

# Author index

Entries refer to chapter number.

- Abad-Zapatero, C., 2.3, 3.3  
 Abdel-Meguid, S. S., 2.3, 3.3  
 Abi-Ezzi, S. S., 3.3  
 Ablov, A. V., 2.5  
 Abrahams, S. C., 2.3, 2.4  
 Abramowitz, M., 2.1  
 Achard, M. F., 4.4  
 Acharya, R., 2.3  
 Adams, M. J., 2.3, 2.4  
 Addison, A. W., 2.3  
 Adlhart, W., 4.2  
 Aeppli, G., 4.4  
 Afanas'ev, A. M., 5.3  
 Agard, D. A., 2.4  
 Agarwal, R. C., 1.3, 2.4  
 Aharonov, Y., 3.3  
 Aharony, A., 4.4  
 Ahlfors, L. V., 1.3  
 Ahmed, F. R., 1.3  
 Åkervall, K., 2.3  
 Akhiezer, N. I., 1.3  
 Akimoto, T., 2.3  
 Al Haddad, M., 5.3  
 Al-Khayat, H. A., 4.5  
 Alben, R., 4.4  
 Albertini, G., 5.3  
 Alden, R. A., 1.3  
 Alexander, L. E., 4.2  
 Alexeev, D. G., 4.5  
 Allegra, G., 2.2  
 Allen, F. H., 3.3  
 Allen, L. J., 4.3  
 Allinger, N. L., 3.3  
 Als-Nielsen, J., 4.4  
 Alston, N. A., 1.3  
 Altermatt, U. D., 1.4  
 Altmann, S. L., 1.5  
 Altomare, A., 2.2  
 Altona, C., 3.3  
 Amador, S., 4.4  
 Amelinckx, S., 4.3  
 Amma, E. L., 3.3  
 Amorós, J. L., 4.2  
 Amorós, M., 4.2  
 Amos, L. A., 2.5  
 An, M., 1.3  
 Anderson, D. C., 3.3  
 Anderson, P. W., 4.4  
 Anderson, S., 3.3  
 Anderson, S. C., 2.5  
 Andersson, B., 4.3  
 Andersson, G., 4.4  
 Ando, M., 5.3  
 Andreeva, N. S., 2.4  
 Andrews, J. W., 2.5  
 Angress, J. F., 4.1  
 Anzenhofer, K., 2.2  
 Apostol, T. M., 1.3  
 Arai, M., 4.2  
 Ardito, G., 2.2  
 Arfken, G., 1.2, 3.4  
 Argos, P., 2.2, 2.3  
 Arif, M., 5.3  
 Arley, N., 3.2  
 Arndt, U. W., 2.4, 4.2  
 Arnold, D. B., 3.3  
 Arnold, E., 2.3  
 Arnold, H., 1.1, 1.3  
 Arnott, S., 4.5  
 Aroyo, M. I., 1.5  
 Arrott, A. S., 5.3  
 Arthur, J., 5.3  
 Artin, E., 1.3  
 Ascher, E., 1.3  
 Ash, J. M., 1.3  
 Ashcroft, N. W., 1.1  
 Ashida, T., 2.4  
 Atkins, E. D. T., 4.5  
 Atwood, D. K., 5.3  
 Au, A. Y., 2.5, 4.2  
 Auslander, L., 1.3  
 Authier, A., 1.4, 5.1  
 Avery, J., 1.2  
 Avilov, A. S., 2.5  
 Avraham, D. ben, 4.5  
 Avrami, M., 2.2  
 Axe, J. D., 4.2  
 Axel, F., 4.6  
 Ayoub, R., 1.3  
 Bacon, G. E., 5.3  
 Badurek, G., 5.3  
 Baer, E., 4.5  
 Bagchi, S. N., 2.3, 4.2, 4.5  
 Baggio, R., 2.2  
 Baird, T., 2.5  
 Bak, H. J., 2.3  
 Bak, P., 4.4  
 Baker, E. N., 1.3, 2.3  
 Baker, T. S., 2.3  
 Baldwin, J. M., 2.5  
 Balibar, F., 5.1  
 Banaszak, L. J., 2.3  
 Bancel, P. A., 4.6  
 Bando, Y., 2.5  
 Banerjee, K., 2.2  
 Bannister, C., 2.5  
 Bansal, M., 1.3  
 Bantz, D., 1.3  
 Barakat, R., 1.3, 2.1  
 Bardhan, P., 4.2  
 Barham, P. J., 4.5  
 Barnea, Z., 1.2  
 Barnes, W. H., 1.3  
 Barois, P., 4.4  
 Barrett, A. N., 1.3  
 Barrington Leigh, J., 4.5  
 Barry, C. D., 3.3  
 Bartels, K., 1.3, 2.3, 2.4  
 Baruchel, J., 5.3  
 Barynin, V. V., 2.5  
 Baryshevskii, V. G., 5.3  
 Basett-Jones, D. P., 2.5  
 Bash, P. A., 3.3  
 Baskaran, S., 4.5  
 Batterman, B. W., 5.1  
 Baturic-Rubcic, J., 4.4  
 Bauer, G., 4.2  
 Bauspiess, W., 5.3  
 Beaglehole, D., 4.4  
 Bean, J. C., 2.5  
 Becker, P. J., 1.2, 5.3  
 Beckmann, E., 2.5  
 Beddell, C., 3.3  
 Bedzyk, M. J., 5.1  
 Beevers, C. A., 1.3, 2.3  
 Beintema, J. J., 2.3  
 Bellamy, H. D., 3.3  
 Bellamy, K., 4.5  
 Bellard, S., 3.3  
 Bellman, R., 1.3  
 Bellocq, A. M., 4.4  
 Belova, N. E., 5.3  
 Belyakov, V. A., 5.3  
 Benattar, J. J., 4.4  
 Bender, R., 2.5  
 Bengtsson, U., 2.3  
 Benguigui, L., 4.4  
 Bennett, J. M., 1.3  
 Bensimon, D., 4.4  
 Bentley, J., 1.2  
 Berberian, S. K., 1.3  
 Berger, J. E., 2.5  
 Bergman, G., 3.2  
 Bergmann, K., 4.4  
 Berliner, R., 5.3  
 Berman, H. M., 1.4  
 Bernstein, F. C., 3.3  
 Bernstein, H. J., 5.3  
 Bernstein, S., 2.1  
 Berry, M. V., 5.2  
 Bertaut, E. F., 1.3, 1.4, 2.2, 3.4  
 Berthou, J., 2.3  
 Bessière, M., 4.2  
 Bethe, H. A., 1.2, 2.5, 5.2  
 Bethge, P. H., 3.3  
 Beurskens, G., 2.2  
 Beurskens, P. T., 2.2, 2.3  
 Beyeler, H. U., 4.2  
 Bhat, T. N., 2.3, 2.4  
 Bhattacharya, R. N., 1.3  
 Bieberbach, L., 1.3  
 Bienenstock, A., 1.3, 1.4  
 Bijvoet, J. M., 2.2, 2.3, 2.4  
 Bilderback, D. H., 5.1  
 Bilhorn, D. E., 2.5  
 Billard, J., 4.4  
 Billard, L., 4.6  
 Bilz, H., 4.1  
 Bing, D. H., 3.3  
 Birgeneau, R. J., 4.4  
 Biswas, A., 4.5  
 Blackman, M., 2.5, 4.1, 5.2  
 Blackwell, J., 4.5  
 Blahut, R. E., 1.3  
 Blech, I., 2.5, 4.6  
 Bleistein, N., 1.3  
 Bley, F., 4.2  
 Blinc, R., 4.4  
 Bloch, F., 1.1, 4.1  
 Bloomer, A. C., 1.3, 2.3, 3.3  
 Blow, D. M., 1.3, 2.2, 2.3, 2.4  
 Bluhm, M. M., 2.3  
 Blume, J., 5.2  
 Blume, M., 5.3  
 Blundell, D. J., 4.5  
 Blundell, T. L., 2.3, 2.4  
 Bochner, S., 1.3  
 Bode, W., 1.3, 2.4  
 Bodo, G., 2.3  
 Boege, U., 2.3  
 Boeuf, A., 5.3  
 Böhm, H., 4.6  
 Böhme, R., 2.2  
 Bokhoven, C., 2.4  
 Bokun, R. Ch., 5.3  
 Bommel, A. J. van, 2.3, 2.4  
 Bondot, P., 1.3  
 Bonnet, M., 5.3  
 Bono, P. R., 3.3  
 Bonse, U., 5.1, 5.3  
 Boon, M., 1.5  
 Booth, A. D., 1.3  
 Borell, A., 2.3  
 Borie, B., 4.2  
 Born, M., 1.2, 1.3, 4.1, 5.1, 5.2  
 Borrmann, G., 5.1  
 Bosman, W. P., 2.2  
 Böttger, H., 4.2  
 Bouckaert, L. P., 1.5  
 Boulay, D. J. du, 1.4, 2.2  
 Bouman, J., 2.2  
 Bourne, P. E., 1.4  
 Boutin, H., 4.1  
 Bowen, D. K., 5.1  
 Boyd, D. B., 3.3  
 Boyer, L., 4.1  
 Boyle, L. L., 1.5  
 Boysen, H., 4.2  
 Bracewell, B. N., 2.5  
 Bracewell, R. N., 1.3  
 Bradler, J., 5.3  
 Bradley, A. J., 2.4  
 Bradley, C. J., 1.5, 4.2  
 Bragg, L., 1.4  
 Bragg, W. H., 1.3  
 Bragg, W. L., 1.3, 2.3, 5.1  
 Brämer, R., 4.2  
 Brand, P., 4.4  
 Brandenburg, N. P., 3.3  
 Braslau, A., 4.4  
 Braun, H., 3.3  
 Braun, P. B., 2.3  
 Bremermann, H., 1.3  
 Bremmer, H., 1.3  
 Brennan, S., 5.1  
 Brice, M. D., 1.3, 3.3  
 Bricogne, G., 1.3, 2.2, 2.3, 2.5, 3.3, 4.5  
 Brigham, E. O., 1.3  
 Brill, R., 1.3  
 Brinkman, W. F., 4.4  
 Brisbin, D., 4.4  
 Brisse, F., 2.5, 4.5  
 Britten, P. L., 1.3, 2.2  
 Brock, J. D., 4.4  
 Brockhouse, B. N., 4.1  
 Brooks, B. R., 3.3  
 Brooks, J. D., 4.4  
 Brown, C. J., 4.5  
 Brown, F., 2.3  
 Brown, G. S., 4.4  
 Brown, H., 1.3  
 Brown, I. D., 1.4  
 Brown, M. D., 3.3  
 Brucolleri, R. E., 3.3  
 Bruijn, N. G. de, 1.3  
 Bruins, E. M., 4.5  
 Bruins Slot, H. J., 2.2  
 Bruinsma, R., 4.4  
 Brümmer, O., 5.1  
 Brünger, A. T., 1.3, 4.5

## AUTHOR INDEX

- Bryan, R. K., 1.3, 4.5  
 Bu, X., 4.6  
 Bubeck, E., 4.2  
 Buch, K. R., 3.2  
 Budai, J., 4.4  
 Buehner, M., 2.3  
 Buerger, M. J., 1.1, 1.4, 2.2, 2.3  
 Bujosa, A., 1.3  
 Bullough, R. K., 2.3  
 Bülow, R., 1.3  
 Bunn, C. W., 4.5  
 Bunshaft, A. J., 3.3  
 Burandt, B., 4.6  
 Burch, S. F., 1.3  
 Burdina, V. I., 2.3  
 Burkert, U., 3.3  
 Burkov, S., 4.6  
 Burla, M. C., 2.2  
 Burnett, R. M., 1.3, 2.3  
 Burnside, W., 1.3  
 Burrus, C. S., 1.3  
 Busetta, B., 2.2  
 Busing, W. R., 1.3, 3.1, 3.4  
 Bussler, P., 2.5  
 Buxton, B., 2.5, 5.2  
 Buxton, B. F., 2.5  
 Buyers, W. J. L., 4.1  
 Byerly, W. E., 1.3  
 Byler, M. A., 4.5  
  
 Cael, J. J., 4.5  
 Caglioti, G., 4.2  
 Cahn, J. W., 2.5, 4.6  
 Caillé, A., 4.4  
 Calabrese, G., 2.2  
 Calvayrac, Y., 4.2  
 Camalli, M., 2.2  
 Cambillau, C., 3.3  
 Campagnari, F., 4.5  
 Campbell, G. A., 1.3  
 Campbell Smith, P. J., 4.5  
 Cannillo, E., 2.4  
 Cantino, M., 4.5  
 Carathéodory, C., 1.3  
 Carlile, C. J., 4.4  
 Carlisle, C. H., 2.3  
 Carlson, J. M., 4.4  
 Carpenter, R. W., 2.5  
 Carroll, C. E., 4.5  
 Carrozzini, B., 2.2  
 Carslaw, H. S., 1.3  
 Cartan, A., 1.3  
 Carter, R. E., 3.3  
 Cartwright, B. A., 3.3  
 Cascarano, G., 2.2  
 Case, A. L., 5.3  
 Casher, A., 1.5  
 Caspar, D. L. D., 2.3, 4.5  
 Castellano, E. E., 2.2  
 Cavicchi, E., 3.3  
 Cenedese, P., 4.2  
 Cesini, G., 5.3  
 Ceska, T. A., 2.5  
 Chacko, K. K., 2.4  
 Chakravarthy, R., 5.3  
 Challifour, J. L., 1.3  
 Chalupa, B., 5.3  
 Champeney, D. C., 1.3  
 Champness, J. N., 1.3, 2.3, 3.3  
 Chan, A. S., 2.5  
 Chan, D. S. K., 1.3  
 Chan, K. K., 4.4  
  
 Chandrasekaran, R., 4.5  
 Chandrasekhar, S., 4.4  
 Chang, S.-L., 5.1  
 Chanzy, H., 2.5, 4.5  
 Chaplot, S. L., 4.1  
 Chapman, D., 4.4  
 Chapuis, G., 4.6  
 Charvolin, J., 4.4  
 Chen, J. H., 4.4  
 Cheng, T. Z., 2.5  
 Chew, M., 4.5  
 Chiang, L. Y., 4.4  
 Chistyakov, R. R., 5.3  
 Chivers, R. A., 4.5  
 Choplin, F., 3.3  
 Chou, C. T., 2.5  
 Chow, M., 2.3  
 Christensen, F., 4.4  
 Chu, K. C., 4.4  
 Chukhovskii, F. N., 5.3  
 Church, G. M., 1.3, 2.4  
 Churchill, R. V., 1.3  
 Cimmino, A., 5.3  
 Cisarova, I., 4.6  
 Clapp, P. C., 4.3  
 Clark, E. S., 4.5  
 Clark, N. A., 4.4  
 Clarke, P. J., 4.2  
 Clarke, R., 4.4  
 Clastre, J., 2.3  
 Clementi, E., 1.2  
 Clews, C. J. B., 1.3, 3.2  
 Clothier, R., 5.3  
 Coates, D., 4.4  
 Cochran, W., 1.1, 1.2, 1.3, 1.4, 2.2, 2.3, 2.5, 3.2, 4.1, 4.5  
 Cockayne, D. J. H., 2.5  
 Cockrell, P. R., 3.3  
 Cohen, J. B., 4.2  
 Cohen, N. C., 3.3  
 Cohen-Tannoudji, C., 1.2  
 Cole, H., 5.1  
 Colella, R., 5.3  
 Colin, P., 3.3  
 Collar, A. R., 5.2  
 Coller, E., 2.2, 2.3  
 Collett, J., 4.4  
 Collins, D. M., 1.3, 2.2, 2.3, 2.4, 3.3  
 Collongues, R., 4.2  
 Colman, P. M., 1.3, 2.3  
 Comarmond, M. B., 2.3  
 Comes, R., 4.2  
 Condon, E. V., 1.2  
 Connolly, M. L., 3.3  
 Conradi, E., 4.2  
 Convert, P., 4.2  
 Cooley, J. W., 1.3  
 Cooper, M. J., 4.2  
 Coppens, P., 1.2, 4.6, 5.3  
 Cordes, A. W., 3.2  
 Corey, R. B., 1.3, 2.3  
 Corfield, P. W. R., 2.3  
 Cork, J. M., 2.4  
 Corliss, A. M., 4.2  
 Coronas, J., 5.2  
 Coster, D., 2.4  
 Cotton, F. A., 3.3  
 Coulson, C. A., 1.2  
 Coulter, C. L., 2.2  
 Courville-Brenasin, J. de, 4.2  
 Cowan, P. L., 5.1  
 Cowan, S. W., 3.3  
  
 Cowley, J. M., 2.5, 4.2, 4.3, 4.5, 5.2  
 Cox, E. G., 1.3  
 Cox, J. M., 2.3, 2.4  
 Coxeter, H. S. M., 1.3  
 Cracknell, A. P., 1.5, 4.2  
 Cramér, H., 1.3, 2.1, 2.5  
 Cramer, R. III, 3.3  
 Creek, R. C., 2.5  
 Crick, F. H. C., 1.3, 2.3, 2.4, 2.5, 4.5  
 Cromer, D. T., 2.3, 2.4  
 Crooker, P. P., 4.4  
 Crowfoot, D., 2.3  
 Crowther, R. A., 1.3, 2.2, 2.3, 2.5, 4.5  
 Crozier, P. A., 2.5  
 Cruickshank, D. W. J., 1.2, 1.3, 2.4  
 Cullen, D. L., 3.3  
 Cullis, A. F., 2.3, 2.4  
 Culver, J. N., 4.5  
 Cummins, H. Z., 4.6  
 Cummins, P. G., 3.4  
 Curtis, C. W., 1.3  
 Curtis, R. J., 4.4  
 Cutfield, J. F., 2.2  
 Czerwinski, E. W., 2.3  
  
