by Dunitz.

- 3.001 Publications by Jack Dunitz, 1947-1960 (33 folders)
- 1.1 The Crystal and Molecular Structure of Certain Dicarboxylic Acids. Part I. Oxalic Acid Dihydrate. *J. Chem. Soc.* (1947): 142-148. [J. D. Dunitz and J. M. Robertson]
- 1.2 The Crystal and Molecular Structure of Certain Dicarboxylic Acids. Part III. Diacetylenedicarboxylic Acid Dihydrate. *J. Chem. Soc.* (1947): 1145-1156. [J. D. Dunitz and J. M. Robertson]
- 1.3 Some Developments in Structural Chemistry. *Oxford Science* 2, 1 (June 1948): 24-34. [J. D. Dunitz and S. C. Wallwork]
- 1.4 Structure of Calciferol. *Nature* 162 (1948): 608-609. [D. Crowfoot and J. D. Dunitz]
- 1.5 The Structure of the Centrosymmetric Isomer of 1:2:3:4-Tetraphenylcyclobutane. *Acta Crystallogr.* 2 (1949): 1-13
- 1.6 The Constitution of the Dimer of Acenaphthylene. *Acta Crystallogr.* 2 (1949): 62. [J. D. Dunitz and L. Weissman]
- 1.7 X-ray Structure Analysis of Complex Organic Compounds. *Research* 3 (1950): 6-12
- 1.8 A Reinvestigation of the Structures of Chlorine Monoxide and Chlorine Dioxide by Electron Diffraction. *J. Amer. Chem. Soc.* 72 (1950): 3108-3112. [J. D. Dunitz and K. Hedberg]
- 1.9 X-ray Analysis of some Antibiotic Substances. *J. Amer. Chem. Soc.* 72 (1950): 4276. [J. D. Dunitz and J. E. Leonard]
- 1.10 The Crystal Structure of Chloramphenicol and Bromamphenicol. *J. Amer. Chem. Soc.* 74 (1952): 995-999
- 1.11 Purpurogallin: by X-ray Fourier Synthesis. *Nature* 169 (1952): 1087
- 1.12 Influence of Chain Length on the Symmetry of Conjugated Molecules. *J. Chem. Phys.* 20 (1952): 1328. [J. D. Dunitz and L. E. Orgel]
- 1.13 Bis-cyclopentadienyl iron: a Molecular Sandwich. *Nature* 171 (1953): 121-122. [J. D. Dunitz and L. E. Orgel]
- 1.14 Crystallography. *Ann. Rep. Chem. Soc. for 1952* 49 (1953): 343-381. [J. H. Robertson and J. D. Dunitz]
- 1.15 Electronic Structure of Metal bis-cyclopentadienyls. *J. Chem. Phys.* 23 (1955): 954-958. [J. D. Dunitz and L. E. Orgel]
- 1.16 Structure of Dithionite. *J. Amer. Chem. Soc.* 78 (1956): 878
- 1.17 The Crystal Structure of Ferrocene. *Acta Crystallogr.* 9 (1956): 373-375. [J. D. Dunitz, L. E. Orgel and A. Rich]
- 1.18 The Structure of Sodium Dithionite and the Nature of the Dithionite Ion. *Acta Crystallogr.* 9 (1956): 579-586
- 1.19 Comments on a Method of Structure Determination. *Acta Crystallogr.* 9 (1956): 537. [J. D. Dunitz and L. E. Orgel]
- 1.20 Stereochemistry of Cupric Compounds. *Nature* 179 (1957): 462-465. [L. E. Orgel and J. D. Dunitz]

- 1.21 Electronic Properties of Transition-metal Oxides - I. Distortions from Cubic Symmetry. *J. Phys. Chem. Solids* 3 (1957): 20-29. [J. D. Dunitz and L. E. Orgel]
- 1.22 Electronic Properties of Transition-metal Oxides - II. Cation Distribution amongst Octahedral or Tetrahedral Sites. *J. Phys. Chem. Solids* 3 (1957): 318-323. [J. D. Dunitz and L. E. Orgel]
- 1.23 Structure of Calciferol. *Chemistry and Industry* (1957): 1148-1149. [D. C. Hodgkin, M. S. Webster and J. D. Dunitz]
- 1.24 Structure of the Cyclododecane Molecule. *Proc. Chem. Soc.* (1958): 348-349. [J. D. Dunitz and H. M. M. Shearer]
- 1.25 The Crystal Structure of the Cuprous Chloride Azomethane Complex. *Acta Crystallogr.* 13(1960): 28-34. [I. D. Brown and J. D. Dunitz]
- 1.26 Structure of the Cyclododecane Molecule: Amendment. *Proc. Chem. Soc.* (1959): 268. [J. D. Dunitz and H. M. M. Shearer]
- 1.27 Les Structures des Cycles de Taille Moyenne. I. Un Examen aux Rayons X de quelques Sels de Cyclononylamine. *Helv. Chim. Acta* 43 (1960): 1-2. [R. F. Bryan et J. D. Dunitz]
- 1.28 Les Structures des Cycles de Taille Moyenne. II. La Structure Cristalline et Moléculaire du Bromure de Cyclononylammonium. *Helv. Chim. Acta* 43 (1960): 3-18. [R. F. Bryan et J. D. Dunitz]
- 1.29 Die Strukturen der mittleren Ringverbindungen. III. Die Struktur des Cyclododecans. *Helv. Chim. Acta* 43 (1960): 18-35. [J. D. Dunitz and H. M. M. Shearer]
- 1.30 Strukturen der mittleren Ringverbindungen. IV. 1,6-trans-Diaminocyclodecandihydrochlorid, trikline Modifikation. *Helv. Chim. Acta* 43 (1960): 760-768. [E. Huber-Buser and J. D. Dunitz]
- 1.31 The Crystal Structure of Diazoaminobenzene Copper (I). *Acta Crystallogr.* 14 (1961): 480-485. [I. D. Brown and J. D. Dunitz]
- 1.32 Röntgenographisch bestimmte Konformationen und Reaktivität mittlerer Ringe. *Angew. Chem.* 72 (1960): 896-902. [J. D. Dunitz and V. Prelog]
- 1.33 Struktur des Cycloheptatrien-molybdän-tricarbonyls, $C_7H_8Mo(CO)_3$. *Helv. Chim. Acta* 43 (1960): 2188-2197. [J. D. Dunitz and P. Pauling]
- 3.002 Publications by Jack Dunitz, 1961-1966 (38 folders)
- 2.1 The Crystal Structure of Chromium (II) Chloride. *Acta Crystallogr.* 14 (1961): 927-929. [J. W. Tracy, N. W. Gregory, E. C. Lingafelter, J. D. Dunitz, H. -C. Mez, R. E. Rundle, C. Scherlinger, H. L. Yakel, Jr. and M. K. Wilkinson]
- 2.2 Kristallographische Daten für das vermutliche 1-Anilino-4-chlor-pyromellitsäure-di-phenylimid. *Helv. Chim. Acta* 44 (1961): 442-444. [J. D. Dunitz, H.-C. Mez, H. Hopff and B. K. Manukian]
- 2.3 Conformation of the Cyclodecane Ring. *Proc. Chem. Soc.* (1961): 463. [E. Huber-Buser, J. D. Dunitz and K. Venkatesan]
- 2.4 Die Strukturen der mittleren Ringverbindungen. V. 1,6-trans-Diaminocyclodecandihydrochlorid. *Helv. Chim. Acta* 44 (1961): 2027-2033. [E. Huber-Buser and J. D. Dunitz]
- 2.5 Die Strukturen der mittleren Ringverbindungen. VI. 1,6-cis-Diaminocyclodecan-dihydrochlorid. *Helv. Chim. Acta* 44 (1961): 2033-2041. [J. D. Dunitz and K. Venkatesan]
- 2.6 Stoffwechselprodukte von Actinomyceten. 32. Mitteilung. Über die Konstitution von Nonactin. *Helv. Chim. Acta* 45 (1962): 129-138. [J. Dominguez, J. D. Dunitz, H. Gerlach and V. Prelog]
- 2.7 Kristallstruktur des Benzol-Addukts des 1, 2, 3, 4-Tetramethyl cyclobutadien-nickel (II) - chlorids. *Helv. Chim. Acta* 45 (1962): 647-665. [J. D. Dunitz, H. -C. Mez, O. S. Mills and H. M. M. Shearer]
- 2.8 Nature of Orientational Defects in Ice. *Nature* 197 (1963): 860-862
- 2.9 The crystal structure of aureomycin (chlortetracycline) hydrochloride. Configuration, bond distances and conformation. *J. Amer. Chem. Soc.* 85 (1963): 851-856. [J. Donohue, J. D. Dunitz, K. N. Trueblood and M. S. Webster]
- 2.10 The Crystal Structure of a Calciferol Derivative. *J. Chem. Soc.* (1963): 4945-4956. [D. C. Hodgkin, B. M. Rimmer, J. D. Dunitz and K. N. Trueblood]
- 2.11 The Supposed Existence of two Molecular Forms in Crystals of Acetyl Choline Bromide. *Acta Chem. Scand.* 17 (1963): 1471-1472
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Box**4. Manuscripts and Lecture Materials, 1946-2006 undated (7 boxes)**