 Dale, D., 2.4  
 Dam, A. van, 3.3  
 Dana, S. S., 4.4  
 Daniel, H., 5.3  
 Daniels, H. E., 1.3  
 Darwin, C. G., 5.1  
 Daubeny, R. de P., 4.5  
 Davey, S. C., 4.4  
 Davidov, D., 4.4  
 Davidson, J. B., 5.3  
 Davies, B. L., 1.5  
 Davies, D. R., 1.3  
 Dawis, P. J., 3.4  
 Dawson, B., 1.2, 2.5  
 Day, D., 4.5  
 Dayringer, H. E., 3.3  
 De Facio, B., 5.2  
 De Gennes, P. G., 4.4  
 De Hoff, R., 4.4  
 De Jeu, W. H., 4.4  
 De Meulenaere, P., 4.3  
 De Ridder, R., 4.3  
 De Vries, H. L., 4.4  
 Dea, I. C. M., 4.5  
 Deans, S. R., 2.5  
 Debaerdemaeker, T., 2.2  
 DeBoissieu, M., 4.6  
 Debye, B., 4.2  
 Debye, P., 4.1  
 Declercq, J.-P., 2.2  
 Dederichs, P. H., 4.2  
 Dehlinger, U., 4.6  
 Deimel, P., 5.3  
 Deisenhofer, J., 1.3, 2.4  
 Delapalme, A., 4.2, 5.3  
 Delaunay, B., 1.5  
 Dellby, N., 4.3  
 Deming, W. E., 3.2  
 Dempsey, S., 3.3  
 Demus, D., 4.4  
 Denny, R., 4.5  
 Denson, A. K., 3.3  
 DeRosier, D. J., 2.5, 4.5  
 DeStrade, C., 4.4  
 DeTitta, G. T., 2.2, 2.5, 4.5  
 Deutsch, M., 4.4  
  
 Dewar, R. B. K., 2.2  
 DeWette, F. W., 3.4  
 Diamond, R., 1.3, 3.3, 4.5  
 Dickerson, R. E., 1.3, 2.2, 2.3, 2.4  
 Diele, S., 4.4  
 Dietrich, H., 1.3  
 Dieudonné, J., 1.3  
 Dijkstra, B. W., 3.3  
 Dimon, P., 4.4  
 Dintzis, H. M., 2.3  
 Dirac, P. A. M., 1.3  
 Dirl, R., 1.5  
 DiSalvo, F. J., 4.4  
 Ditchfield, R., 1.2  
 Diu, B., 1.2  
 Djurek, D., 4.4  
 Dobrott, R. D., 2.3  
 Dodson, E., 2.3, 2.4  
 Dodson, E. J., 1.3, 2.2, 2.3, 3.3  
 Dodson, G. G., 2.2, 2.3, 3.3  
 Doesburg, H. M., 2.2  
 Doi, K., 5.3  
 Dokashenko, V. P., 5.3  
 Dolata, D. P., 3.3  
 Dolling, C., 4.1  
 Dolling, G., 4.2  
 Doman, E., 4.4  
 Dong, W., 2.5  
 Donohue, J., 1.3, 2.3  
 Donovan, B., 4.1  
 Dorner, B., 4.2  
 Dorner, C., 4.2  
 Dorset, D. L., 2.5, 4.5  
 Doubleday, A., 3.3  
 Doucet, J., 4.4  
 Douglas, A. S., 2.2  
 Downing, K. H., 2.5  
 Dowty, E., 1.4  
 Doyle, P. A., 4.3, 4.5  
 Dräger, J., 4.6  
 Drenth, J., 4.5  
 Drits, V. A., 2.5  
 Duane, W., 1.3  
 Dubernat, J., 4.2  
 Dubois, J. C., 4.4  
 Duce, D. A., 3.3  
 Duke, G. M., 2.3  
 Dumrongrattana, S., 4.4  
 Duncan, W. J., 5.2  
 Dunitz, J. D., 1.2  
 Dunmur, D. A., 3.4  
 Durrant, J. L. A., 4.4  
 Dvoryankin, V. F., 2.5  
 D'yakon, I. A., 2.5  
 Dym, H., 1.3  
 Dyott, T. M., 3.3  
  
 Eades, J. A., 2.5  
 Eaker, D., 2.3  
 Ebel, J. P., 2.3  
 Edmonds, J. W., 2.2, 2.5, 4.5  
 Edwards, O. S., 4.2  
 Egert, E., 2.2, 2.3  
 Eichhorn, F., 5.3  
 Eiland, P. F., 1.3  
 Einstein, A., 4.1  
 Einstein, J. E., 2.4  
 Eisenberg, D., 2.2, 2.3, 2.4  
 Eklundh, J. O., 1.3  
 Elder, M., 4.5  
 Eliopoulos, E. E., 3.3  
 Eller, G. von, 2.2

## AUTHOR INDEX

- Elyutin, N. O., 5.3  
 Emery, V. J., 4.2  
 Enderle, G., 3.3  
 Endoh, H., 2.5  
 Endres, H., 4.2  
 Engel, P., 1.3  
 Englander, M., 5.3  
 Entin, I. R., 5.3  
 Epstein, J., 4.2  
 Erdélyi, A., 1.3  
 Erickson, H. P., 2.5  
 Erickson, J. W., 2.3  
 Eschenbacher, P. W., 1.3  
 Estermann, M., 4.6  
 Etheridge, J., 5.2  
 Etherington, G., 4.4  
 Evans, A. C., 3.3  
 Evans, N. S., 2.5  
 Evans, P., 2.4  
 Evans, P. R., 3.3  
 Evans-Lutterodt, K. W., 4.4  
 Evjen, H. M., 3.4  
 Ewald, P. P., 1.1, 1.3, 1.4, 3.4, 5.1  
 Exelby, D. R., 2.5  
  
 Faber, T. E., 4.4  
 Faetti, S., 4.4  
 Faggiani, R., 2.1  
 Fåk, B., 5.3  
 Fan, C. P., 4.4  
 Fan, H.-F., 2.2, 2.5  
 Farach, H. A., 3.3  
 Farber, A. S., 4.4  
 Farkas, D. R., 1.3  
 Farrants, G., 1.4, 2.5  
 Farrants, G. W., 3.3  
 Favin, D. L., 1.3  
 Fayard, M., 4.2  
 Fedotov, A. F., 2.5  
 Fehlhammer, H., 2.3  
 Feig, E., 1.3  
 Feil, D., 1.2  
 Feiner, S. K., 3.3  
 Feldkamp, L. A., 4.1  
 Feldmann, R. J., 3.3  
 Feltynowski, A., 2.5  
 Fender, B. E. F., 4.2  
 Ferraris, G., 2.5  
 Ferrel, R. A., 4.3  
 Ferrin, T. E., 3.3  
 Fewster, P. F., 5.1  
 Feynman, R., 5.2  
 Fields, P. M., 4.3  
 Filman, D. J., 2.3  
 Finch, J. T., 2.5  
 Fingerland, A., 5.1  
 Finkelstein, K. D., 5.3  
 Finkenstadt, V. L., 4.5  
 Fischer, J., 2.3  
 Fischer, K., 1.2  
 Fischer, W., 1.4  
 Fisher, J., 2.2  
 Fisher, P. M. J., 4.3  
 Fiske, S. J., 2.2  
 Fitzgerald, P. M. D., 1.4, 2.3  
 Flack, H. D., 4.2  
 Flautt, T. J., 4.4  
 Fleming, R. M., 4.4  
 Fletterick, R. J., 2.3, 3.3  
 Flook, R. J., 2.4  
 Fock, R., 5.2  
 Foldy, L. L., 2.5  
  
 Foley, J. D., 3.3  
 Folkhard, W., 1.3  
 Fontaine, D. de, 4.2  
 Fontell, K., 4.4  
 Fontes, E., 4.4  
 Ford, G. C., 2.3  
 Ford, L. O., 3.3  
 Forgany, S. K. E., 2.5  
 Fornberg, A., 1.3  
 Forst, R., 4.2  
 Forsyth, J. B., 1.3, 4.2  
 Forsyth, V. T., 4.5  
 Fortier, S., 2.2  
 Fortuin, C. M., 3.4  
 Foster, R. M., 1.3  
 Foucher, P., 4.4  
 Fouret, P., 4.2  
 Fouret, R., 4.2  
 Fout, G. S., 2.3  
 Fowler, R. H., 1.3  
 Fowweather, F., 1.3  
 Fox, G., 2.3  
 Frank, F. C., 4.4  
 Frank, J., 2.5  
 Frankenberger, E. A., 2.3  
 Franklin, R. E., 4.5  
 Franulovic, K., 4.4  
 Franx, M., 2.1  
 Fraser, H. L., 2.5  
 Fraser, R. D. B., 4.5  
 Frazer, R. A., 5.2  
 Freeman, A. J., 1.2, 4.3  
 Freeman, H. C., 2.4  
 Freer, A. A., 2.2  
 Freer, S. T., 1.3, 2.4  
 Freiser, M. J., 4.4  
 French, A. D., 4.5  
 French, S., 2.1, 2.2, 2.4  
 Frey, F., 4.2  
 Frey, S., 2.5  
 Fridborg, K., 2.3  
 Fridrichsons, J., 2.3  
 Friedel, G., 1.3, 4.4  
 Friedlander, F. G., 1.3  
 Friedlander, P. H., 1.3  
 Friedman, A., 1.3  
 Frobenius, G., 1.3  
 Frost, J. C., 4.4  
 Frost-Jensen, A., 4.6  
 Fry, E., 2.3  
 Fryer, J. R., 2.5, 4.5  
 Fuess, H., 5.3  
 Fujii, Y., 4.1  
 Fujimoto, F., 2.5, 4.3, 5.2  
 Fujinaga, M., 2.3  
 Fujiwara, K., 2.5, 5.2  
 Fujiyoshi, Y., 2.5  
 Fukuhara, A., 2.5, 5.2  
 Fukuyama, K., 2.3  
 Fuller, W., 4.5  
 Furie, B., 3.3  
 Furie, B. C., 3.3  
 Furusaka, M., 4.2  
  
 Gabor, D., 2.5  
 Gähler, R., 5.3  
 Galerme, Y., 4.4  
 Gallagher, T. M., 2.3  
 Gallo, L., 3.3  
 Gallop, J. R., 3.3  
 Gallwitz, U., 4.5  
 Gane, P. A. C., 4.4  
  
 Gannon, M. G. J., 4.4  
 Garcia-Golding, F., 4.4  
 Garcia-Granda, S., 2.2  
 Gardner, K. H., 4.5  
 Garland, C. W., 4.4  
 Garland, Z. G., 4.4  
 Garrido, J., 2.3  
 Gasparoux, H., 4.4  
 Gassmann, J., 1.3, 2.3, 2.4, 2.5  
 Gatti, M., 4.4  
 Gaughan, J. P., 4.4  
 Gautier, F., 4.2  
 Gavrilov, V. N., 5.3  
 Gay, R., 2.3  
 Gaykema, W. P. J., 2.3  
 Gebhard, W., 4.5  
 Geddes, A. J., 3.3  
 Gehlen, P., 4.2  
 Gehring, K., 2.5  
 Geil, P. H., 4.5  
 Geisel, T., 4.2  
 Gelder, R. de, 2.2  
 Gel'fand, I. M., 1.3  
 Geller, M., 3.3  
 Gentleman, W. M., 1.3  
 Georgopoulos, P., 4.2  
 Gerhard, O. E., 2.1  
 Gerlach, P., 4.2  
 Germain, G., 2.2, 2.5  
 Germian, C., 4.4  
 Gerold, V., 4.2  
 Giacobuzzo, C., 2.1, 2.2  
 Giarrusso, F. F., 3.3  
 Gibbs, J. W., 2.3  
 Giegé, R., 2.3  
 Gilbert, P. F. C., 2.5  
 Gill, P. E., 3.3  
 Gillan, B. E., 4.2  
 Gilli, G., 2.4  
 Gilliland, G. L., 3.3  
 Gillis, J., 1.3, 2.2  
 Gilmore, C. J., 2.2, 2.5, 4.5  
 Gilmore, R., 5.2  
 Gingrich, N. S., 1.3, 4.2  
 Girling, R. L., 3.3  
 Gjønnes, J., 2.5, 4.3, 5.2  
 Gjønnes, K., 2.5  
 Glaeser, R. M., 2.5  
 Glasser, M. L., 3.4  
 Glatigny, A., 3.3  
 Glauber, R., 2.5  
 Glazer, A. M., 4.2  
 Glück, M., 1.5  
 Glucksman, M. J., 4.5  
 Go, N., 3.3  
 Godréche, C., 4.6  
 Goedkoop, J. A., 1.3, 2.2  
 Goldman, A. I., 4.6  
 Goldstine, H. H., 1.3  
 Golovchenko, J. A., 5.1  
 Goncharov, A. B., 2.5  
 Gonzalez, A., 4.5  
 Good, I. J., 1.3  
 Goodby, J. J., 4.4  
 Goodby, J. W., 4.4  
 Goodman, P., 2.5, 5.2  
 Gordon, R., 2.5  
 Gosling, R. G., 4.5  
 Gossling, T. H., 3.3  
 Gould, R. O., 2.2  
 Gouyet, J. F., 4.6  
 Graaf, H. de, 4.5  
  
 Graaff, R. A. G. de, 2.2  
 Grabcev, B., 4.2  
 Graeff, W., 5.3  
 Gragg, J. E., 4.2  
 Gramlich, V., 2.2  
 Gransbergen, E. F., 4.4  
 Grant, D. F., 2.2  
 Gratias, D., 2.5, 4.6, 5.2  
 Grau, U. M., 2.3  
 Gray, G. W., 4.4  
 Green, D. W., 2.3, 2.4  
 Green, E. A., 2.2, 2.4  
 Greenall, R. J., 4.5  
 Greenhalgh, D. M. S., 1.3  
 Greer, J., 3.3  
 Gress, M. D., 1.3  
 Grenander, U., 1.3  
 Griffith, J. P., 2.3  
 Grimm, H., 1.3, 4.2  
 Grinstein, G., 4.4  
 Gross, L., 1.3  
 Grosse-Kunstedt, R. W., 1.4  
 Grubb, D. T., 4.5  
 Grzanic, G., 2.5  
 Gu, Y.-X., 2.2  
 Guagliardi, A., 2.2  
 Gubbens, A. J., 4.3  
 Guessoum, A., 1.3  
 Guigay, J. P., 5.3  
 Guillon, D., 4.4  
 Guinier, A., 4.2  
 Gull, S. F., 1.3  
 Gunning, J., 2.5  
 Gunther, L., 4.4  
 Gur, Y., 1.5  
 Gurskaya, G. V., 2.5  
 Guru Row, T. N., 1.2  
 Gutierrez, G. A., 4.5  
 Guyot-Sionnest, P., 4.4  
  
 Hadamard, J., 1.3  
 Haefner, K., 4.2  
 Haibach, T., 4.6  
 Hall, I. H., 4.5  
 Hall, M., 1.3  
 Hall, S. R., 1.4, 2.2  
 Halla, F., 4.2  
 Halperin, B. I., 4.4  
 Hamilton, W. A., 5.3  
 Hamilton, W. C., 2.3, 2.4, 3.1, 3.2, 4.5  
 Hancock, H., 2.2  
 Handelsman, R. A., 1.3  
 Hansen, N. K., 1.2  
 Hao, Q., 2.2  
 Harada, J., 4.2  
 Harada, Y., 2.3, 2.5, 4.3  
 Harburn, G., 4.2  
 Harding, M. M., 2.2, 2.3  
 Hardman, K. D., 3.3  
 Hardouin, F., 4.4  
 Hardy, G. H., 1.3  
 Harford, J., 4.5  
 Harker, D., 1.3, 2.1, 2.2, 2.3, 2.4  
 Harrington, M., 2.3  
 Harris, D. B., 1.3  
 Harris, M. R., 3.3  
 Harrison, S. C., 1.3, 2.3  
 Harrison, W. A., 4.1  
 Hart, M., 5.1, 5.3  
 Hart, R. G., 2.4  
 Hartman, P., 1.3

## AUTHOR INDEX

- Hartree, D. R., 1.2  
Hartsuck, J. A., 2.3  
Hasegawa, K., 4.5  
Haseltine, J. H., 4.4  
Hashimoto, H., 2.5  
Hashimoto, S., 4.2, 4.3  
Hass, B. S., 3.3  
Hastings, C. Jr, 3.4  
Hastings, J. B., 5.3  
Hastings, J. M., 4.2  
Hata, Y., 2.4  
Hatch, D. M., 1.5  
Haubold, H. G., 4.2  
Hauptman, H., 1.3, 2.1, 2.2, 2.3, 2.4, 2.5, 4.5  
Hausdorff, F., 4.6  
Havelka, W., 2.5  
Havighurst, R. J., 1.3  
Hayakawa, M., 4.2  
Hazen, E. E., 3.3  
Heap, B. R., 3.3  
Hearmon, R. F. S., 4.1  
Hearn, A. C., 1.4  
Hecht, H. J., 2.3  
Hecht, H.-J., 2.2  
Hehre, W. J., 1.2  
Heideman, M. T., 1.3  
Heil, P. D., 4.5  
Heinermann, J. J. L., 2.2  
Heiney, P. A., 4.4, 4.6  
Helfrich, W., 4.4  
Helliwell, J. R., 2.2, 2.4  
Hellner, E., 4.2  
Helms, H. D., 1.3  
Hende, J. van den, 1.3  
Henderson, R., 2.3, 2.5  
Hendricks, S., 4.2, 4.5  
Hendrickson, W. A., 1.3, 2.2, 2.3, 2.4  
Hendrikx, Y., 4.4  
Hennion, B., 4.2  
Herglotz, G., 1.3  
Herman, G. T., 2.5  
Hermann, C., 1.3, 4.6  
Hermans, J., 3.3  
Herriot, J. R., 2.4  
Herrmann, K. H., 2.5  
Hetherington, C. J. D., 2.5  
Hewitt, J., 2.5  
Heymann, J. A. W., 2.5  
Higgs, H., 3.3  
High, D. F., 2.3, 2.4  
Hildebrandt, G., 5.1  
Hills, G. J., 2.5  
Hirsch, P. B., 2.5, 4.5, 5.1, 5.2  
Hirschman, I. I. Jr, 1.3  
Hirshfeld, F. L., 1.2, 2.3  
Hirt, A., 2.5  
Hirth, J. P., 4.4  
Hitchcock, P. B., 4.4  
Hjertén, S., 2.3  
Ho, M.-H., 2.5  
Ho, M.-S., 2.5  
Hodgkin, D. C., 2.2, 2.3, 2.4  
Hodgson, K. O., 2.4  
Hodgson, M. L., 1.3  
Hofmann, D., 4.5  
Hogle, J., 2.3, 3.3  
Hohlwein, D., 4.2  
Høier, R., 2.5, 4.3, 5.2  
Hol, W. G. J., 2.3, 3.3  
Holbrook, S. R., 1.3, 2.4  
Holmes, K. C., 4.5  
Honegger, A., 3.3  
Honjo, G., 4.3  
Hopfinger, A. J., 3.3, 4.5  
Hopgood, F. R. A., 3.3  
Hoppe, W., 1.3, 2.2, 2.3, 2.4, 2.5  
Horalik, L., 5.3  
Horjales, E., 3.3  
Hörmander, L., 1.3  
Horn, P. M., 4.4, 4.6  
Horne, M. A., 5.3  
Hornreich, R. M., 4.4  
Hornstra, J., 2.3  
Horstmann, M., 2.5  
Hosemann, R., 2.3, 4.2, 4.5  
Hoser, A., 4.2  
Hoshino, S., 5.3  
Hosoya, S., 5.3  
Hosur, M. V., 2.3  
Houston, T. E., 3.3  
Hovmöller, S., 1.4, 2.5  
Howells, E. R., 2.1  
Howells, R. G., 2.2  
Howie, A., 2.5, 4.3, 4.5, 5.2  
Hrdlička, Z., 5.3  
Hsiung, H., 4.4  
Hu, H., 4.5  
Hu, H. H., 2.5  
Huang, C., 3.3  
Huang, C. C., 4.4  
Huang, K., 1.3, 4.1  
Hubbard, R. E., 3.3  
Huber, R., 1.3, 2.3, 2.4  
Hudson, L., 4.5  
Hudson, P. J., 3.3  
Hughes, D. E., 1.3  
Hughes, E. W., 1.3, 2.2, 2.3  
Hughes, J. F., 3.3  
Hughes, J. J., 2.3, 2.4  
Hull, S. E., 2.2  
Hüller, A., 4.2  
Hummelink, T., 3.3  
Hummelink-Peters, B. G., 3.3  
Hümmer, K., 5.1  
Humphreys, C. J., 2.5, 4.3, 5.2  
Hunsmann, N., 2.5  
Huntingdon, H. B., 4.1  
Hurley, A. C., 1.2, 2.5, 5.2  
Huse, D. A., 4.4  
Iannelli, P., 4.5  
Ibers, J. A., 2.4, 4.2  
Iijima, S., 4.3  
Iizumi, M., 4.2  
Imamov, R. M., 2.5  
Immirzi, A., 1.3  
Imry, Y., 4.4  
Indenbom, V. L., 5.3  
Ingersent, K., 4.4  
Ingram, V. M., 2.3, 2.4  
Iolin, E. M., 5.3  
Irwin, M. J., 2.2  
Isaacs, N. W., 1.3, 2.2, 2.4, 3.3  
Ishihara, K. N., 4.6  
Ishii, T., 4.2  
Ishikawa, I., 5.3  
Ishikawa, Y., 4.2  
Ishizuka, K., 2.5  
Isoda, S., 2.5, 4.5  
Israel, R., 2.2  
Ito, T., 3.2  
Ivanova, M. I., 4.5  
Iwata, H., 4.2  
Jach, T., 5.1  
Jack, A., 1.3, 2.4  
Jacobson, R. A., 2.3  
Jacques, J., 4.4  
Jaeger, J. C., 1.3  
Jagodzinski, H., 4.2  
James, R. W., 1.2, 1.3, 2.3, 4.2, 5.1  
Jan, J.-P., 1.5  
Janner, A., 1.3, 2.5, 4.2, 4.6  
Janot, Chr., 4.6  
Jansen, L., 1.5  
Janssen, T., 1.3, 1.5, 2.5, 4.2, 4.6  
Jap, B. K., 2.5  
Jaric, M. V., 4.6  
Jarvis, L., 3.3  
Jaynes, E. T., 1.3, 2.2  
Jefferey, J. W., 4.2  
Jeffery, B. A., 2.3  
Jeffrey, G. A., 1.3  
Jensen, L. H., 1.3, 2.3, 2.4  
Jih, J. H., 2.3  
Johannisen, H., 2.3  
Johnson, A. W. S., 2.5, 5.2  
Johnson, C. K., 1.2, 3.1, 3.3  
Johnson, D. H., 1.3  
Johnson, D. L., 4.4  
Johnson, H. W., 1.3  
Johnson, J. E., 2.3, 3.3  
Johnson, L. N., 2.3, 2.4, 3.3  
Johnson, R. W., 1.3  
Jolles, P., 2.3  
Jones, B., 4.4  
Jones, P. M., 2.5  
Jones, R., 4.2, 4.5  
Jones, R. C., 4.2  
Jones, T. A., 2.3, 3.3  
Josefsson, T. W., 4.3  
Joyez, G., 4.2  
Jürgensen, H., 1.3  
Just, W., 4.2  
Kabsch, W., 3.3, 4.5  
Kac, M., 1.3  
Kadečková, S., 5.3  
Kaenel, R. A., 1.3  
Kagan, Yu., 5.3  
Kainuma, Y., 4.3, 5.2  
Kaiser, H., 5.3  
Kakinoki, J., 4.2  
Kalantar, A. H., 3.2  
Kaldor, U., 2.1  
Kalning, M., 4.6  
Kam, Z., 2.5  
Kamada, K., 5.3  
Kambe, K., 2.5, 5.2  
Kamer, G., 2.3  
Kamper, J., 2.3  
Kannan, K. K., 2.3  
Kansy, K., 3.3  
Kaplan, D. R., 5.1  
Kaplan, M., 4.4  
Kara, M., 1.2  
Karbach, A., 4.5  
Karle, I. L., 2.2  
Karle, J., 1.3, 2.1, 2.2, 2.3, 2.4, 2.5  
Kármán, T. von, 4.1  
Karplus, M., 1.3, 3.3  
Karrass, A., 1.3  
Kartha, G., 2.3, 2.4  
Kasper, J. S., 1.3, 2.2  
Kasting, G. B., 4.4  
Katagawa, T., 5.1  
Katayama, K., 4.5  
Kato, K., 4.6  
Kato, N., 5.1, 5.3  
Katsube, Y., 2.4  
Katz, L., 3.3  
Katznelson, Y., 1.3  
Kawaguchi, A., 4.5  
Kearsley, S. K., 3.3  
Kek, S., 4.6  
Keller, A., 4.5  
Keller, J., 4.2  
Kelley, B., 4.4  
Kelly, B. A., 4.4  
Kelton, K. F., 4.6  
Kendall, M., 1.2, 2.1  
Kendrew, J. C., 1.3, 2.3, 2.4  
Kennard, O., 3.1, 3.3  
Kennedy, J. M., 1.5  
Ketelaar, J. A. A., 2.3  
Khinchin, A. I., 1.3  
Kiefer, J. E., 1.3, 2.1  
Kikuta, S., 5.1, 5.3  
Kim, S.-H., 1.3, 2.4  
Kirichuk, V. S., 2.5  
Kirkland, E. J., 2.5  
Kiselev, N. A., 2.5  
Kitagaku, M., 4.3  
Kitagawa, Y., 2.4  
Kitaigorodskii, A. J., 4.1  
Kitaigorodsky, A. I., 4.2  
Kitamura, N., 4.3  
Kittel, C., 4.4  
Kitz, N., 1.3  
Kjeldgaard, M., 3.3  
Klapperstück, M., 4.4  
Klar, B., 5.3  
Klechkovskaya, V. V., 2.5  
Klein, A. G., 5.3  
Kleinstück, K., 5.3  
Kleman, M., 4.6  
Klimkovich, S., 1.4  
Klug, A., 1.3, 2.2, 2.3, 2.5, 3.3, 4.5  
Klug, H. P., 4.2  
Kluyver, J. C., 1.3  
Knoell, R. V., 2.5  
Knol, K. S., 2.4  
Knowles, J. W., 5.3  
Kobayashi, S., 4.4  
Kobayashi, T., 2.5  
Koch, E., 1.1, 1.4  
Koch, M. H. J., 2.2  
Kodera, S., 4.3  
Koellner, M., 5.3  
Koetzle, T. F., 2.4, 3.3  
Kogiso, M., 2.5, 5.2  
Kohn, V. G., 5.1  
Kohra, K., 5.1, 5.3  
Kolar, H., 2.5  
Kolba, D. P., 1.3  
Komada, T., 2.5  
Komura, Y., 4.2  
Konnert, J. H., 1.3, 2.4  
Kopka, M. L., 2.3  
Kopp, S., 2.5, 4.5  
Korekawa, M., 4.2, 4.6  
Korn, D. G., 1.3  
Korpiun, P., 5.3  
Kortan, A. R., 4.4  
Kossel, W., 2.5

## AUTHOR INDEX

- Kosterlitz, J. M., 4.4  
 Kosykh, V. P., 2.5  
 Kovacs, A. J., 4.5  
 Kovalchuk, M. V., 5.1  
 Kovalev, O. V., 1.5  
 Krabbendam, H., 2.2  
 Krahl, D., 2.5, 4.3  
 Kraut, J., 1.3, 2.3, 2.4  
 Kress, W., 4.1  
 Kreuger, R. J., 5.2  
 Krishna, P., 4.2  
 Krivanek, O. L., 4.3  
 Krivoglaz, M. A., 4.2, 4.3  
 Kroon, J., 2.2  
 Kruse, F. H., 1.3  
 Kühlbrandt, W., 2.5  
 Kühne, T., 2.5  
 Kuhs, W. F., 1.2  
 Kukla, D., 2.4  
 Kulda, J., 5.3  
 Kulidzhanov, F. G., 5.3  
 Kuligin, A. K., 2.5  
 Kulka, D., 1.3  
 Kuntz, I. D., 3.3  
 Kunz, C., 4.2  
 Kuriyan, J., 1.3  
 Kurki-Suonio, K., 1.2  
 Kutznetsov, P. I., 1.2  
 Kuvdaldin, B. V., 5.3  
 Kuwabara, S., 2.5  
 Kvardakov, V. V., 5.3  
  
 Lacour, T. F. M., 1.3  
 Ladbroke, B. D., 4.4  
 Lagomarsino, S., 5.3  
 Lajzėrowicz, J., 2.2  
 Lajzerowicz, J., 4.4  
 Lakshminarayanan, A. V., 2.5  
 Laloe, F., 1.2  
 Lambert, D., 5.3  
 Lambert, M., 4.4  
 Lambiotte, J. J. Jr, 1.3  
 Lancon, F., 4.6  
 Lanczos, C., 1.3  
 Landau, H. J., 1.3  
 Landau, L. D., 4.4  
 Lando, J. B., 4.5  
 Lang, A. R., 5.1  
 Lang, S., 1.3  
 Lang, W. W., 1.3  
 Langer, R., 2.5  
 Langridge, R., 3.3, 4.5  
 Langs, D. A., 2.2, 2.5, 4.5  
 Larine, M., 1.4  
 Larmor, J., 1.3  
 Lattman, E. E., 2.3, 2.4  
 Lau, H. Y., 4.2  
 Laue, M. von, 1.1, 1.3, 2.5, 5.1  
 Laval, J., 4.1  
 Laves, R., 4.2  
 Lavoine, J., 1.3  
 Lawson, K. D., 4.4  
 Leadbetter, A. J., 4.4  
 Leapman, R. D., 4.3  
 Lechner, R. E., 4.2  
 Lederer, F., 3.3  
 Ledermann, W., 1.3, 4.1  
 Lee, E. J., 4.5  
 Lee, S. D., 4.4  
 Leenhouts, J. I., 2.3  
 Lefebvre, J., 4.1, 4.2  
 Lefebvre, S., 4.2  
 Lefeld-Sosnowska, M., 5.1  
 Legg, M. J., 1.3  
 Lehmann, M., 5.3  
 Lehmann, M. S., 1.3, 2.2  
 Lehmpfuhl, G., 4.3  
 Lele, S., 4.2  
 Lemoine, G., 3.3  
 Lentz, P. J. Jr, 2.3  
 Lepault, J., 2.5  
 Lerner, F. Ya., 2.5  
 Lesk, A. M., 3.3  
 Leslie, A. G. W., 1.3, 2.3, 3.3  
 Lessinger, L., 2.2  
 Leung, P., 1.2  
 Levanyuk, A. P., 4.4  
 Levut, A. M., 4.4  
 Levens, S. A., 1.3  
 Levine, D., 4.6  
 Levinthal, C., 3.3  
 Levitov, L. S., 4.6  
 Levitt, M., 1.3, 2.4, 3.3  
 Levy, H. A., 1.2, 1.3, 3.1  
 Li, D. X., 2.5  
 Li, F. H., 2.5  
 Li, J. Q., 2.5  
 Liang, K. S., 4.4  
 Liebert, L., 4.4  
 Liebert, L. E., 4.4  
 Liebman, G., 2.5  
 Lien, S. C., 4.4  
 Lieth, C. W. van der, 3.3  
 Lievert, L., 4.4  
 Lifchitz, A., 1.3, 2.3  
 Lifshitz, E. M., 4.4  
 Lifson, S., 3.3  
 Lighthill, M. J., 1.3  
 Lijk, L. J., 3.3  
 Liljas, L., 2.3, 3.3  
 Liljefors, T., 3.3  
 Linares-Galvez, J., 5.3  
 Lindegaard, A., 4.4  
 Lindsey, J., 2.3  
 Link, V., 4.4  
 Linnik, I. Ju., 1.3  
 Lipanov, A. A., 4.5  
 Lipkowitz, K. B., 3.3  
 Lippert, B., 2.1  
 Lipscomb, W. N., 2.2, 2.3  
 Lipson, H., 1.1, 1.2, 1.3, 1.4, 2.1, 2.3, 4.2, 4.5  
 Litster, J. D., 4.4  
 Litvin, D. B., 2.3  
 Liu, J., 4.5  
 Liu, Y.-W., 2.5  
 Livanova, N. B., 2.5  
 Livesey, A. K., 1.3  
 Loane, R. F., 4.3  
 Lobachev, A. N., 2.5  
 Lobanova, G. M., 2.5  
 Lobert, S., 4.5  
 Lock, C. J. L., 2.1  
 Lockhart, T. E., 4.4  
 Lomer, T. R., 2.1  
 Lomont, J. S., 1.5  
 Lonsdale, K., 1.3  
 Lontovitch, M., 5.2  
 Looijenga-Vos, A., 4.6  
 Lorenz, M., 4.5  
 Lotz, B., 2.5, 4.5  
 Love, W., 1.3  
 Love, W. E., 2.2, 2.3  
 Love, W. F., 1.5  
 Lovell, F. M., 1.3  
 Lovesey, S. W., 4.2  
 Lövgren, S., 2.3  
 Lowde, R. D., 5.3  
 Lu, C., 1.3  
 Luban, M., 4.4  
 Lubensky, T. C., 4.4  
 Lucas, B. W., 4.2  
 Luck, J. M., 4.6  
 Ludewig, J., 5.1  
 Luenberger, D. G., 3.3  
 Luić, M., 2.2  
 Lunin, V. Yu., 1.3  
 Luo, M., 2.3  
 Lurie, N. A., 4.1  
 Lushington, K. J., 4.4  
 Luther, P., 4.5  
 Luty, T., 4.1  
 Luzzati, V., 2.3, 4.4  
 Lybanon, M., 3.2  
 Lynch, D. F., 2.5, 5.2  
  