- 4.001 Manuscripts of Articles by Jack Dunitz, 1946-1991 (30 folders) [This series contains a diverse collection of manuscripts and lecture materials, including a number of transparencies, drawings for slides and other visual aids created by Dunitz for use in presentation. Included in this series are several pieces written by Dunitz on the life and work of notable scientists, including Linus Pauling, John Montearth Robertson and Vladimir Prelog.]
- 1.1 Typescripts: "Verse", 1946-1952 1990 [Series of poems, some of them parodies of other works, written by Dunitz. Titles include *The Research Student's Lament*, *Our Worlds Came in Collision*, *Lines Addressed to Dr. Orgel* and *Of Molecules and Men*.]
- 1.2 Typescript: *The Tragical Comedie of Dr. Faustus. Or "Scientia vincit omnia."* Stage play written by J. D. Dunitz and C. E. Harrold. ["vaguely adapted from the 'Faustus' play of Christopher Marlow, esq."] Composed for the Caltech-Biology Biology Christmas party, 1950
- 1.3 Typescript, Correspondence, Referee's Report: *Electronic Structure of Metal Bis-Cyclopentadienyls*, by Jack Dunitz and Leslie Orgel, March 1953
- 1.4 Typescript, Notes, Correspondence: *The Crystal Structure of Ferrocene*, by Jack Dunitz, Leslie Orgel and Alexander Rich, 1954-1955
- 1.5 Manuscript, Correspondence, Referee's Report: *Stereochemistry of Cupric Compounds*, 1956-1957
- 1.6 Typescript: *Crystals*, 1957
- 1.7 Manuscripts, Notes, Correspondence: *Molecular Energetics Drafts*, ca. 1958 [Series of untitled manuscripts for a proposed book.]
- 1.8 Manuscript: *Lattices*, ca. 1950s
- 1.9 Manuscript: *Scattering of X-rays by Matter*, ca. 1950s
- 1.10 Manuscript, Typescripts, Correspondence, Notes: *The Nature of Orientational Defects in Ice*, November 1962
- 1.11 Typescript: Untitled discussion of the determination of molecular structure by X-ray diffraction methods, ca. 1962
- 1.12 Typescripts, Correspondence, Referee's Report: *Configuration, Conformation and Chirality*, 1965
- 1.13 Typescript, Notes, Correspondence: *Silver Fluoride - Preparation from Silver Carbonate*, 1965-1967
- 1.14 Typescript: *The Crystal Structure of Dibenzyl Phosphoric Acid, A Correction*, by Jack Dunitz and J. S. Rollett, 1968
- 1.15 Typescript, Notes, Correspondence, Visual Aids: *Molecular Basis of Alkali Cation Transport by Macrocyclic Antibiotics of the Valinomycin Group*, by Jack Dunitz and A. D. McLachlan, April 1969
- 1.16 Manuscript, Correspondence: *Pentagon (in Space) with All Angles and All Distances Equal Must Be Planar*, 1971
- 1.17 Typescript, Notes: *Non-empirical SCF calculations on hydrogenlike molecules: the effect of nuclear charge on binding energy and bond length*, by Jack Dunitz and T. K. Ha, 1972
- 1.18 Typescript: *The Early History of Silver Cyanate and Fulminate*, by Doyle Britton and Jack Dunitz, ca. 1970s
- 1.19 Typescript, Correspondence, Referees' Reports, Background Materials: *Electron Density Distribution in the Organic Superconductor (TMTSF)₂AsF₆: Fact and Fancy*, December 1983