 Ma, S. K., 4.4  
 McCall, M. J., 3.3  
 McClellan, J. H., 1.3  
 McCourt, M. P., 2.5, 4.5  
 McDonald, W. S., 2.4  
 McEwen, B., 2.5  
 MacGillavry, C. H., 1.3, 4.5  
 Machin, P. A., 3.3  
 McIntyre, G. J., 1.2  
 Mackay, A. L., 2.2, 3.3  
 MacKay, M., 2.3  
 McKean, H. P., 1.3  
 McLachlan, A. D., 3.3  
 McLachlan, D., 2.3, 2.5  
 MacLane, S., 1.3  
 McLean, J. D., 2.5  
 McMahan, B., 1.4  
 McMillan, W. L., 4.4  
 McMullan, R. K., 3.3  
 MacNicol, D. D., 2.5  
 McPherson, A., 2.4  
 McQueen, J. E., 3.3  
 MacRae, T. P., 4.5  
 McWhan, D. B., 4.4  
 Mada, H., 4.4  
 Madelung, E., 3.4  
 Madhav Rao, L., 5.3  
 Magdoff, B. S., 2.3  
 Magnus, W., 1.3  
 Mahendrasingam, A., 4.5  
 Maher, D. M., 2.5  
 Maier, W., 4.4  
 Main, P., 1.3, 2.2, 2.3, 2.5  
 Makowski, L., 4.5  
 Malgrange, C., 5.1, 5.3  
 Malik, K. M. A., 4.4  
 Maling, G. C., 1.3  
 Mallikarjunan, M., 3.3  
 Malthête, J., 4.4  
 Maly, K., 4.6  
 Mandelkern, L., 4.5  
 Mandelkew, E., 4.5  
 Mani, N. V., 2.4  
 Manley, R. St. J., 2.5  
 Mannami, M., 2.5  
 Mansfield, J., 2.5  
 Marchington, B., 1.3  
 Mardix, S., 4.2  
 Marel, R. P. van der, 2.1  
 Marigo, A., 4.2  
 Marinder, B. O., 2.5  
 Mark, H., 2.4  
 Markham, R., 2.5  
 Marks, L. D., 4.3  
 Marsh, R. E., 3.2  
 Marson, F., 4.4  
 Martin, P. C., 4.4  
 Martinez-Miranda, L. J., 4.4  
 Martorana, A., 4.2  
 Marumo, F., 1.2  
 Marvin, D. A., 1.3, 4.5  
 Marynissen, H., 4.4  
 Masaki, N., 5.3  
 Maslen, V. W., 1.2  
 Maslen, W. V., 4.3  
 Mason, R., 4.4  
 Mason, S. A., 4.5  
 Massidda, V., 3.4  
 Mastryukov, V. S., 2.5  
 Materlik, G., 1.2, 5.1  
 Mathews, F. S., 3.3  
 Mathiesen, S., 4.4  
 Mathieson, A. McL., 2.3  
 Matsubara, E., 4.2  
 Matsuda, T., 2.5  
 Matthews, B. W., 1.3, 2.3, 2.4  
 Mauguen, Y., 2.2, 2.4  
 Mauritz, K. A., 4.5  
 Max, N. L., 3.3  
 Mayer, S. W., 1.3  
 Mayers, D. F., 4.3  
 Mazeau, K., 4.5  
 Mazid, M. A., 4.4  
 Mazkedian, S., 5.3  
 Mazuré-Espejo, C., 5.3  
 Mazzarella, L., 2.3, 2.4  
 Meiboom, S., 4.4  
 Meichle, M., 4.4  
 Melone, S., 5.3  
 Mendiratta, S. K., 5.3  
 Menke, H., 4.2  
 Menzer, G., 2.3  
 Mermin, N. D., 1.1, 2.5, 4.6  
 Mersereau, R. M., 1.3, 2.5  
 Merwe, J. H. van der, 4.4  
 Messiah, A., 5.2  
 Meyer, C. E., 4.3  
 Meyer, E. F., 3.3  
 Meyer, G., 2.5  
 Meyer, R. B., 4.4  
 Michalec, R., 5.3  
 Midgley, P. A., 2.5  
 Mierzejewski, A., 4.1  
 Mighell, A. D., 2.3  
 Mikula, P., 5.3  
 Millane, R. P., 4.5  
 Miller, A., 4.5  
 Miller, D. P., 4.5  
 Miller, G. H., 4.5  
 Miller, J. R., 3.3  
 Miller, P., 2.5  
 Miller, R. C., 2.2, 4.5  
 Miller, S. C., 1.5  
 Mimori-Kiyosue, Y., 4.5  
 Minakawa, N., 5.3  
 Minor, I., 2.3  
 Mitra, A. K., 4.5  
 Mitsui, T., 4.5  
 Miyako, S., 2.5  
 Miyano, K., 4.4  
 Miyazaki, M., 2.5  
 Mo, Y. D., 2.5

## AUTHOR INDEX

- Moliere, G., 4.3  
 Moliterni, A. G. G., 2.2  
 Möllenstedt, G., 2.5  
 Moncrief, J. W., 2.2, 2.3  
 Moncton, D. E., 4.4  
 Montroll, E. W., 1.3  
 Moodie, A. F., 2.5, 5.2  
 Moon, P. B., 2.4  
 Mooney, P. E., 4.3  
 Moore, D. H., 1.3  
 Moore, P. B., 2.5  
 Moras, D., 2.3  
 More, M., 4.2  
 Morffew, A. J., 3.3  
 Mori, M., 4.3  
 Moriguchi, S., 2.5  
 Morimoto, C. N., 3.3  
 Morinaga, M., 4.2  
 Moring, I., 2.3  
 Morris, R. L., 1.3  
 Moser, W. O. J., 1.3  
 Mosley, A., 4.4  
 Moss, B., 2.5  
 Moss, G., 1.2  
 Moss, S. C., 4.2, 4.3  
 Mosser, A. G., 2.3  
 Motherwell, W. D. S., 3.3  
 Motohashi, H., 5.3  
 Moussa, F., 4.4  
 Muirhead, H., 2.3, 2.4  
 Mukamel, D., 4.4  
 Mukherjee, A. K., 2.2  
 Müller, H., 4.2  
 Müller, U., 4.2  
 Munn, R. W., 3.4  
 Murakami, W. T., 2.3  
 Murdock, W. L., 1.3  
 Murray, W., 3.3  
 Murthy, M. R. N., 2.3  
 Muus, I. T., 4.5  
 Myller-Lebedeff, W., 2.1  
  
 Nagabhushana, C., 4.4  
 Nagasawa, T., 2.5, 5.2  
 Naiki, T., 2.5  
 Nakatsu, K., 2.3  
 Namba, K., 4.5  
 Nambudripad, R., 4.5  
 Narayan, R., 1.3, 2.2, 2.4  
 Nathans, R., 4.2  
 Natterer, F., 1.3  
 Navaza, J., 1.3, 2.2  
 Nave, C., 1.3, 4.5  
 Navia, M. A., 2.4  
 Nawab, H., 1.3  
 Naya, S., 2.2, 4.5  
 Neisser, J. Z., 4.5  
 Nelson, D. E., 1.3  
 Nelson, D. R., 4.4  
 Nelson, H. M., 1.5  
 Neto, A. M. F., 4.4  
 Neubert, M. E., 4.4  
 Neubüser, J., 1.3  
 Newham, R. J., 3.4  
 Newman, W. M., 3.3  
 Niall, H. D., 3.3  
 Nicholson, P. B., 4.5  
 Nicholson, R. B., 2.5, 5.2  
 Nigam, G. D., 2.1  
 Niggli, A., 1.3  
 Niimura, N., 4.2  
 Nijboer, B. R. A., 3.4  
  
 Nitta, I., 2.2  
 Nityananda, R., 1.3, 2.2  
 Nixon, P. E., 2.3  
 Nonoyama, M., 4.3  
 Nordman, C. E., 1.3, 2.2, 2.3  
 North, A. C. T., 2.3, 2.4, 3.3  
 Norton, D. A., 2.2  
 Nunzi, A., 2.2  
 Nussbaumer, H. J., 1.3  
  
 Öberg, B., 2.3  
 Oberhettinger, F., 1.3  
 Oberteuffer, J. A., 5.3  
 Oberti, R., 2.4  
 Ocko, B. M., 4.4  
 Oda, T., 2.2  
 O'Donnell, T. J., 3.3  
 Oesterheld, D., 2.5  
 Ogata, C. M., 2.2  
 Ogawa, T., 2.5  
 Ohara, M., 4.5  
 Ohshima, K., 4.2, 4.3  
 Ohtsuki, Y. H., 4.3, 5.1  
 Oikawa, T., 4.3  
 Okaya, J., 2.2  
 Okaya, Y., 2.2, 2.3, 2.4  
 O'Keefe, M. A., 2.5  
 Olafson, B. D., 3.3  
 Olmer, P., 4.1  
 Olsen, A., 2.5  
 Olsen, K. W., 2.3  
 Olson, A. J., 1.3, 2.3, 3.3  
 Olthof-Hazekamp, R., 1.4, 2.2  
 Omura, T., 4.3  
 Ono, A., 2.5  
 Onsager, L., 1.3, 4.4  
 Opat, G. I., 5.3  
 Opdenbosch, N. van, 3.3  
 Oppenheim, A. V., 2.5  
 Ord, K., 2.1  
 Orlov, S. S., 2.5  
 Orlova, E. V., 2.5  
 Ørmen, P.-J., 1.2  
 Ott, H., 2.2  
 Ottensmeyer, F. P., 2.5  
 Overhauser, A. W., 4.2, 5.3  
  
 Paciorek, W. A., 4.6  
 Paley, R. E. A. C., 1.3  
 Palleschi, V., 4.4  
 Palmenberg, A. C., 2.3  
 Palmer, R. A., 2.3, 2.4  
 Palmer, S. B., 5.3  
 Pan, M., 2.5  
 Pan, Q., 2.5  
 Pandey, D., 4.2  
 Paoletti, A., 4.2  
 Paradossi, G., 4.5  
 Park, H., 4.5  
 Parks, T. W., 1.3  
 Parmon, V. S., 2.5  
 Parodi, O., 4.4  
 Parthasarathy, R., 2.3, 2.4  
 Parthasarathy, S., 2.1, 2.2, 2.4  
 Parthé, E., 4.3  
 Pashley, D. W., 2.5, 4.5, 5.2  
 Patel, J. R., 5.1  
 Pattabiraman, N., 3.3  
 Pattanayek, R., 4.5  
 Patterson, A. L., 1.1, 1.3, 2.3, 2.4, 4.2  
 Patterson, C., 5.3  
  
 Paturle, A., 1.2  
 Pätzold, H., 4.3  
 Pauling, L., 1.3, 2.3  
 Pavlovitch, A., 4.6  
 Pawley, G. S., 4.1  
 Pearl, L. H., 3.3  
 Pearson, K., 1.3  
 Pease, M. C., 1.3  
 Peerdeman, A. F., 2.2, 2.3, 2.4  
 Peierls, R. E., 4.4  
 Peisl, J., 4.2  
 Penning, P., 5.1  
 Penrose, R., 4.6  
 Penzkofer, B., 4.2  
 Pepinsky, R., 1.3, 2.2, 2.3, 2.4  
 Perez, S., 2.5, 4.5  
 Perham, R. N., 4.5  
 Perrier de la Bathie, R., 5.3  
 Pershan, P. S., 4.4  
 Perutz, M. F., 2.3, 2.4  
 Petef, G., 2.3  
 Peters, C., 1.3  
 Petrascheck, D., 5.3  
 Petricek, V., 4.6  
 Pétroff, J. F., 5.3  
 Petrov, V. V., 1.3  
 Petřílka, V., 5.3  
 Petsko, G. A., 1.3, 3.3  
 Pezerat, H., 4.2  
 Pfaff, G., 3.3  
 Phillips, D. C., 2.1, 2.3, 2.4, 3.3  
 Phillips, J. C., 2.4  
 Phillips, S. E. V., 3.3  
 Phizackerley, R. P., 2.4  
 Phong, B. T., 3.3  
 Pickworth, J., 2.3  
 Pielartzik, H., 4.5  
 Pietila, L.-O., 3.4  
 Pietronero, L., 4.2  
 Pietsch, U., 2.5  
 Pifferi, A., 2.2  
 Pigram, W. J., 4.5  
 Pilling, D. E., 1.3  
 Pindak, R., 4.4  
 Pink, M. G., 3.3  
 Pinsker, Z. G., 2.5, 5.1  
 Pirie, J. D., 4.1  
 Piro, O. E., 2.2  
 Platas, J. G., 2.2  
 Plotnikov, A. P., 2.5  
 Plotnikov, V. P., 2.5  
 Podjarny, A. D., 2.2, 2.3, 2.4  
 Podurets, K. M., 5.3  
 Pogany, A. P., 2.5  
 Pokrovsky, V. L., 4.4  
 Polder, D., 5.1  
 Polidori, G., 2.2  
 Poljak, R. J., 2.3  
 Pollack, H. O., 1.3  
 Pond, R. C., 2.5  
 Poole, C. P., 3.3  
 Popa, N. C., 4.1  
 Pople, J. A., 1.2  
 Popp, D., 4.5  
 Porter, T. K., 3.3  
 Portier, R., 2.5, 5.2  
 Potenzzone, R., 3.3  
 Potterton, E. A., 3.3  
 Potts, R. B., 1.3  
 Pouget, J. P., 4.2  
 Powell, B. M., 4.2  
 Prandl, W., 4.2  
  
 Press, W., 4.2, 4.6  
 Preston, A. R., 2.5  
 Prick, A. J., 2.2  
 Prins, J. A., 2.4, 4.2, 5.1  
 Prosen, R. J., 1.3, 2.3  
 Prost, J., 4.4  
 Pryor, A. W., 4.1, 4.6  
 Puliti, P., 5.3  
 Purisima, E. O., 3.3  
 Pustovskikh, A. I., 2.5  
 Pynn, R., 4.1  
  
 Quandalle, P., 1.3  
 Quiucho, F. A., 3.3  
 Qurashi, M. M., 1.3  
  
 Rabinovich, D., 2.1, 2.3  
 Rabinovich, S., 2.1  
 Rabson, D. A., 4.6  
 Rackham, G. M., 2.5  
 Rader, C. M., 1.3  
 Radermacher, M., 2.5  
 Radha, A., 4.5  
 Radhakrishnan, R., 3.3  
 Radi, G., 2.5  
 Radon, J., 2.5  
 Radons, W., 4.2  
 Rae, A. D., 2.2  
 Raghavacharyulu, I. V. V., 1.5  
 Raghavan, N. V., 2.4  
 Raghavan, R. S., 2.4  
 Raimondi, D. L., 1.2  
 Raitman, E. A., 5.3  
 Raiz, V. Sh., 2.4  
 Raja, V. N., 4.4  
 Rajagopal, H., 2.4  
 Ralph, A., 2.2  
 Ralph, A. C., 2.2  
 Ramachandran, G. N., 2.2, 2.3, 2.4, 2.5, 5.1  
 Raman, C. V., 4.1  
 Raman, S., 2.2, 2.3, 2.4  
 Ramaseshan, S., 2.3, 2.4  
 Rango, C. de, 2.2, 2.4  
 Rao, R. R., 1.3  
 Rao, S. N., 2.3  
 Rao, S. T., 3.3  
 Rasmussen, K., 3.4  
 Ratna, B. R., 4.4  
 Rauch, H., 5.3  
 Raum, K., 5.3  
 Ravelli, R., 2.2  
 Rawiso, M., 4.4  
 Rayleigh (J. W. Strutt), Lord, 1.3, 2.1  
 Rayment, I., 2.3, 3.3  
 Read, R. J., 2.3  
 Rees, A. L. G., 2.5  
 Reid, T. J. III, 2.3  
 Reif, F., 1.3  
 Reijen, L. L. van, 1.3  
 Reiner, I., 1.3  
 Reiss-Husson, F., 4.4  
 Remillard, B., 4.5  
 Renninger, M., 5.1  
 Reuber, E., 2.5  
 Revol, J. F., 2.5  
 Rez, P., 2.5, 4.3, 5.2  
 Rhyner, J., 4.6  
 Ricci, R., 4.2  
 Rice, S. O., 1.3  
 Richardson, J. S., 3.3

## AUTHOR INDEX

- Richardson, R. M., 4.4  
Rickert, S. E., 4.5  
Riekel, C., 4.2  
Riesz, M., 1.3  
Rietveld, H. M., 4.2  
Rimmer, B., 2.3  
Rivard, G. E., 1.3  
Robertson, J. H., 2.3  
Robertson, J. M., 1.3, 2.3, 2.4, 3.2  
Robinson, G., 1.3, 3.2  
Rodewald, M., 4.3  
Rodgers, J. R., 3.3  
Rodgers, J. W., 2.4  
Rodrigues, A. R. D., 5.3  
Roetti, C., 1.2  
Rogers, D., 2.1, 2.2, 2.3  
Rokhsar, D. S., 4.6  
Rollett, J. S., 1.3, 3.3  
Rosen, J., 1.5  
Rosenstein, R. D., 2.3  
Rosshirt, E., 4.2  
Rossmann, M. G., 1.3, 2.2, 2.3, 2.4, 3.3  
Rossouw, C. J., 4.3  
Roux, D., 4.4  
Rowlands, D., 2.3  
Rowlands, R. J., 4.5  
Rozenfeld, A., 2.5  
Rueckert, R. R., 2.3  
Ruedenberg, K., 1.2  
Rugman, M., 4.4  
Ruland, W., 4.2  
Rust, H.-P., 2.5  
Rustichelli, F., 5.3  
Ruston, W. R., 4.2  
Rybnikar, F., 4.5  
Rydén, L., 2.3  
Ryskin, A. I., 2.5
- Sabine, T. M., 4.2  
Sackmann, H., 4.4  
Sadashiva, B. K., 4.4  
Sadoc, J. F., 4.4  
Sadova, N. I., 2.5  
Safinya, C. R., 4.4  
Safran, S. A., 4.4  
Sahni, V. C., 4.1  
Saito, P., 2.5  
Saito, Y., 2.3  
Saka, T., 5.1  
Sakabe, K., 2.2  
Sakabe, N., 2.2  
Sakurai, K., 4.2  
Salamon, M. B., 4.2  
Sande, G., 1.3  
Sander, B., 5.3  
Sandonis, J., 5.3  
Sands, D. E., 1.1, 3.1  
Sarko, A., 4.5  
Sasada, Y., 2.3, 3.3  
Sato, H., 4.2  
Satow, Y., 2.4  
Saupe, A., 4.4  
Sauvage, M., 4.3, 5.3  
Sayre, D., 1.3, 2.2, 2.4, 2.5, 4.5  
Scaringe, P. R., 4.2  
Scaringe, R. P., 2.5  
Schacher, G. E., 3.4  
Schaetzing, R., 4.4  
Schapink, F. W., 2.5  
Schärpf, O., 4.2
- Schenk, H., 2.2  
Scheraga, H. A., 3.3  
Scheringer, C., 1.2  
Schem, R., 5.3  
Scherzer, O., 2.5  
Schevitz, R. W., 2.2, 2.3, 2.4  
Schilling, J. W., 2.3  
Schiske, P., 2.5  
Schlenker, M., 5.3  
Schmatz, W., 4.2  
Schmid, S., 2.5  
Schmidt, H. H., 5.3  
Schmidt, T., 2.3  
Schmidt, W. C. Jr., 3.3  
Schneider, A. I., 4.5  
Schoenborn, B. P., 2.4  
Schofield, P., 4.1  
Schomaker, V., 1.1, 1.2, 1.3, 2.3, 2.5, 3.2  
Schoone, J. C., 2.4  
Schramm, H. J., 2.5  
Schroeder, M. R., 1.3  
Schuessler, H. W., 1.3  
Schulz, H., 1.2, 4.2  
Schulze, G. E. R., 5.3  
Schumacker, R. A., 3.3  
Schuster, S. L., 4.1  
Schutt, C. E., 1.3, 2.3  
Schwager, P., 1.3, 2.4  
Schwartz, L., 1.3  
Schwartz, L. H., 4.2  
Schwartzman, A., 2.5  
Schwarzenbach, D., 1.2  
Schwarzenberger, R. L. E., 1.3  
Schweizer, J., 5.3  
Scott, W. R., 1.3  
Scraba, D. G., 2.3  
Scudder, M. L., 2.4  
Sears, V. F., 4.2, 5.3  
Sedláková, L., 5.3  
Seidl, E., 5.3  
Seitz, E., 4.2  
Seitz, F., 1.4  
Sekii, H., 2.5, 5.2  
Sellar, J. R., 5.2  
Selling, B. H., 2.3  
Semiletov, S. A., 2.5  
Senechal, M., 4.6  
Sethna, J. P., 4.4  
Sha, B.-D., 2.5  
Shaffer, P. A. Jr., 1.3  
Shakked, Z., 2.1, 2.3  
Shankland, K., 2.5, 4.5  
Shannon, C. E., 1.3  
Shannon, M. D., 2.5  
Shao-Hui, Z., 2.2  
Shappell, M. D., 2.3  
Shashidhar, R., 4.4  
Shashua, R., 2.1  
Sheat, S., 2.3  
Shechtman, D., 2.5, 4.6  
Sheldrick, G. M., 2.2, 2.3  
Shen, Y. R., 4.4  
Shenefelt, M., 1.3  
Sheriff, S., 2.4  
Sherry, B., 2.3  
Sherwood, J. N., 4.2  
Shilov, G. E., 1.3  
Shil'shtein, S. Sh., 5.3  
Shimanouchi, T., 3.3  
Shipley, C. G., 4.4  
Shirane, G., 4.1, 4.2
- Shmueli, U., 1.1, 1.3, 1.4, 2.1, 3.1, 3.2  
Shoemaker, C. B., 2.3  
Shoemaker, D. P., 1.3, 2.3  
Shoemaker, V., 2.5  
Shohat, J. A., 1.3  
Shore, V. C., 2.4  
Shortley, G. H., 1.2  
Shotton, M. W., 4.5  
Shtrikman, S., 4.4  
Shull, C. G., 5.3  
Sicignano, A., 2.3  
Siddons, D. P., 5.3  
Sidorenko, S. V., 2.5  
Sieber, W., 3.3  
Siegel, B. M., 2.5  
Sieker, L. C., 2.4  
Sigaud, G., 4.4  
Sigler, P. B., 2.2, 2.3, 2.4  
Sikka, S. K., 2.4  
Sikorski, A. Z., 2.5  
Silcox, J., 4.3  
Siliqi, D., 2.2  
Silverman, H. F., 1.3  
Sim, G. A., 2.2, 2.3, 4.5  
Simerska, M., 2.2  
Simonov, V. I., 2.2, 2.3  
Simpson, P. G., 2.3  
Singh, A. K., 2.3, 2.4  
Singleton, R. C., 1.3  
Sinha, S. K., 4.4  
Sint, L., 2.2  
Sippel, D., 5.3  
Siripitayananon, J., 4.2  
Sirota, E. B., 4.4  
Sirota, M. I., 2.5  
Sivardiére, J., 5.3  
Sjögren, A., 2.5  
Skehel, J. J., 2.3  
Skilling, J., 1.3  
Skoglund, U., 2.3  
Skoulios, A., 4.4  
Skuratovskii, I. Y., 4.5  
Slater, L. S., 1.5  
Slepian, D., 1.3  
Sluckin, T. J., 4.4  
Sly, W. G., 1.3  
Smaalen, S. van, 4.6  
Small, D., 4.4  
Smith, A. B. III, 4.4  
Smith, D. J., 2.5  
Smith, G., 3.3  
Smith, G. S., 4.4  
Smith, G. W., 4.4  
Smith, J. L., 2.2, 2.3  
Smith, T., 4.1  
Smits, J. M. M., 2.2  
Smoluchowski, R., 1.5  
Sneddon, I. N., 1.3  
Soboleva, A. F., 2.5  
Socolar, J. E. S., 4.6  
Soeter, N. M., 2.3  
Sokol'skii, D. V., 5.3  
Solitar, D., 1.3  
Solomon, L., 4.4  
Somenkov, V. A., 5.3  
Soni, R. P., 1.3  
Sorensen, L. B., 4.4  
Spagna, R., 2.2  
Spargo, A. E. C., 2.5  
Sparks, C. J., 1.2, 4.2  
Sparks, R. A., 1.3, 3.3
- Speake, T. C., 1.3  
Speakman, J. C., 2.3  
Spek, A. L., 2.2  
Spence, J. C. H., 2.5, 4.3  
Spiegel, M. R., 2.1  
Spink, J. A., 2.5  
Sprang, S. R., 3.3  
Sprecher, D. A., 1.3  
Springer, T., 4.2, 4.4  
Sprokel, G. E., 4.4  
Sproull, R. F., 3.3  
Squire, J. M., 4.5  
Squires, G. L., 1.2, 4.1, 5.3  
Srinivasan, R., 2.1, 2.2, 2.4  
Staden, R., 1.3, 2.3, 3.3  
Stanley, E., 2.2, 4.5  
Stark, W., 4.5  
Stassis, C., 5.3  
States, D. J., 3.3  
Staudenmann, J. L., 5.3  
Stauffacher, C. V., 2.3  
Steeds, J. W., 2.5  
Stegemeyer, H., 4.4  
Steger, W., 4.2  
Stegun, I. A., 2.1  
Steigemann, W., 1.3, 2.4  
Stein, Z., 2.1  
Steinberger, I. T., 4.2  
Steinhardt, P. J., 4.6  
Steinkilberg, M., 2.5  
Steinrauf, L. K., 2.3  
Steitz, T. A., 2.3  
Stephanik, H., 5.1  
Stephen, M. J., 4.4  
Stephens, P. W., 4.4, 4.6  
Stephenson, G. B., 4.4  
Steurer, W., 4.6  
Stevens, E. D., 1.2  
Stewart, A. T., 4.1  
Stewart, R. F., 1.2  
Stokes, H. T., 1.5  
Storks, K. H., 4.5  
Stout, G. H., 1.3, 2.3  
Stragler, H., 4.4  
Strahs, G., 2.3  
Strandberg, B., 2.3  
Strandberg, B. E., 1.3, 2.3, 2.4  
Strässler, S., 4.2  
Stratonovich, R. L., 1.2  
Stroud, R. M., 2.4  
Stroud, W. J., 4.5  
Strzelecki, L., 4.4  
Stuart, A., 1.2, 2.1  
Stuart, D., 2.3  
Stubbs, G., 4.5  
Stubbs, G. J., 4.5  
Sturkey, J., 5.2  
Sturtevant, J. M., 4.5  
Su, Z., 1.2  
Suck, D., 2.3, 3.3  
Sundaralingam, M., 3.3  
Sundaram, K., 3.3  
Sundberg, M., 2.5  
Suresh, K. A., 4.4  
Suryan, G., 1.3  
Sussman, J. L., 1.3, 2.4  
Sutcliffe, D. C., 3.3  
Sutherland, I. E., 3.3  
Suzuki, E., 4.5  
Suzuki, H., 4.5  
Swaminathan, S., 3.3  
Swanson, S. M., 3.3

## AUTHOR INDEX

- Swartzrauber, P. N., 1.3  
 Swoboda, M., 4.3  
 Symmons, M. F., 4.5  
 Szegő, G., 1.3  
 Szillard, L., 2.4
- Tadokoro, H., 4.5  
 Taftø, J., 2.5, 4.3  
 Taguchi, I., 2.2  
 Tajbaksh, A. R., 4.4  
 Takagi, S., 2.5, 5.1, 5.3  
 Takahashi, H., 5.2  
 Takahashi, T., 5.3  
 Takaki, Y., 4.2  
 Takano, T., 1.3  
 Takenaka, A., 3.3  
 Takeuchi, Y., 2.3, 2.4  
 Talapov, A. L., 4.4  
 Tamarkin, J. D., 1.3  
 Tanaka, K., 1.2  
 Tanaka, M., 2.5, 5.2  
 Tanaka, N., 2.3, 2.4, 4.3  
 Tanaka, S., 4.5  
 Tanji, T., 2.5  
 Tanner, B. K., 5.1  
 Tardieu, A., 4.4  
 Tarento, R. J., 4.4  
 Tasset, F., 5.3  
 Tasumi, M., 3.3  
 Tatarinova, L. I., 4.5  
 Tate, C., 2.2  
 Taupin, D., 5.3  
 Taylor, C. A., 1.3, 1.4, 4.2  
 Taylor, D. J., 2.2  
 Taylor, G. H., 4.4  
 Taylor, R., 3.1  
 Taylor, W. J., 2.3  
 Tchoubar, D., 4.2  
 Teeter, M. M., 2.3, 2.4  
 Teller, E., 4.2, 4.5  
 Temperton, C., 1.3  
 Templeton, D. H., 2.4  
 Templeton, L. K., 2.4  
 Ten Eyck, L. F., 1.3  
 Terauchi, M., 2.5  
 Terwilliger, T. C., 2.3, 2.4  
 Teworte, R., 5.1  
 Thaler, R. M., 2.5  
 Thierry, J. C., 2.3  
 Thoen, J., 4.4  
 Thomas, D. J., 3.3  
 Thomas, K. M., 4.4  
 Thompson, J. G., 2.5  
 Thomsen, K., 3.3  
 Thon, F., 2.5  
 Thouless, D. G., 4.4  
 Thuman, P., 2.2  
 Tibbals, J. E., 4.2  
 Tikhonov, V. I., 1.2  
 Tinh, N. H., 4.4  
 Tirion, M., 4.5  
 Titchmarsh, E. C., 1.3  
 Tivol, W. F., 2.5  
 Tivol, W. T., 4.5  
 Tjian, R., 3.3  
 Tobacman, W., 2.5  
 Toeplitz, O., 1.3  
 Tolimieri, R., 1.3  
 Tollin, P., 2.3  
 Tolstov, G. P., 1.3  
 Tomimitsu, H., 5.3  
 Toner, J., 4.4
- Tong, L., 2.3  
 Toniolo, L., 4.2  
 Tonomura, A., 2.5  
 Toupin, R., 2.2  
 Tournarie, M., 2.5, 5.2  
 Tramontano, A., 3.3  
 Traub, W., 2.2  
 Trèves, F., 1.3  
 Trommer, W. E., 2.3  
 Tronrud, D. E., 1.3  
 Trueblood, K. N., 1.1, 1.2, 1.3, 2.3  
 Truter, M. R., 1.3  
 Tsernoglou, D., 3.3  
 Tsipursky, S. I., 2.5  
 Tsirelson, V. G., 2.5  
 Tsoucaris, G., 2.2, 2.4  
 Tsuda, K., 2.5  
 Tsuji, M., 2.5, 4.5  
 Tsukihara, T., 2.3, 3.3  
 Tsuprun, V. L., 2.5  
 Tucciarone, A., 4.2  
 Tucker, R. C., 2.3  
 Tukey, J. W., 1.3  
 Tulinsky, A., 2.4  
 Turberfield, K. C., 4.2  
 Turner, J., 3.3  
 Turner, J. N., 2.5  
 Turner, P. S., 2.5, 4.5  
 Typke, D., 2.5
- Uchida, Y., 4.3  
 Ueki, T., 2.4  
 Ueno, K., 2.5  
 Uhrich, M. L., 1.3  
 Ungaretti, L., 2.4  
 Unge, T., 2.3  
 Unwin, P. N. T., 2.5  
 Uragami, T., 5.1  
 Usha, R., 2.3  
 Ushigami, Y., 5.3  
 Utemisov, K., 5.3  
 Uyeda, N., 2.5  
 Uyeda, R., 2.5, 4.3
- Vaara, I., 2.3  
 Vacher, R., 4.1  
 Vagin, A. A., 2.5  
 Vainshtein, B. K., 2.5, 4.2, 4.5  
 Van Dael, W., 4.4  
 Van der Pol, B., 1.3  
 Van der Putten, N., 2.2  
 Van Heel, M., 2.5  
 Van Hove, L., 4.1, 4.3  
 Van Tendeloo, G., 4.3  
 Vand, V., 1.3, 2.5, 4.5  
 Varady, W. A., 4.4  
 Varghese, J. N., 1.3, 2.2  
 Varnum, J. C., 2.3  
 Vaucher, C., 4.4  
 Vaughan, M. R., 2.5  
 Vaughan, P. A., 2.2  
 Vedani, A., 3.3  
 Venkataraman, G., 4.1  
 Venkatesan, K., 2.4  
 Vereijken, J. M., 2.3  
 Vermin, W. J., 2.2  
 Vibert, P. J., 4.5  
 Vicković, I., 2.2  
 Vijayan, M., 2.3, 2.4  
 Vilkov, L. V., 2.5  
 Villain, J., 4.4  
 Vincent, R., 2.5
- Viterbo, D., 2.2  
 Vlachavas, D. S., 2.5  
 Von der Lage, F. C., 1.2  
 Vonderviszt, F., 4.5  
 Voronova, A. A., 2.5  
 Vos, A., 2.4  
 Vrána, M., 5.3  
 Vriend, G., 2.3  
 Vries, T. A. de, 2.3  
 Vrublevskaya, Z. V., 2.5  
 Vulis, M., 1.3
- Wagner, E. H., 5.1  
 Waho, T., 4.3  
 Wakabayashi, K., 4.5  
 Walian, P. J., 2.5  
 Walker, C. B., 4.1  
 Waller, I., 1.2  
 Walsh, G. R., 3.3  
 Wang, B. C., 1.3, 2.3, 2.4  
 Wang, D. N., 2.5  
 Wang, H., 4.5  
 Wang, J., 4.4  
 Wang, X. J., 4.4  
 Wang, Z. L., 4.3  
 Ward, J. C., 1.3  
 Ward, K. B., 2.3  
 Warme, P. K., 3.3  
 Warren, B., 1.3  
 Warren, B. E., 1.3, 4.2, 4.4  
 Warren, S., 4.5  
 Warshel, A., 3.3  
 Waser, J., 1.3, 1.4, 3.1, 3.2  
 Watanabe, D., 2.5, 4.2, 4.3  
 Watanabe, E., 2.5  
 Watenpaugh, K. D., 1.4, 2.4  
 Watson, D. G., 3.3  
 Watson, G. L., 1.3  
 Watson, G. N., 1.3  
 Watson, H. C., 2.3  
 Watson, K. J., 1.2  
 Weckert, E., 5.1  
 Weeks, C. M., 2.2, 4.5  
 Weintraub, H. J. R., 3.3  
 Weinzierl, J. E., 2.2, 2.3, 2.4  
 Weiss, A. H., 4.4  
 Weiss, G. H., 1.3, 2.1  
 Weiss, R., 2.3  
 Weiss, R. J., 1.2  
 Weissberg, A. M., 2.2  
 Welberry, T. R., 4.2, 4.5  
 Welch, P. D., 1.3  
 Wells, M., 1.3, 1.4  
 Welsh, L. C., 4.5  
 Wenk, H.-R., 2.5  
 Wentowska, K., 4.4  
 Werner, S. A., 4.2, 5.3  
 Wesolowski, T., 3.3  
 West, J., 1.3  
 Westbrook, J. D., 1.4  
 Weyl, H., 1.3  
 Weymouth, J. W., 4.1  
 Whelan, M., 4.3  
 Whelan, M. J., 2.5, 4.3, 4.5, 5.2  
 White, J. G., 2.3  
 White, P., 2.2  
 White, T. J., 2.5  
 Whitfield, H. J., 2.5, 5.2  
 Whittaker, E. J. W., 1.3  
 Whittaker, E. T., 1.3, 3.2  
 Widder, D. V., 3.4  
 Widom, H., 1.3
- Wiener, N., 1.3  
 Wigner, E. P., 1.5  
 Wiley, D. C., 2.3  
 Wilfing, A., 5.3  
 Wilke, W., 4.2  
 Wilkins, M. H. F., 4.5  
 Wilkins, S. W., 1.3, 2.2  
 Williams, D. E., 3.4, 4.1  
 Williams, G. J. B., 3.3  
 Williams, R. M., 4.4  
 Williams, T. V., 3.3  
 Willis, B. T. M., 1.2, 4.1, 4.6  
 Willoughby, T. V., 3.3  
 Wilson, A. J. C., 1.3, 2.1, 2.2, 2.3, 2.4, 2.5, 4.2, 4.5  
 Wilson, E. B., 1.1  
 Wilson, I. A., 2.3  
 Wilson, I. J., 2.5  
 Wilson, K. S., 2.1, 2.2  
 Wilson, S. A., 5.3  
 Windsor, C. G., 4.2  
 Winkler, F. K., 1.3, 2.3  
 Winkor, M. J., 4.4  
 Winograd, S., 1.3  
 Winter, W. T., 4.5  
 Wintgen, G., 1.5  
 Wintner, A., 1.3  
 Wipke, W. T., 3.3  
 Withers, R. L., 2.5, 4.2  
 Wittmann, J. C., 2.5, 4.5  
 Wolf, E., 5.1  
 Wolf, J. A., 1.3  
 Wolff, P. M. de, 2.2, 2.5, 4.2, 4.6  
 Wonacott, A. J., 2.4, 4.5  
 Wondratschek, H., 1.3, 1.5, 2.2  
 Wong, S. F., 4.2  
 Woodward, I., 2.3, 2.4  
 Woolfson, M. M., 1.3, 2.1, 2.2, 2.3, 2.5  
 Wooster, W. A., 4.2  
 Wright, D. C., 4.6  
 Wright, M. H., 3.3  
 Wrighton, P. G., 4.4  
 Wrinch, D. M., 2.3  
 Wu, T. B., 4.2  
 Wu, X.-J., 2.5  
 Wuensch, B. J., 4.2  
 Wunderlich, B., 4.5  
 Wunderlich, J. A., 2.3  
 Wyckoff, H. W., 1.3, 2.3, 4.5  
 Wynn, A., 3.3
- Xiang, S.-B., 2.5  
 Xiaodong, Z., 1.4  
 Xu, P. R., 4.3
- Yagi, N., 4.5  
 Yamamoto, A., 4.6  
 Yamashita, I., 4.5  
 Yang, Y. W., 1.2  
 Yao, J.-X., 2.2, 2.5  
 Yelon, W. B., 5.3  
 Yessik, M., 4.2  
 Yip, S., 4.1  
 Yonath, A., 2.2  
 York, B., 2.2  
 Yoshioka, H., 4.3  
 Yosida, K., 1.3  
 Young, A. P., 4.4  
 Young, C. Y., 4.4  
 Young, R. A., 4.2