- 1.20 Typescript, Notes: *Measurement of the State of Ionicity of the Atoms in Lithium Fluoroberyllate, a Conventionally Ionic Crystal*, ca. 1985
- 1.21 Typescript: *Science Students*, letter to the editor of *The Economist* by Jack Dunitz, September 15, 1987
- 1.22 Typescripts: *Edward Wesley Hughes (1904-1987)*, ca. 1988
- 1.23 Typescript: *Personal Reminiscences*, [re: the life and work of Alexander Isaakovich Kitaigorodsky], ca. 1989 [Written as a preface for a special issue of *Acta Chimica Hungarica*, "Models in Chemistry - A. I. Kitaigorodskii Memorial Issue."]
- 1.24 Typescript: *Conformational Polymorphism of Ferrocene*, by Carolyn Brock, Daniel Selski, Emily Maverick and Jack Dunitz, ca. 1989
- 1.25 Typescript: *Distance Geometry and Molecular Conformation*, by G. M. Crippen and T. F. Havel. *John Wiley and Sons*, 1989
- 1.26 Manuscript, Typescript: *Structural Variability of Aliphatic Nitro Groups*, Yasushi Kai and Jack Dunitz, ca. 1980s
- 1.27 Typescript: *John Monteath Robertson (1900-1989)*, ca. 1990
- 1.28 Typescript: *The Cambridge Structural Database as a New Scientific Tool*, February 7, 1991
- 1.29 Typescript: *Linus Pauling - Born 1901, Still Going Strong*, May 1991
- 1.30 Typescript, Notes, Correspondence: *Racemates and Conglomerates: Wallach's Rule*, by Carolyn P. Brock, W. Bernd Schweizer and Jack D. Dunitz, ca. 1991
- 4.002 Manuscripts of Articles by Jack Dunitz, 1994-2006 undated (29 folders)
- 2.1 Typescript, Correspondence: *Linus Pauling (1901-1994); Some Personal Recollections*, September 1994
- 2.2 Typescript, Correspondence: *A New Look at Proton Transfer Dynamics Along the Hydrogen Bonds in Amides and Peptides*, December 1994
- 2.3 Typescript, Correspondence: *Linus Pauling, 1901-1994*, ca. 1994
- 2.4 Typescript: *LINUS CARL PAULING, 29 [sic] February 1901 - 19 August 1994, Elected For. Mem. R. S. 1948*, ca. 1994
- 2.5 Typescript: *LINUS CARL PAULING, 28 February 1901 - 19 August 1994*, ca. 1994
- 2.6 Typescript, Correspondence, Background Materials: *A New Look at Proton Transfer Dynamics Along the Hydrogen Bonds in Amides and Peptides*, 1994-1995
- 2.7 Typescript, Correspondence, Background Materials: *Right and Left in Chiral Crystals*, February 1995
- 2.8 Correspondence, Background Materials: *Disappearing Polymorphs*, ca. 1995
- 2.9 Typescript, Correspondence, Background Materials: Letter to the Editor of *Chemical and Engineering News*. [re: changes in the publication policy enforced by the *Journal of the American Chemical Society*], June 13, 1996 [Published in the *International Union of Crystallography Newsletter*, 4, 3 (1996): 4.]
- 2.10 Typescript, Correspondence: *Potassium Channels: the Dubious Role of $K^{+..pi}$ Interactions*, by Robin Taylor and Jack Dunitz, March 1996
- 2.11 Typescript: *Force of Nature: the Life of Linus Pauling*, by Thomas Hager. 1995. *New York: Simon & Schuster*. 721 pp., 1996
- 2.12 Typescript, Notes, Correspondence, Figures: *Chemical Reaction Paths. IX. Visualization of Four-Dimensional Stereoisomerization Paths for Ph4X Molecules*, ca. 1997
- 2.13 Typescript: *Verner Schomaker (1914-1997)*, ca. 1997
- 2.14 Typescript: *Dorothy Crowfoot Hodgkin: an Introduction to her Work and Personality*, ca. 1997
- 2.15 Typescript: *Recollections of Pre-Prebiotic Leslie Orgel*, ca. 1997
- 2.16 Typescript: *Kenneth N. Trueblood (1920-1998)*, ca. 1998
- 2.17 Typescript: *Encounters with Bragg*, ca. 1990s
- 2.18 Typescript: *Right and Left at the Brgerstock Conference 1973*, ca. 1990s
- 2.19 Typescript: *Ewald - Sommerfeld - von Laue anecdote*, ca. 1990s
- 2.20 Assorted untitled Dunitz typescripts and research materials re: the life and work of Linus Pauling, ca. 1990s
- 2.21 Typescripts, Correspondence: *Vladimir Prelog, 23 July 1906 - 7 January 1998*, by Duilio Arigoni, Jack Dunitz and Albert Eschenmoser, 2000
- 2.22 Typescripts, Galley Proofs, Correspondence, Background Materials: *Pauling's left-handed alpha-helix*, June 2001
- 2.23 Typescript: *Sir John Meurig Thomas at 70*, 2002
- 2.24 Typescript: *Light is a Messenger: The life and science of William Lawrence Bragg*, by Dr. Graeme K Hunter. *Oxford University Press*, 2004