## AUTHOR INDEX

- Yu, L. J., 4.4  
Yuan, B.-L., 4.5  
Zachariasen, W. H., 1.3, 1.4, 2.4,  
5.1, 5.3  
Zak, J., 1.5  
Zalkin, A., 2.4  
Zanotti, G., 2.2  
Zarka, A., 5.3  
Zaschke, H., 4.4  
Zassenhaus, H., 1.3  
Zechmeister, K., 1.3, 2.5  
Zegenhagen, J., 5.1  
Zeilinger, A., 5.3  
Zeitler, E., 2.5  
Zelenka, J., 5.3  
Zelepukhin, M. V., 5.3  
Zelwer, C., 2.2  
Zemanian, A. H., 1.3  
Zemlin, F., 2.5  
Zenetti, R., 4.2  
Zernike, F., 4.2  
Zeyen, C., 4.2, 5.3  
Zhang, W. P., 2.5  
Zhao, Z. X., 2.5  
Zheng, C.-D., 2.2, 2.5  
Zhong, Z.-Y., 2.5  
Zhukhlistov, A. P., 2.5  
Ziman, J. M., 1.1  
Zobetz, E., 4.6  
Zolotoyabko, E., 5.3  
Zou, J.-Y., 3.3  
Zucker, I. J., 3.4  
Zucker, U. H., 1.2  
Zugenmaier, P., 4.5  
Zuo, J. M., 2.5  
Zvyagin, B. B., 2.5  
Zwick, M., 1.3, 2.3, 2.4  
Zygmund, A., 1.3

# Subject index

- A posteriori* probability, 423  
*A priori* probability, 415  
*Ab initio* phase determination, 261  
  for proteins, 231  
Abbe theory, 282  
Abel summation procedure, 45  
Abelian groups, 40, 73  
Aberrations, 282  
Absolute configuration, 264, 267  
Absolutely integrable functions, 27  
Absorbing crystals, 536, 545–547  
Absorption coefficient, 541, 546  
  effective, 536  
  linear, 535  
  phenomenological, 281  
Absorption edge, 266  
Absorption function, 445  
Absorption in electron diffraction, 312  
Accelerated convergence, 385  
  formula *via* Patterson function, 389  
Acceptance domain, 492  
Acentric reflections, 69  
Acoustic modes, 402  
Action, 64  
Additive reindexing, 57  
Adiabatic approximation, 400  
Adjusted coefficients, 167  
Affine change of coordinates, 35  
Affine change of variables, 39  
Affine space-group type, 163  
Affine transformation, 105  
Agarwal's FFT implementation of the Fourier method, 90  
Alfalfa mosaic virus, 250  
Algebra of functions, 70  
Algebraic integers, 73, 76  
Algebraic method of reconstruction, 318  
Algebraic number theory, 77  
Aliasing, 46–47, 86  
Allowed origins, 210  
'Almost everywhere', 27  
Analytical electron microscope, 285  
Analytical methods of probability theory, 94  
Angle between two vectors, 348  
Angles  
  Eulerian, 252, 362  
  spherical, 252  
Anisotropic displacement tensors, 6  
Anisotropic fluid, 449  
Anisotropic Gaussian atoms, 60  
Anisotropic temperature factors, 69  
Anisotropic weights, 355  
Annular dark-field detector, 283  
Anomalous absorption, 541, 562  
Anomalous difference, 270, 272  
Anomalous dispersion (scattering), 246–247, 264–266  
  integration with direct methods, 232  
  Patterson function, 248  
Anomalous scatterers, 60–61, 69, 247, 266, 268  
Anomalous transmission effect, 541  
Anti-nodes of standing waves, 541  
Antiferromagnetic domains, 564  
Antisymmetric tensor, 6  
Aperiodic crystal, 486  
  ideal, 486  
Aperiodic structure, 486  
Apparent noncrystallographic symmetry, 255  
Approximate helix symmetry, 469  
Approximations  
  adiabatic, 400  
  Bethe, second, 280  
  Born, first-order, 10, 279  
  Born, second-order, 11  
  Born–Oppenheimer, 18  
  Edgeworth, 23  
  forward-scattering, 280  
  harmonic, 400  
  kinematical, 58, 279–280, 309, 326, 481, 561  
  phase-grating, 556  
  phase-object, 280, 445  
  projected charge-density, 283  
  projection, 286, 553  
  saddlepoint, 94–95  
  seven-beam, 556  
  small-angle-scattering, 278  
  three-beam, 556  
  two-beam, 280, 553  
  two-beam dynamical, 326  
  weak-phase-object, 283  
Area detector, 275  
Argand diagram, 264  
Arithmetic classes, 66  
  of representations, 66  
Arithmetic crystal class, 164  
Arms of star, 165  
Artificial temperature factor, 87, 92  
Aspherical-atom form factor, 15  
Associated actions in function spaces, 65  
Associativity properties of convolution, 92  
Assumption of independence, 205  
Assumption of uniformity, 199, 205  
Asymmetric carbon atom, 267  
Asymmetric images, 314  
Asymmetric unit, 64, 67, 166  
  noncrystallographic, 244  
Asymmetry ratio, 539  
Asymptotic distribution of eigenvalues of  
  Toeplitz forms, 43, 63  
Asymptotic expansions  
  and limit theorems, 95  
  of Gram–Charlier and Edgeworth, 97  
Atom-centred spherical harmonic expansion,  
  14  
Atomic characteristic functions, 206  
Atomic electron densities, 70  
Atomic error matrix, 358  
Atomic force-constant matrix, 401  
Atomic form factor, 10  
  X-ray, 275  
Atomic scattering factor, 10, 265  
  spherical, 10  
Atomic scattering length, 11  
Atomic surface, 486, 492  
Atomic temperature factor, 18  
Autocorrelation, 61  
Autocorrelation function, 320  
Automated Patterson-map search, 321  
Automorphism, 65–66  
Average difference cluster method, 429  
Average intensity  
  of general reflections, 190  
  of zones and rows, 191  
Average multiples for point groups, 193  
Average periodic structure, 409  
Averaged electron density, 261  
Axial disorder, 429  
Back-projection method of reconstruction, 318  
Back-shift correction, 89  
Back surface, 547  
Background diffraction, accurate subtraction  
  of, 473  
Backward convolution theorem, 43, 70  
Bacterial rhodopsin, 262  
Banach spaces, 28  
Band-limited function, 47  
Base-centred lattices, 83  
Bases  
  Cartesian, 7  
  contravariant, 5  
  covariant, 5  
  direct and reciprocal, relationships between, 3  
  mutually reciprocal, 2–3  
  primitive, 163  
  reference, choice of, 7  
Basic crystallographic computations, 84  
Basic domain, 166  
Basic structure, 487  
Basis vectors, contravariant, 348  
Bayesian statistical approach to the phase  
  problem, 98  
Beevers–Lipson factorization, 55, 71  
Beevers–Lipson strips, 71, 86  
Bessel's inequality, 45  
Best Fourier, 84, 272  
Best phase, 272  
Best plane, 353  
Beta distribution  
  first kind, 197  
  second kind, 197  
Bethe approximation, second, 280  
Biaxial nematic order, 452  
Bieberbach theorem, 64  
Bijvoet differences, 248  
Bijvoet equivalents, 268–269  
Bijvoet pair, 267–268  
*Bilder*, 382  
Binary systems, distortions in, 433  
Binding energy, 265  
Bloch-wave formulation, 555  
Bloch waves, 278, 536  
Bloch's theorem, 9, 401  
  alternative form of, 9  
Blow and Crick formulation, 271  
Body-centred lattices, 83  
Body-diagonal axes, 113  
Bond angles, 379  
Bond orientational order, 449  
Booth's differential Fourier syntheses, 88  
Booth's method of steepest descents, 89  
Borie–Sparks method, 434  
Born approximation  
  first-order, 10, 279  
  second-order, 11  
Born series, 279, 555  
  expansion, 445  
Born–Oppenheimer approximation, 18  
Born–von Kármán theory, 400  
Borrmann effect, 281, 541  
Borrmann triangle, 548  
Boundary conditions, 536, 546  
  at exit surface, 542  
Bounded projections, 63, 85  
Bounded subset, 26  
Bragg case, 539  
Bragg condition, symmetric, 287

## SUBJECT INDEX

- Bragg–Lipson charts, 86  
 Bragg's law, departure of incident wave  
     from, 538  
 Branch, 401  
 Bravais lattices  
     centred, 105  
     direct and reciprocal, 105  
 Bright-field disc, 288  
 Bright-field image intensity, 311  
 Brillouin zone, 9, 401  
     first, 165  
 Bulk plasmon excitation, 278  
 Burg entropy, 64  
 Burnside's theorem, 66  
 Butterfly loop, 51
- Calculus**  
     of asymmetric units, 73  
     operational, 28  
 Carpet of cross-vectors, 250  
 Cartesian basis, 7  
 Cartesian coordinate system, 348  
 Cartesian frames of reference, 5  
 Cartesian product, 26, 40  
 Cartesian system, transformation to, 3  
 Cauchy kernel, 45  
 Cauchy sequence, 27  
 Cauchy–Schwarz inequality, 27, 45  
 Cauchy's theorem, 95  
 CBED (convergent-beam electron  
     diffraction), 285  
 Cell constants, 475  
 Central-limit theorem, 95, 194  
     Lindeberg–Lévy version, 199  
 Centre-of-mass translational displacements, 437  
 Centre of symmetry, 289  
     false, 100  
 Centred Bravais lattice, 105  
 Centred lattices, 68  
 Centric reflections, 68  
 Centring  
     effect of, 191  
     translations, 106  
     type, 106  
 Centrosymmetric projections, 242  
 Centrosymmetry  
     determination of, 292  
     status of, 108  
 Cesàro sum, 44  
 Chain rule, 91  
 Chain trace, 384  
 Change-of-basis matrix, 107  
 Change of crystal axes, 104  
 Channelling pattern, 447  
 Characteristic functions, 94, 192, 204  
     atomic, 206  
*CHARMM*, 384  
*Chem-X*, 384  
*CHEMGRAF*, 381  
 Chemical correctness of polypeptide fold, 261  
 Chinese remainder theorem (CRT), 51, 57, 76  
     for polynomials, 54, 77  
     reconstruction, 52  
     reconstruction formula, 54  
 Chirality, 267  
 Choice of reference bases, 7  
 Cholesteryl iodide, 240  
 $\alpha$ -Chymotrypsin, 260  
 Circular harmonic expansions, 93  
 Classical Thomson scattering, 10  
 Classification of crystallographic groups, 66  
 Clebsch–Gordan coefficients, 18
- Closed point group, 248  
 Closed subset, 26  
 Cluster model, 448  
 Clustering, 429  
 Clusters, 411  
 Cochran's Fourier method, 89  
 Cocycle, 79  
 Coherence, 376  
 Coherence length, 467  
 Coherent scattering, 404  
 Column part, 163  
 Communication, statistical theory of, 96  
 Commutative ring, 51  
 Compact subset, 26  
 Compact support, 26, 36, 43  
     distributions with, 31, 39, 41–42, 45  
 Complement of the incomplete gamma  
     function, 386–387  
 Complete normed space, 28  
 Complete vector spaces, 27  
 Completely reducible matrix group, 163  
 Complex antisymmetric transforms, 80  
 Complex scattering factor, 246  
 Complex symmetric transforms, 80  
 Components of vector products, 349  
 Components of vectors, 5  
 Composite lattice, 385, 388  
 Composite structure, 489  
 Compound nucleus, 11  
 Compound transformations, 371  
 Compton scattering, 405  
 Computational and algebraic aspects of mutually  
     reciprocal bases, 4  
 Computer-adapted space-group symbols, 102,  
     106, 112  
 Computer-algebraic languages, 106  
 Computer architecture, 50, 58  
 Condensed ring systems, 379  
 Conditional pair probability, 415  
 Conforming/non-conforming disorder, 429  
 Conformons, 374  
 Conjugacy classes of subgroups, 65  
 Conjugate and parity-related symmetry, 79  
 Conjugate distribution, 96–97  
 Conjugate families of distributions, 98  
 Conjugate gradient method, 378  
 Conjugate symmetry, 35, 39  
 Conjugation, 65  
 Connectivity  
     drawing, 377  
     implied, 377  
     logical, 377  
     structural, 377  
 Connectivity tree, 382  
 Consistency condition, 38  
 Constant **Q** mode, 405  
 Constraints on interpretation of Patterson  
     functions, 248  
 Continuous diffraction on layer lines, 473  
 Contragredient, 39  
     of a matrix, 35  
 Contravariant bases, 5  
 Contravariant basis vectors, 348  
 Contravariant components, 5  
 Conventional coefficients, 167  
 Convergence  
     accelerated, 385  
     accelerated, formula *via* Patterson  
         function, 389  
     of distributions, 31  
     of Fourier series, 44  
 Convergence method, 227
- Convergence-accelerated direct sum, 387  
 Convergent-beam electron diffraction  
     (CBED), 285  
     principal-axis pattern symmetries, 296  
     space-group determination by, 285  
 Conversion of translations to phase shifts, 35  
 Convolution, 61, 235  
     associativity properties of, 92  
     cyclic, 49, 53  
     of distributions, 33  
     of Fourier series, 43  
     of probability densities, 94  
     of two distributions, 34  
 Convolution property, 35, 49  
 Convolution techniques, 324  
 Convolution theorem, 36–37, 41–42, 44, 63, 94,  
     98  
     backward version, 43, 70  
     forward version, 43, 61, 70  
 Convolution theorems with crystallographic  
     symmetry, 70  
 Cooley–Tukey algorithm, 50, 58, 71  
     vector-radix version, 55  
 Cooley–Tukey factorization,  
     multidimensional, 55–56, 74  
 Coordinate systems  
     Cartesian, 348  
     natural, 348  
 Coordinates  
     affine change of, 35  
     fractional, 41, 59, 252  
     homogeneous, 360, 363  
     non-standard, 41  
     screen, 368, 370  
     spherical polar, 252  
     standard, 41, 59, 67  
     transformation of, 5, 7, 33  
     world, 368  
 Copolymers, random, 470  
 Core of discrete Fourier transform matrix, 77  
 Correction-factor approach, 199, 208  
 Correlated lattice disorder, 472  
 Correlation, 61  
 Correlation functions, 70, 92, 243, 405, 415, 444  
     short-range-order, 429  
 Correlation length, 452  
     pretransitional lengthening of, 453  
 Correlations  
     intermolecular, 437  
     librational–librational, 437  
     vibrational–librational, 437  
 Coset averaging, 46–47  
 Coset decomposition, 46, 55  
 Coset reversal, 56  
 Cosets, 46, 67  
     left, 64  
     right, 64  
 Cosine strips, 71  
 Coulombic energy, 385  
 Coulombic lattice energy, 385, 389  
 Covariance, 350  
     interatomic, 354  
 Covariances, 354  
 Covariant bases, 5  
 Covariant components, 5  
 Cowpea mosaic virus, 250  
 Critical angle, 456  
 Critical scattering, 453  
 Cross correlation, 70  
 Cross-correlation function, 314  
 Cross-Patterson vectors, 251  
 Cross-rotation function, 92

## SUBJECT INDEX

- Cross-vectors, 242
  - carpet of, 250
- CRT (Chinese remainder theorem), 51, 57, 76
  - for polynomials, 54, 77
  - reconstruction, 52
  - reconstruction formula, 54
- Cruickshank's modified Fourier method, 90
- Crystal axes, change of, 104
- Crystal class, arithmetic, 164
- Crystal defects, 292
  - in thin films, 445
- Crystal periodicity, 59
- Crystal structure imaging, 284
- Crystal symmetry, 64
- Crystal systems, 66, 108
- Crystal-B phase, 460
- Crystal-E phase, 462–463
- Crystal-G phase, 462
- Crystal-H phase, 463
- Crystal-J phase, 462
- Crystal-K phase, 463
- Crystalline approximant, 486
- Crystallographic applications of Fourier transforms, 58
- Crystallographic discrete Fourier transform, 72
  - algorithms, 71
- Crystallographic extension of the Rader/Winograd factorization, 76
- Crystallographic Fourier transform theory, 59
- Crystallographic group action, 74
  - in real space, 67
  - in reciprocal space, 68
- Crystallographic groups, 64
  - classification of, 66
- Crystallographic statistics, 199
- Crystallographic symmetry, 248
- Cubic groups, 83
- Cubic space groups, 102
- Cumulant expansion, 22
- Cumulant-generating functions, 95, 193
- Cumulative distribution functions, 196
- Cuprous chloride azomethane complex, 238
- Cyclic convolution, 49, 53
- Cyclic (even) permutation of coordinates, 102–103, 107
- Cyclic groups, 66
- Cyclic symmetry, 77
- Cyclotomic polynomials, 54
- Cylindrically averaged diffraction patterns, 471
- Cylindrically averaged Patterson function, 475
  
- Dark-field discs, 287
- Data flow, 58
- Data handling, Hall symbols in, 107
- Data space, 367, 369, 371–372
- de la Vallée Poussin kernel, 44
- Debye model, 402
- Debye theory, 400
- Debye–Waller factor, 453, 542
- Decagonal phase, 503
- Decimation, 26, 47, 51
  - and subdivision of period lattices, duality between, 46
  - in frequency, 51, 56, 79
  - in time, 51, 79
  - period, 47
- Decimation matrix, 55–56, 73
- Decomposition, 72
  - coset, 46, 55
- Deconvolution of a Patterson function, 240
- Defects, 278, 429
  
- Defocus
  - optimal, 311
  - Scherzer, 283
  - Scherzer, conditions, 311
- Deformed crystal, 540
- Delta functions, 26
  - Dirac, 29, 386
  - periodic, 206
  - transforms of, 39
- Density modification, 84, 324
- Density modulation, 496
  - harmonic, 496
  - symmetric rectangular, 497
- Density of nuclear matter, 2
- Deoxyhaemoglobin, 261
- Depth cueing, 371, 381
- Derivatives
  - for model refinement, 88
  - for variational phasing techniques, 87
- Detectors
  - annular dark-field, 283
  - area, 275
- Determinantal formulae, 223
- Determinantal inequalities, 63
- Deviation parameter, 539–541
- Diamond's real-space refinement method, 92
- Dielectric susceptibility, 535, 550
  - Fourier expansion of, 535
- Difference Fourier analysis, 474
- Difference Fourier synthesis, 270, 477
- Difference Fourier technique, 270
- Difference Patterson functions, 244–245
  - isomorphous, 244
- Differential syntheses, 36, 63, 90
- Differentiation, 26, 35
  - and multiplication by a monomial, 39
  - of distributions, 31
  - under the duality bracket, 31
- Differentiation identities, 49
- Differentiation property, 98
- Diffraction
  - by helical structures, 93, 467
  - dynamical, 325
- Diffraction beams, intensities of, 308
- Diffraction conditions, 59
- Diffraction imaging techniques, 564
- Diffraction patterns, cylindrically averaged, 471
- Diffraction point-group tables, 290
- Diffraction relations, 2
- Diffraction vector, 2
- Diffractionometers, optical, 314
- Diffuse scattering, 443
  - elastic, 407
  - inelastic, 407
  - measurement of, 438
  - of X-rays, 407
  - thermal, 407
- Digit reversal, 51, 56, 58
- Digital electronic computation of Fourier series, 71
- Dihedral symmetry, 77
- Dimension of a representation, 163
- Dipalmitoylphosphatidylcholine, 464
- Dipole moment, 389
- Dirac delta function, 29, 386
- Direct and reciprocity symmetries, 286
- Direct Bravais lattice, 105
- Direct inspection of structure-factor equation, 100
- Direct lattice, 2, 5, 41, 106, 164
- Direct-lattice sum, 388
  
- Direct methods, 94, 102, 270, 320
  - in macromolecular crystallography, 231
  - integration with anomalous-dispersion techniques, 232
  - integration with isomorphous replacement techniques, 232
- Direct-methods packages, 230
- Direct metric, 4
- Direct phase determination, 36
  - for proteins, *ab initio*, 231
  - in electron crystallography, 320
- Direct reconstruction, methods of, 317
- Direct space, 163
- Direct-space crystal lattice, 386
- Direct-space sum, 385
- Direct-space transformations, 104
- Direct unit-cell parameters, 4
- Direction cosines of plane normal, 357
- Dirichlet kernel, 44
  - spherical, 60, 84
- Disc symmetries, internal, 292
- Discotic phases, 463
- Discrete Fourier transform matrix, core of, 77
- Discrete Fourier transformation, 45
- Discrete Fourier transforms, 25, 72
  - algorithms, 71
  - matrix representation of, 49
  - numerical computation of, 49
  - properties of, 49
- Discretization, 317
- Dislocations, 457
- Disorder, 443
  - axial, 429
  - conforming/non-conforming, 429
  - from turns, twists and torsions of chains, 429
  - lattice, 471
  - lattice, correlated, 472
  - longitudinal, 428
  - orientational, 436
  - substitutional, 447, 471
  - two-dimensional, 425
- Disordered fibres, 467
- Dispersion corrections, 265, 268, 535
- Dispersion effects, 266
- Dispersion energy, 385
- Dispersion equations, 278
- Dispersion surface, 537, 555, 560
- Displacement modulations, 418
- Displacive modulation, 496
  - harmonic, 497
- Display space, 368, 371–373, 376
- Distance function, 28
- Distribution function, 420
  - cumulative, 196
- Distributions
  - associated with locally integrable functions, 30
  - beta, first kind, 197
  - beta, second kind, 197
  - conjugate, 96–97
  - conjugate families of, 98
  - convergence of, 31
  - convolution of, 33–34
  - definition of, 30
  - differentiation of, 31
  - division of, 33
  - electron-magnetization, 11
  - Fourier transforms of, 38
  - gamma, 197
  - Gaussian, 272
  - hypersymmetric, 196
  - ideal acentric, 195

## SUBJECT INDEX

- Distributions
  - ideal centric, 196
  - integration of, 32
  - lattice, 42, 45–46
  - maximum-entropy, 36, 97
  - motif, 59
  - multiplication of, 32
  - non-ideal, 199, 203
  - of finite order, 30
  - of random atoms, 96
  - of sums, averages and ratios, 197
  - operations on, 31
  - periodic, 41, 43, 59
  - probability density, 192
  - probability density, ideal, 195
  - support of, 31
  - $T$  on  $\Omega$ , 30
  - tempered, 36, 38, 40, 45, 68
  - tensor products of, 33
  - theory of, 25, 28
  - with compact support, 31, 39, 41–42, 45
- Divided differences, 556
- Division of distributions, 33
- Division problem, 33
- Docking, 383
- Domain
  - basic, 166
  - minimal, 166
  - of influence, 165
  - representation, 166
- Domain structure, 383
- Double-phased synthesis, 265
- Double-sorting technique, 261
- Drawing connectivity, 377
- Dual, topological, 30–31, 38–39
- Dual relationships, 2
- Duality
  - between differentiation and multiplication by a monomial, 63
  - between periodization and sampling, 42
  - between sections and projections, 40
  - between subdivision and decimation of period lattices, 46
- Duality bracket, 38
- Duality product, 31
- Dummy indices, 5
- Dynamic parallax, 369, 383
- Dynamical approximation, two-beam, 326
- Dynamical diffraction, 325, 445
  - theory, 280, 534
  - two-beam, formulae, 281
- Dynamical matrix, 401
- Dynamical scattering effects, 321
- Dynamical scattering factor, 446
- Dynamical shape function, 556
- Dynamical theory, 280, 534
  - fundamental equations, 536
  - of neutron diffraction, 557
  - plane-wave, 538
  - solution of, 540
- Dynamics, 9
  - of three-dimensional crystals, 400
- $E$  maps, interpretation of, 228
- Edgeworth approximation, 23
- Edgeworth series, 95
- EDSA (electron-diffraction structure analysis), 306
- Effect of centring, 191
- Effective absorption coefficient, 536
- Effective potential-energy function, 479
- Effects of symmetry on the Fourier image, 99
- Eigenspace decomposition of  $L^2$ , 36
- Eigenvalue, 554
- Eigenvalue decomposition, 378
- Einstein model, 402
- Elastic component of X-ray scattering, 10
- Elastic constants, measurement of, 406
- Elastic diffuse scattering, 407
- Electromagnetic electron lenses, 278, 282
- Electron band theory of solids, 537
- Electron crystallography, 320
  - direct phase determination, 320
  - of polymers, 481
  - of proteins, 321
  - three-dimensional structure determination by, 323
- Electron density, 2, 8, 17, 100, 272
  - averaged, 261
  - real-space averaging of, 250, 261
- Electron-density calculations, 69
- Electron-density maps, Fourier synthesis of, 84
- Electron diffraction, 443
  - sign conventions, 279–280
- Electron-diffraction data
  - for crystal-structure determination, 481
  - three-dimensional, 324, 484
- Electron-diffraction patterns
  - geometric theory of, 309
  - polycrystal, 308
  - single-crystal, 306
  - texture, 307, 326
- Electron-diffraction structure analysis (EDSA), 306
- Electron distribution, atomic, radial dependence of, 12
- Electron lenses, electromagnetic, 278, 282
- Electron-magnetization distribution, 11
- Electron micrographs
  - Fourier transform of, 325, 482
  - phase information from, 322
- Electron-microscope image contrast, 445
- Electron-microscope imaging, 443
- Electronic analogue computer X-RAC, 71
- Electronic structure, 9
- Electrons, interaction with matter, 277
- Electrostatic energy, 385
- Electrostatic potential, 2
- Electrostatic properties of molecular surfaces, 380
- Embedding method,  $n$ -dimensional, 487
- Enantiomer, 267
- Enantiomeric ambiguity, 237
- Enantiomorph definition, 227
- Enantiomorphic images, weak, 238
- Enantiomorphic solutions, 237
- Energy minimization, 380, 382, 384
- Entire functions, 36
- Entrance surface, 547
- Entropy, 87
- Envelope, 248
- Envelope functions, 283
- Epitaxial orientation techniques, 482
- Equal-amplitude assumption, 479
- Equal distribution, 43
- Equivalent matrix groups, 163
- Equivalent reflections, 267
- Error matrix, atomic, 358
- Error propagation, 353
- Errors, 271
  - root-mean-square, 273
  - systematic, 351
- Essential bounds, 43
- Essentially bounded function, 27
- Euclidean algorithm, 46, 54, 62
- Euclidean norm, 26
- Euclidean space, 26
- Eulerian angles, 252, 362
- Eulerian space, 253
- Eulerian space groups, 254
  - rotation-function, 256
- Eulerian symmetry elements, 254
- Even (cyclic) permutation of coordinates, 102–103, 107
- Ewald result, 385
- Ewald wave, 536
- Exchange between differentiation and multiplication by monomials, 94
- Exchange between multiplication and convolution, 26
- Excitation error, 552
- Excitations
  - bulk plasmon, 278
  - inner-shell, 278
  - interband, 278
  - intra-band, 278
- Explicit-origin space-group notation, 112
- Explicit space-group symbols, 107–109
- Exploration of parameter space by molecular model building, 474
- Exponential coefficient, 14
- Exsolution, 416
- Extended resolution, 261
- External fields, effect on neutron scattering, 562
- External modes, 402
- Extinction, 546
- Extinction conditions, real-space interpretation of, 291
- Extinction distance, 539–541
- Extinction factors, 561
- Extinction rules for symmetry elements, 291
- Face-centred lattices, 83
- Face-diagonal axes, 113
- Factor group, 65, 67
- Factorization, 72
- False centre of symmetry, 100
- Fast Fourier transform (FFT), 71
- Fast rotation function, 255
- Feedback method, 244
- Fejér kernel, 44
  - spherical, 60
- Fermi pseudo-potential, 557
- Fermi surface, 448
- FFT (fast Fourier transform), 71
- $F_{HLE}$ , 270
- $F_{HUE}$ , 270
- Fibonacci chain, 491
- Fibonacci sequence, 490
- Fibre axis, 467
- Fibre diffraction, 40, 474
  - $R$  factor, 480
  - specimens for, 467
  - X-ray, 466
- Fibres
  - axially periodic, transform of, 93
  - disordered, 467
  - macromolecular, 479
  - noncrystalline, 467, 469, 474
  - partially crystalline, 471
  - polycrystalline, 467, 469, 474
- Field of a  $\mathbf{k}$  vector, 171
- Field emission gun, 285
- Figures of merit, 227, 272
- Films
  - freely suspended, 456

## SUBJECT INDEX

- Films
  - smectic, 456
- Filtered image, 314
- Filtering
  - iterative low-pass, 473
  - rotational, 314
- Finite field, 53
- Finite space group, 164
- First Brillouin zone, 165
- First-order Born approximation, 10, 279
- First-order perturbation theory, 353
- Flight time, neutron, 563
- Flipping ratio, 561
- Fluctuations from an average periodic structure, 409
- Focusing of neutron beams, 563
- Force-constant matrix, atomic, 401
- Form factor, 60
  - aspherical-atom, 15
  - atomic, 10
  - atomic, X-ray, 275
  - geometric, 501
  - Kikuchi-line, 446
- FORTRAN, 106
- FORTRAN interface, 106
- FORTRAN interpreter, 107
- Forward convolution theorem, 43, 61, 70
- Forward scattering, 552
- Forward-scattering approximation, 280
- Four-dimensional vector, 366
- Fourier analysis, 59
  - and filtration in reciprocal space, 313
- Fourier approach, 208
- Fourier coefficient, 44, 265
- Fourier convolution theorem, 10
- Fourier cotransform, 34
- Fourier cotransformation, 40
- Fourier expansion, 2
  - of dielectric susceptibility, 535
- Fourier images, 99, 284
  - effects of symmetry on, 99
- Fourier map, 265
- Fourier method, 203
  - Agarwal's FFT implementation of, 90
- Fourier representation, 274
- Fourier series, 25
  - convergence of, 44
  - convolution of, 43
  - digital electronic computation of, 71
  - electron density and its summation, 60
- Fourier space, 101
  - symmetry in, 105
- Fourier summations, 101
  - space-group-specific, 101
- Fourier synthesis, 59, 268, 272
  - best, 272
  - of electron-density maps, 84
- Fourier transformation
  - discrete, 45
  - for reconstruction, 318
  - inverse, 35, 40
  - mathematical theory of, 25
- Fourier transforms, 25, 34, 386
  - crystallographic applications, 58
  - crystallographic, discrete, 72
  - crystallographic, theory of, 59
  - discrete, 25
  - discrete, core of matrix, 77
  - discrete, matrix representation of, 49
  - discrete, numerical computation of, 49
  - discrete, properties of, 49
  - exchange of subdivision and decimation, 47
- Fourier transforms
  - in  $L^1$ , 35
  - in  $L^2$ , 36
  - in polar coordinates, 93
  - in  $\mathcal{L}$ , 37
  - inverse, 8
  - kernels of, 35
  - of a distribution, 38
  - of electron micrographs, 325, 482
  - of periodic distributions, 41
  - of tempered distributions, 38–39
  - tables of, 38
  - tensor product property of, 71
  - various writings of, 38
- Fourier-transform space, 386
- Fourier–Bessel series, 205
- Fourier–Bessel structure factors, 468
- Fractal atomic surface, 493
- Fractal sequence, 494
- Fractional coordinates, 41, 59, 252
- Fréchet space, 28
- Freely suspended films, 456
- Fresnel reflection law, 456
- Friedel equivalent, 264, 266
- Friedel pair, 267
- Friedel's law, 60, 68, 70, 246, 278
- Frobenius congruences, 66, 68
- Frodo*, 383
- Fubini's theorem, 28, 35, 38
- Function spaces
  - associated actions in, 65
  - topology in, 28
- Functional derivative, 91
- Functions of polynomial growth, 40
- Fundamental domain, 64, 66–67
- Fundamental equations of dynamical theory, 536
- Fundamental region, 165
- Fundamental relationships, 3
- Fused-ring systems, 384
  
- G*-invariant function, 65
- Gamma distribution, 197
- Gamma function, 386
  - incomplete, 386, 389–390
- Gamma radiation, 274–275
- Gaussian atomic densities, 58
- Gaussian atoms, 67–68, 86
  - anisotropic, 60
- Gaussian distribution, 272
- Gaussian function, 38
  - standard, 37, 39
- Gaussian plane, general, 356
- Gaussian weights, 355
- Gaussians, 92
- General conditions for possible reflections, 100
- General Gaussian plane, 356
- General  $\mathbf{k}$  vector, 165
- General linear change of variable, 35
- General multivariate Gaussians, 37
- General reflections, average intensity of, 190
- General topology, 28
- General translation function, 258
- Generalized multiplexing, 82
- Generalized Patterson function, 409
- Generalized Rader/Winograd algorithms, 83
- Generalized structure-factor formalism, 23
- Generalized support condition, 34
- Geometrical form factor, 501
- Geometric redundancies, 62
- Geometric structure factors, 101, 120
  
- Geometric theory of electron-diffraction patterns, 309
- Gibbs phenomenon, 44, 60
- GKS (Graphical Kernel System), 361
- GKS-3D (Graphical Kernel System for Three Dimensions), 361
- Glide line, projected, 289
- Glide planes, horizontal, 289
- Global crystallographic algorithms, 82
- Glyceraldehyde-3-phosphate dehydrogenase, 249, 261–262
- Good algorithm, 51
- Good factorization, multidimensional, 76
- Goodness of fit, 359
- Gram–Charlier series, 22, 95
- Gram–Schmidt process, 367, 379
- GRAMPS*, 381
- Graphical Kernel System (GKS), 361
- Graphical Kernel System for Three Dimensions (GKS-3D), 361
- Graphics, 360
- Gravity, 563–564
- Green's theorem, 32, 86
- GRIP*, 382
- Group actions, 64, 72
  - crystallographic, 74
  - crystallographic, real space, 67
  - crystallographic, reciprocal space, 68
- Group characters, 82
- Group cohomology, 74
- Group extensions, 66
- Group of units, 50
- Group ring
  - integral, 74
  - module over, 25
- Group–subgroup relationship, 103
- Groups, 64
- GS (glide–screw) bands, 286
- Guide*, 383
  