- 2.25 Typescript, Correspondence, Referee's Report: *Exercises in Prognostication: Crystal Structures and Protein Folding*, 2004
- 2.26 Typescript, Correspondence: *Are Crystal Structure [sic] Predictable?*, ca. 2004
- 2.27 Typescript: *1905 Anno Mirabilis: Albert Einstein's Influence on Modern Chemistry*, 2005
- 2.28 Typescript: The Pauling Catalogue, *Oregon State University Libraries, Corvallis, OR, 2007, 6 vol., \$125*, 2006
- 2.29 Typescripts: "Stories", undated [Series of short fiction stories written by Dunitz. Titles include *Orpheus und Eurydice, Julia's Japanese Story, Captain Marinette - The Story of a Sailor, Bruno Leaves Home, Idomeno, Re di Creta, Astrochem* and *A Mysterious Visitor.*]
- 4.003 Lectures by Jack Dunitz, 1953-1976 (14 folders)
- 3.1 Manuscript: Untitled discussion of the application of quantum mechanics to chemistry, with special focus on the Molecular Orbital method, ca. 1953
- 3.2 Manuscript: *Cyclopentadienyl Talk*, ca. 1956
- 3.3 Typescript: *Distortions from Cubic Symmetry*, 1957
- 3.4 Typescript, Background Materials: Untitled discussion of cyclobutadiene, 1959
- 3.5 Typescripts: Untitled lecture on contemporary developments in crystallography, Inaugural Lecture, Swiss Federal Institute of Technology, Zurich, Switzerland, ca. 1959 [English and German-language typescripts.]
- 3.6 Manuscripts: X-ray analysis lectures, ca. 1950s [Extensive series of lecture manuscripts discussing the specifics of x-ray analysis.]
- 3.7 Manuscript: *Structural Investigations of Some Antibiotic Substances*, ca. 1960s
- 3.8 Notebook: *X-Ray Diffraction Lectures - Disorder*, ca. 1960s
- 3.9 Typescript: *Role of Diffraction Methods in Conformational Analysis*, J. M. Robertson Symposium, Glasgow, Scotland, September 1970
- 3.10 Typescript, Notes, Background Materials: *A Simple Selection Rule for Electrocyclic Reactions*, ca. 1970
- 3.11 Typescript, Notes: *The Future of Crystallography as an Academic Discipline*, lecture delivered in London, England, November 24, 1972
- 3.12 Manuscript, Notes: Untitled lecture on complexes of alkali and alkaline earth complexes with organic ligands, ca. 1972
- 3.13 Typescript: *Organische Chemie*, Eschenmoser lecture, Basel, Switzerland, March 26, 1976
- 3.14 Manuscript, Correspondence, Program, Background Materials: *Chemical Research*, International Agrarisch Centrum, Wageningen, The Netherlands, May 26, 1976
- 4.004 Lectures by Jack Dunitz, 1977-2006 undated (31 folders)
- 4.1 Typescript, Notes: *Von Kristallstrukturen zu chemischen Reaktionswegen*. Keynote Speech, Annual General Meeting of the German Chemical Society, Munich, Germany, September 14, 1977
- 4.2 Manuscript: Untitled lecture on non-bonded interactions, ca. 1970s
- 4.3 Typescript, Background Materials: *The Cyclohexane Ring*, ca. 1970s
- 4.4 Manuscript: Untitled lecture on the need to reconsider the initial classification of primary processes related to 3-coordinated and 5-coordinated species. Presented at the "Idea Centenary", ca. 1970s
- 4.5 Manuscript Notes re: untitled lecture on irregular coordination, ca. 1970s
- 4.6 Manuscript: *Physical Methods in Structure Analysis: Structure Analysis by X-ray Diffraction - Scope and Limitation*, ca. 1970s
- 4.7 Typescript, Notes: *Crystal Structure and Chemical Reactivity*, ca. 1970s
- 4.8 Typescript: Untitled lecture on the physical and chemical properties of medium-sized alicyclic rings, ca. 1970s
- 4.9 Typescript: *Unverrichtete Dinge*, ["Empty handed"] talk delivered at a celebration held at ETH Zürich, July 7, 1989
- 4.10 Typescript, Correspondence, Background Materials: *After-dinner Talk at the Symposium in Memory of David Ginsburg, Haifa, September 19, 1989*
- 4.11 Typescript: untitled German-language remarks delivered at a meeting of the Swiss Technion Society, December 5, 1990
- 4.12 Lecture Notes, Photograph, Program: Eighteenth Course on Static, Kinematic and Dynamic Aspects of Crystal and Molecular Structure, International School of Crystallography. Erice, Italy. Hans-Beat Bürgi and Jack D. Dunitz, directors, May 30 - June 9, 1991 [Includes a group photo of all who attended the conference in Erice. Dunitz is seated in the front row, sixth from left.]

- 4.13 Typescript, Program, Visual Aids: *Phase Transitions in Molecular Crystals: A Chemical Viewpoint, Forty Years of Ferrocene and From Crystal Data Towards Chemical Reaction Paths*, Robert Burns Woodward Lectureship, Harvard University, April 14 - May 11, 1992
- 4.14 Typescript: *Scientists and their Social Responsibility*, manuscript prepared for a meeting of Fundacion BBV, Bilbao, Spain, ca. September 1992
- 4.15 Typescript: untitled lecture on Dorothy Hodgkin and Linus Pauling. Published in *Dorothy Hodgkin and Linus Pauling: A Tribute*, talks presented at the Montreal meeting of the American Crystallographic Association, July 25, 1995
- 4.16 Typescript: untitled reminiscence of Alexander Rich on the occasion of his receipt of an unknown award. Eugene, Oregon, October 28, 1995
- 4.17 Typescript: *Symmetry Considerations in Chemistry*. Symposium on "Symmetry throughout the Sciences," Washington, D. C., November 25-27, 1997 [Annotated "contains 'Dunitz's Conjecture'."]
- 4.18 Typescript: *Thoughts on European Culture and Unity*, meeting of Fundacion BBV, Bilbao, Spain, October 4-5, 1998
- 4.19 Typescripts: *Scientific Research - Panacea or Pandora's Box* [alternatively titled by Dunitz as "Spain Talk."], ca. 1990s [Folder also contains a thematically related partial typescript titled "BBV Lecture."]
- 4.20 Manuscript: Untitled discussion of mathematical puzzles and Linus Pauling, ca. 1990s
- 4.21 Typescript: *Max Perutz, 1914-2002*, ca. 2002
- 4.22 Typescript: untitled remarks delivered at a symposium held in celebration of Dunitz's eightieth birthday, 2003
- 4.23 Abstract, Program: *Are Crystal Structures Predictable?* Conference on Non-Covalent Interactions in Chemistry and Biology, University of Cambridge, September 16, 2004
- 4.24 Typescript: *CCDC Dinner*. Remarks made at the fortieth anniversary celebration of the Cambridge Crystallographic Data Centre, September 23, 2005
- 4.25 Typescript, Background Materials: *Edgar Heilbronner, 1921-2006*, 2006
- 4.26 Typescript: *Sydney Brenner*, ca. 2000s
- 4.27 Typescript: *The Golden Age at Caltech*, ca. 2000s
- 4.28 Manuscript: *Notes on Hydrogen Bonding*, undated
- 4.29 Manuscript: Untitled introduction to x-ray crystallographic analysis, undated
- 4.30 Manuscript: Untitled discussion of the relationship between crystal chemistry and the electronic structure of ions, undated
- 4.31 Assorted non-Dunitz quotations for use in presentations and articles, undated
- 4.005 Lecture Transparencies, ca. 2000 (5 folders)
- 5.1 Lecture Transparencies re: crystal structure, ca. 2000
- 5.2 Lecture Transparencies re: general and organic chemistry, ca. 2000 [Text primarily in German.]
- 5.3 Lecture Transparencies re: history of crystallography, ca. 2000
- 5.4 Lecture Transparencies re: phase transitions and polymorphism, ca. 2000
- 5.5 Lecture Transparencies re: symmetry, ca. 2000
- 4.006 Assorted Transparencies, Figures and Visual Aids, undated (1 folder)
- 6.1 Assorted Transparencies, Figures and Visual Aids, undated
- 4.007 Drawings for Slides, undated (1 folder)
- 7.1 Drawings for Slides, undated [Drawings created for eventual conversion into lecture transparencies.]

Box

5. Research Notes and Notebooks, 1941-1989 (5 boxes)

Series 5 consists of research notes, arranged alphabetically by subject, and research notebooks, arranged chronologically. The diversity of topics represented in this series are indicative of the many scientific interests maintained by Dunitz over the course of his career.

- 5.001 Research Notes, 1946-1950 1953-1954 1966 1970 (9 folders)
- 1.1 Notes, Background Materials re: "Couper's Compound", 1966 1970 [Includes x-ray crystallographic photographs labeled "Cooper's Compound."]

- 1.2 Notes re: crystal structure determinations, ca. 1950s [Includes examinations of adamantane, cyclohexane, cyclohexene and cyclooctadiene among others.]
- 1.3 Notes re: electromagnetism, ca. 1950s
- 1.4 Notes re: hemoglobin, 1953-1954
- 1.5 Notes: "Method of Finding Maximum of Fourier Peak by Least Squares (Shoemaker)", ca. 1950s [Notes on a technique devised by David Shoemaker.]
- 1.6 Notes: "Molecular Statics", 1949-1950
- 1.7 Notes re: nitrogen, ca. 1950s
- 1.8 Notes re: research reports, 1946-1949
- 1.9 Notes re: ribonucleic acid, 1953
- 1.10 Notes re: statistical thermodynamics, 1946 [Notes primarily from a lecture delivered by W. C. Orr.]
- 1.11 Notes re: sulphur, ca. 1950s
- 1.12 Notes: "Waves", ca. 1950s
- 5.002 Research Notebooks, 1941-1946 (6 folders)
 - 2.1 Research Notebook: "Mathematics: Calculus, Infinite Series", 1941-1942
 - 2.2 Research Notebook: "Mathematics: 3 Dimensional Coordinate Geometry, Partial Differentiation", 1944
 - 2.3 Research Notebook: "Mathematics: Integral Calculus (Adv.), Differential Equations", 1944-1945
 - 2.4 Research Notebook: "Acetylene Dicarboxylic Acid Dihydrate, Diacetylene Dicarboxylic Acid Dihydrate, Research Book I", 1944-1946
 - 2.5 Research Notebook: "Physics; Triple Bond Calculations", 1944-1946
 - 2.6 Research Notebook: "Acetylene Dicarboxylic Acid Dihydrate, Diacetylene Dicarboxylic Acid Dihydrate, Research Book II", 1945
- 5.003 Research Notebooks, 1948-1951 (6 folders)
 - 3.1 Research Notebook: "Electron Diffraction of Gas Molecules", 1948-1949
 - 3.2 Research Notebook: "Calciferol Iodo-Nitro Benzoate", 1948-1949
 - 3.3 Untitled Research Notebook, 1949-1950 [Notebook is primarily devoted to a detailed exploration of the structures of chloromycetin, bromamphenicol and aureomycin. Also includes notes on terramycin hydrochloride and isoplasmicide.]
 - 3.4 Research Notebook: "Stercobilin Hydrochloride", 1949-1951 [Also contains notes titled "Dimerisation Product of Acenaphthylene."]
 - 3.5 Untitled Research Notebook, 1950 [Contains notes on quantum mechanics, the movement of electrons and the structure of the hydrogen molecule. Also contains notes on bond orbital hybridization, optics and the "4 electron problem."]
 - 3.6 Untitled Research Notebook, ca. 1951 [Contains notes on Pauling's "Nature of the Chemical Bond" as well as a comparison of the valence bond and molecular orbital theories of chemical structure as utilized in colleague's publications.]
- 5.004 Research Notebooks, 1952-1955 (6 folders)
 - 4.1 Untitled Research Notebook, 1952 [First interior page is titled "Elementary Thermodynamics Notes."]
 - 4.2 Untitled Research Notebook, 1952-1953 [Contains analyses of various crystal structures and notes on colleagues' structural chemistry publications.]
 - 4.3 Untitled Research Notebook, 1953-1954 [Contains notes on nucleic acids and proteins, as well as colleagues' structural chemistry research.]
 - 4.4 Research Notebook: "Misc Notes", 1954-1955 [Contains notes on nucleic acids, hemoglobin, proteins and model building. Also contains notes on angular momentum and the movement of electrons.]
 - 4.5 Research Notebook: "NIH Exp 54-55", 1954-1955 [First interior page is titled "Experiments in Molecular Complex Formation Among Purines, Pyrimidines, etc." Also includes notes on nucleic acids and experiments on Na₂S₂O₄.]
 - 4.6 Research Notebook: "Misc 55", 1955 [Contains notes on light scattering, molecular orbitals and assorted crystal structure determinations. Also contains work on ferrocene, sodium hydrosulfite and chromium dibenzene.]
- 5.005 Research Notebooks, 1956 1967-1968 1970-1989 (7 folders)
 - 5.1 Untitled Research Notebook, 1956 [Contains Dunitz's daily log of work that he has conducted as well as notes on colleagues' publications on a variety of topics.]
 - 5.2 Research Notebook: "Diffractionmeter", 1967-1968

- 5.3 Untitled Research Notebook, 1970-1974 1982 1985 [Contains notes and calculations on a number of topics related to crystal structure.]
- 5.4 Research Notebook: "Mo Theorie", 1971-1972
- 5.5 Research Notebook: "Pentagons", June 1972
- 5.6 Research Notebook: "Literature", 1973-1978
- 5.7 Research Notebook: "Mathematics", 1973-1989

Box**6. Subject Files, 1927-2008 (19 boxes)**

The subject files held in series 6 consist of notes and subject-specific publications collected and organized by Dunitz over time.

- 6.001 Subject Files: A, 1927-2002 (4 folders)
 - 1.1 Notes, Publications re: alkali cation complexes, 1969-2002
 - 1.2 Notes, Publications re: amino acids, 1969-2002
 - 1.3 Notes, Publications re: aromatic compounds, 1956-1987
 - 1.4 Notes, Publications re: atomic motion in solids, 1927-2000
- 6.002 Subject Files: B, 1948-2004 (5 folders)
 - 2.1 Publications re: bicyclobutanes, 1977-1982
 - 2.2 Notes, Publications re: biochemistry, 1948-2004
 - 2.3 Publications re: biographical sketches, 1948-2004 [Collected biographical materials related to various scientists.]
 - 2.4 Publications re: Bond Energy Bond Order (BEBO) method, 1960-1968
 - 2.5 Notes, Publications re: bonds, orbitals and lone pairs, 1951-1999
- 6.003 Chirality [1 of 2], 1964-2004 (1 folder)
 - 3.1 Notes, Publications re: chirality [1 of 2], 1964-2004
- 6.004 Chirality [2 of 2], 1975-2001 (1 folder)
 - 4.1 Notes, Publications re: Chirality [2 of 2], 1975-2001
- 6.005 Subject Files: Co - Cr, 1940-2000 (2 folders)
 - 5.1 Notes, Publications re: conformational analysis, 1940-1986
 - 5.2 Notes, Publications re: crystal structure determination, 1953-2000
- 6.006 Subject Files: E, 1969-2003 (3 folders)
 - 6.1 Publications: "Eccentric Articles", 1981-2003 [Articles relating to chemistry which Dunitz found to be outlandish. Dunitz has annotated one article as "Rubbish!"]
 - 6.2 Notes, Publications re: electron density, 1969-1990
 - 6.3 Publications re: electron diffraction, 1970-1990
- 6.007 Ferrocene [1 of 2], 1952-2005 (2 folders)
 - 7.1 Notes, Publications re: ferrocene and other metallocenes, 1953-2005
 - 7.2 Notes, Publications re: ferrocene and other metallocenes, 1952-2001
- 6.008 Ferrocene [2 of 2], 1953-1991 (1 folder)
 - 8.1 Publications re: ferrocene and other metallocenes, 1953-1991
- 6.009 Subject Files: Fo - G, 1949-1983 (2 folders)
 - 9.1 Notes, Publications re: force constants and reaction paths, 1960-1983
 - 9.2 Notes, Publications re: group theory, 1949-1976
- 6.010 History of Chemistry, 1938-1967 2003 (2 folders)
 - 10.1 Publications re: history of chemistry, 1938-1967 [Files includes photocopy of A. L. Patterson's lengthy handwritten account of his 1926 visit to England.]
 - 10.2 Publications re: history of DNA, 2003
- 6.011 Subject Files: Hy, 1953-2008 (3 folders)
 - 11.1 Notes, Publications re: hydrogen bonding, 1964-2008
 - 11.2 Notes, Publications re: hydrogen gas, 1953-1972
 - 11.3 Notes, Publications re: hydrolysis, 1972-1980
- 6.012 Subject Files: I - Mi, 1950-1991 (4 folders)

- 12.1 Notes, Publications re: ice, 1958-1965
- 12.2 Publications re: lithium compounds, 1950-1991
- 12.3 Publications re: methadone, 1973-1974
- 12.4 Notes, Publications re: middle rings, 1956-1969
- 6.013 Molecular Geometry, 1944-1983 (1 folder)
- 13.1 Notes, Publications, Visual Aids re: molecular geometry, 1944-1983
- 6.014 Subject Files: N - Pa, 1956-2005 (4 folders)
- 14.1 Publications re: neutron diffraction, 1972
- 14.2 Notes, Publications re: nitroso compounds, 1956-1982
- 14.3 Notes, Publications re: organic conductors, 1978-1991
- 14.4 Publications re: packing in chemical structures, 1962-2005
- 6.015 Phase Transitions, 1957-2001 (1 folder)
- 15.1 Notes, Publications re: phase transitions, 1957-2001
- 6.016 Subject Files: Pol - R, 1940-2007 (3 folders)
- 16.1 Notes, Publications re: polymorphism, 1940-2007
- 16.2 Notes, Publications re: potassium ion channels, 1981-2001
- 16.3 Publications re: reactivity of organic solids, 1990
- 6.017 Subject Files: Sp - St, 1942-1998 (2 folders)
- 17.1 Notes, Publications re: space groups, 1942-1998
- 17.2 Notes, Publications re: structure correlation, 1965-1998
- 6.018 Subject Files: St - Sy, 1935-2006 (2 folders)
- 18.1 Notes, Publications re: structure - miscellaneous, 1935-2006
- 18.2 Notes, Publications re: symmetry, 1962-1981
- 6.019 Subject Files: T - X, 1937-2002 (7 folders)
- 19.1 Notes, Publications re: tetrahedra, 1956-1976
- 19.2 Notes, Publications re: tobacco mosaic virus, 1952-1955
- 19.3 Publications re: travel, 1943-1948
- 19.4 Notes, Publications re: vitamin B12, 1959-1982
- 19.5 Publications re: vitamin C, 1953-1977
- 19.6 Publications re: Woodward-Hoffman rules, 1937-1972
- 19.7 Notes, Publications re: x-ray analysis, 1957-2002