- Haemoglobin, 242, 264, 269
  - horse, 243
- Half-bake*, 231
- Hall symbols, 107, 112, 115
  - in data handling, 107
  - in software, 107
- Hankel transform, 93
- Hardy's theorem, 38
- Harker diagram, 248, 265, 271–272
- Harker lines, 240
- Harker peaks, 71
- Harker planes, 240
  - special, 240
- Harker sections, 239–240
- Harmonic approximation, 400
- Harmonic density modulation, 496
- Harmonic displacive modulation, 497
- HDD (high-dispersion diffraction), 306
- Heavy atoms, 268
- Heavy-atom-derivative data sets, scaling of, 246
- Heavy-atom derivatives, 269
- Heavy-atom distribution, 270
- Heavy-atom location, 239
  - three-dimensional methods, 243
- Heavy-atom lower estimate, 248
- Heavy-atom parameters, 270
- Heavy-atom sites, 242
- Heavy-atom substitution, 245
- HEED (high-energy electron diffraction), 306
- Heisenberg's inequality, 38, 84
- Helical structures, 429
  - diffraction by, 93, 467

## SUBJECT INDEX

- Helical symmetry, 93, 317, 467, 475  
 approximate, 469  
 Helix repeat units, 468  
 Hermann–Mauguin space-group symbol, 103  
 Hermite function, 37, 95  
 multivariate, 37, 92  
 Hermite polynomials, three-dimensional, 22  
 Hermitian-antisymmetric transforms, 80  
 Hermitian form, 43  
 Hermitian symmetry, 60, 69, 79  
 Herringbone packing, 462  
 Hexagonal axes, 103  
 Hexagonal family, 103  
 Hexagonal groups, 83  
 Hexagonal space groups, 103  
 Hexatic phase, 458  
 in two dimensions, 457  
 tilted, 458  
 Hexatic-B phase, 460  
 Hexokinase, 261  
 Hidden-line algorithms, 376  
 Hidden-surface algorithms, 376  
 High-dispersion diffraction (HDD), 306  
 High-energy electron diffraction (HEED), 306  
 High-resolution electron diffraction (HRED), 306  
 High-resolution electron microscopy (HREM), 310  
 High-voltage limit, 556  
 Higher-order Laue zone (HOLZ), 292  
 Highlighting, 376  
 Hilbert space, 27, 34, 45  
 Hologram, in-line, 285  
 Holohedral point group, 166  
 Holosymmetric space group, 166  
 HOLZ (higher-order Laue zone), 292  
 Homogeneous coordinates, 360, 363  
 Homogeneous symmetric polynomial, 556  
 Homometric pair, 237  
 Homometric structures, 237  
 Homomorphism, 163  
 Horizontal glide plane, 289  
 Horizontal mirror plane, 289  
 Horse haemoglobin, 243  
 HRED (high-resolution electron diffraction), 306  
 HREM (high-resolution electron microscopy), 310  
 Hybridization, 384  
 HYDRA, 383  
 Hydrogen bonding, 381, 383–384  
 Hydrophobic properties of molecular surfaces, 380  
 Hyperatoms, 487  
 Hypercrystal, 486, 488  
 Hypersymmetric distributions, 196  
 Hypothetical atoms, 87
- Icosahedral phase, 509  
 Ideal acentric distributions, 195  
 Ideal aperiodic crystal, 486  
 Ideal centric distributions, 196  
 Ideal crystal, 163, 486  
 Ideal probability density distributions, 195  
 Idempotents, 52  
 Image averaging in real space, 313  
 Image contrast, electron-microscope, 445  
 Image detection, 240  
 Image enhancement, 310, 313  
 Image intensity, bright-field, 311  
 Image of a function by a geometric operation, 26
- Image processing in transmission electron microscopy, 310  
 Image reconstruction, 310  
 Image resolution, 284  
 Image restoration, 310–311  
 Images  
 asymmetric, 314  
 filtered, 314  
 with point symmetry, 314  
 Immunoglobulin, 260  
 Implication theory, 239  
 Implicit function theorem, 53  
 Implied connectivity, 377  
 Improper rotation axes, 248  
 Improper rotations, 108, 113  
 In-disc symmetries, 287  
 In-line hologram, 285  
 Incident wave, departure from Bragg's law, 538  
 Incoherent inelastic scattering, 404  
 Incoherent scattering, 404  
 inelastic, 404  
 Incommensurability, 452  
 Incommensurate intergrowth structure, 489  
 Incommensurately modulated structure, 487  
 Incomplete gamma function, 386, 389  
 complement of, 386–387  
 evaluation of, 390  
 Independence, assumption of, 205  
 Index, 64  
 Index of refraction, 535  
 Indicator functions, 32, 41, 46, 61, 84–85  
 Individual symmetry elements, observation of, in CBED patterns, 288  
 Induction formula, 96  
 Inductive limit, 30  
 Inelastic component of X-ray scattering, 10  
 Inelastic diffuse scattering, 407  
 Inelastic neutron scattering, 404  
 Inelastic scattering, 278, 443  
 diffuse, 407  
 neutron, 404  
 Inequalities among structure factors, 217  
 Inner-shell excitations, 278, 444  
*Insight*, 381  
*Insight II*, 384  
 Instrumental resolution, 285  
 Integral group ring, 74  
 Integral representation, 64  
 theory, 66  
 Integrals  
 Lebesgue, 27  
 Riemann, 27  
 Integrated intensity, 544, 546–547  
 Integration  
 by parts, 31  
 Lebesgue's theory of, 29  
 of anomalous-dispersion techniques with direct methods, 232  
 of distributions, 32  
 of isomorphous replacement techniques with direct methods, 232  
 Intensities of diffraction beams, 308  
 Intensities of plane waves  
 in reflection geometry, 545  
 in transmission geometry, 541  
 Intensities of reflected and refracted waves, 542  
 Intensity differences, 266  
 Intensity statistics, 97  
 Interaction between symmetry and decomposition, 73  
 Interaction between symmetry and factorization, 73
- Interaction matrix, 240  
 Interaction of electrons with matter, 277  
 Interaction of X-rays with matter, 534  
 Interatomic covariance, 354  
 Interatomic vectors, 61  
 Interband excitation, 278  
 Interference function, 62  
 spherical, 251  
 Interferometry, neutron, 563  
 Intermolecular correlations, 437  
 Internal disc symmetries, 292  
 Internal modes, 402  
 Interpolation formula, 46  
 Interpolation kernel, 85  
 Interpretation of  $E$  maps, 228  
 Intraband excitation, 278  
 Intramolecular energy terms, 390  
 Intrinsic component of translation part of space-group operation, 100  
 Invariance of  $L^2$ , 36  
 Inverse Fourier transform, 8  
 Inverse Fourier transformation, 35, 40  
 Inverse rotation operator, 99  
 Ionic crystal, electrostatic energy of, 385  
 Irreducible matrix group, 163  
 Irreps, 162  
 Ising model, 64  
 Isometry, 36  
 Isometry property, 36  
 Isomorphism, 163, 271, 273  
 lack of, 245  
 Isomorphous addition, 264  
 Isomorphous crystals, 265  
 Isomorphous differences, 270, 273  
 Isomorphous heavy-atom derivatives, 478  
 Isomorphous replacement, 242, 264  
 difference Patterson functions, 242, 244  
 multiple, 271  
 single, 244, 265  
 techniques, integration of direct methods with, 232  
 Isomorphous synthesis, 265  
 Isotropic harmonic oscillator, three-dimensional, 18  
 Isotropic temperature factors, 68  
 Isotropy subgroups, 64, 67  
 Iteration method of reconstruction, 318  
 Iterative low-pass filtering, 473
- Jacobians, 33, 49  
 Joint probability distribution of structure factors, 97  
 Juxtaposition of chains, 476
- k** vector  
 general, 165  
 special, 165  
 uni-arm, 167  
 Kernels, 55  
 of Fourier transformations, 35  
 Kikuchi-line contrast, 446  
 Kikuchi-line form factor, 446  
 Kinematical approximation, 58, 279–280, 309, 326, 481, 561  
 Kinematical diffraction  
 formulae, 281  
 intensities, 281  
 Kinematical  $R$  factor, 483  
 Kinematical scattering, 279  
 Klug peaks, 255  
 Known structural fragment, use of, 260, 321

## SUBJECT INDEX

- Kronecker symbol, 5  
 ‘Kubic Harmonics’, 14
- LACBED (large-angle convergent-beam electron diffraction), 285
- Lagrange multiplier, 87, 97, 356
- Lagrange’s theorem, 64
- LALS*, 476
- Lamellar domains with long-range order, 416–417
- Landau–Peierls effect, 453–454
- Langmuir troughs, 482
- Languages  
   computer-algebraic, 106  
   numerically and symbolically oriented, 102
- Large-angle convergent-beam electron diffraction (LACBED), 285
- Large values of  $\mu_{ot}$ , 549
- Larmor precession, 558
- Lattice, 40  
   base-centred, 83  
   body-centred, 83  
   centred, 68  
   composite, 385, 388  
   direct, 2, 5, 41, 106, 164, 386  
   face-centred, 83  
   non-primitive, 67  
   non-standard, 40  
   non-standard period, 42  
   one-dimensional, 454  
   period, 41, 59, 64  
   primitive, 66  
   reciprocal, 2, 5, 42, 46, 59, 106, 164  
   residual, 46  
   rhombohedral, 83  
   standard, 40  
   translation, 163
- Lattice disorder, 471  
   correlated, 472
- Lattice distributions, 42, 45–46
- Lattice-dynamical model, 400
- Lattice energy, Coulombic, 385, 389
- Lattice mode, 66
- Lattice-parameter mapping, 534
- Lattice plane, 2, 350
- Lattice sum, 43
- Lattice transform, 386
- Lattice-translation subgroup, 108
- Lattice type, 108
- Laue case, 538
- Laue circle patterns, 291
- Laue equations, 2
- Laue groups, 100
- Laue point, 538
- Laue scattering, 432
- Laue techniques, monochromatic, 439
- Laue zones, higher-order, 292
- Layer lines, continuous diffraction on, 473
- Lead, 269
- Least resolvable distance, 284
- Least-squares adjustment of observed positions, 356
- Least-squares determination of phases, 229
- Least-squares method, multivariate, 88
- Least-squares plane, 353  
   proper, 355
- Least-squares refinement, 270
- Lebesgue integral, 27
- Lebesgue’s theory of integration, 29
- LEED (low-energy electron diffraction), 306
- Left action, 64–65, 68, 74
- Left cosets, 64
- Left representation, 68
- Leibnitz’s formula, 387
- Length  
   of a function, 27  
   of a vector, 348
- Lennard–Jones potential, 406
- L’Hospital’s rule, 387
- Libration, 19
- Libration tensor, 19
- Librational–librational correlations, 437
- Lifchitz’s reformulation, 91
- Lifshitz point, 455
- Lindeberg–Lévy version of the central-limit theorem, 199
- Line drawings, 375
- Linear absorption coefficient, 535
- Linear change of variable, general, 35
- Linear forms, 30
- Linear functionals, 28
- Linear transformation, 7
- Linearity, 35, 49
- Linearization formulae, 70
- Linearly semidependent phases, 212
- Linked-atom least-squares (*LALS*) system, 476
- Liouville’s theorem, 36
- Liquid crystals, 449
- Lissajous curve, 96
- Little co-group, 165, 167
- Little group, 165
- Local ordering, 429
- Locally integrable functions, 30  
   distributions associated with, 30
- Locally summable function of polynomial growth, 39
- Location-dependent component of translation part of space-group operation, 100
- Locked rotation function, 255
- Logical connectivity, 377
- Lone pairs, 384
- Long-range order (LRO), 415, 450  
   positional, 449
- Longitudinal disorder, 428
- Lorentz point, 537
- Low-angle scattering, 419
- Low-energy conformational changes, 480
- Low-energy electron diffraction (LEED), 306
- $L^p$  spaces, 27
- LRO (long-range order), 450  
   positional, 449
- Lytotropic phase, 451
- Lysozyme, 243
- MACCS*, 384
- Macromolecular crystallography, 264  
   direct methods in, 231
- Macromolecular fibre structures, 479
- Macromolecular refinement techniques, 92
- Macromolecular structures, direct determination of, 481
- MAD (multiwavelength anomalous diffraction), 233
- Madelung constant, 385
- Magic-integer methods, 228
- Magnetic domains, 564
- Magnetic scattering, 11, 559
- Main reflections, 488
- Manganese, 268
- Many-beam case, 536
- Mapping, 26
- Mathematical theory of Fourier transformation, 25
- Matrices of mixed scalar products, 8
- Matrix algebra, 252
- Matrix groups, 163  
   completely reducible, 163  
   equivalent, 163  
   irreducible, 163  
   reducible, 163  
   unitary, 163
- Matrix part, 163
- Matrix representation, 99  
   of discrete Fourier transform, 49
- Maximum determinant rule, 223
- Maximum entropy, 97, 325
- Maximum-entropy distributions, 36  
   of atoms, 97
- Maximum-entropy methods, 94, 230
- Maximum-entropy theory, 97
- Maximum function, 241
- Maximum likelihood, 325
- Maxwell’s equations, 534, 550
- MBD (microbeam diffraction), 306
- MDIR (multidimensional isomorphous replacement), 478
- MDKINO*, 381
- Mean-field theory, 451
- Mean values, 351
- Measurement of diffuse scattering, 438
- Meijer’s *G* function, 196
- Mercury, 269
- Mesomorphic structures, scattering from, 449
- Metric  
   direct, 4  
   reciprocal, 4
- Metric space, 26, 28
- Metric tensors, 4–5
- Metrizability, 26
- Metrizable topology, 28
- Micelle, 449
- Microanalysis, 277–278
- Microbeam diffraction (MBD), 306
- Microdiffraction, 447–448
- MIDAS*, 381
- Middle of reflection domain, 539
- Minimal domain, 166
- Minimization function, 271
- Minimum function, 241
- MIR (multiple isomorphous replacement), 271  
   phases, 250
- MIRAS (multiple isomorphous replacement with anomalous scattering), 233
- Mirror image, 267
- Mirror plane  
   horizontal, 289  
   vertical, 289
- MM2/MMP2*, 384
- MMS-X*, 382
- Modified peaklist optimization, 231
- Modified tangent formula, 229
- Modulated phases, 452
- Modulated smectic-A phase, 455
- Modulated smectic-C phase, 455
- Modulated structure, 487
- Modulation function, 487
- Module, 74  
   over a group ring, 25
- Molbuild*, 384
- Molecular averaging by noncrystallographic symmetry, 85
- Molecular axis, 467
- Molecular dynamics, 384
- Molecular-dynamics refinement, 479
- Molecular envelope, 32, 61, 85–86
- Molecular mechanics, 379



## SUBJECT INDEX

- Molecular model building, 476  
 Molecular modelling, 6, 360  
 Molecular orientational order, 449  
 Molecular origin, 261  
 Molecular replacement, 235, 248, 260–261, 274  
     real-space, 261  
 Molecular rotation, 460  
 Molecular structure, position of a known, 259  
 Molecular surfaces, hydrophobic and electrostatic properties of, 380  
 Moment-generating functions, 36, 95  
 Moment-generating properties, 94  
     of  $\bar{F}$ , 63  
 Moments of a distribution, 94  
 Monochromatic Laue techniques, 439  
 Monochromators, 563  
     polarizing, 560  
 Monoclinic family, 103  
 Monoclinic groups, 82  
 Monoclinic space groups, 103  
 Mosaic crystals, 534  
 Mosaic model, 561  
 Mosaicity, 306  
 Motif, 41–43  
 Motif distribution, 59  
 Multicritical point, 455  
 Multidimensional algorithms, 55  
 Multidimensional Cooley–Tukey factorization, 55–56, 74  
 Multidimensional factorization, 55  
 Multidimensional Good factorization, 76  
 Multidimensional isomorphous replacement (MDIR), 478  
 Multidimensional prime factor algorithm, 56  
 Multidimensional structure, 380  
 Multi-index, 27, 36–37  
 Multi-index notation, 27  
 Multiple diffuse scattering, 445  
 Multiple isomorphous replacement (MIR), 271  
     phases, 250  
 Multiple isomorphous replacement with anomalous scattering (MIRAS), 233  
 Multiple reciprocal cell, 106  
 Multiple scattering, 443  
 Multiple-wavelength method, 274  
 Multiplexing, generalized, 82  
 Multiplexing–demultiplexing, 79  
 Multiplication by a monomial, 26  
 Multiplication of distributions, 32  
 Multiplicative group of units, 53  
 Multiplicative reindexing, 57  
 Multiplicity, 101, 167  
 Multiplicity corrections, 242  
 Multiplier functions, 40  
 Multipliers, 42  
     Lagrange, 87, 97, 356  
 Multi-Slater determinant wavefunction, 18  
 Multislice, 284, 555  
     calculations, 447  
     computer programs, 447  
 Multislice recurrence relation, 555  
 Multivariate Gaussian, 43  
 Multivariate Hermite functions, 37, 92  
 Multivariate least-squares method, 88  
 Multiwavelength anomalous diffraction (MAD), 233  
 Mutually reciprocal bases, 2–3  
     computational and algebraic aspects of, 4  
 Mutually reciprocal triads, 2  
 Myoglobin, 242, 264, 269  
  
*n*-dimensional embedding method, 487  
*n*-shift rule, 90  
*n*-torus  
     non-standard, 41  
     standard, 40  
 Natural coordinate system, 348  
 Negative peaks, 243  
 Nematic order  
     biaxial, 452  
     uniaxial, 452  
 Nematic phase, 449, 451  
 Nested algorithms, 58  
 Nested neighbourhood principle, 218  
 Nesting, 57  
     of Winograd small FFTs, 56  
 Net distortions, 429  
 Neutron absorption, 558  
 Neutron beams, focusing of, 563  
 Neutron crystallography, 275  
 Neutron diffraction, 463  
     dynamical theory of, 557  
 Neutron flight time, 563  
 Neutron interferometry, 563  
 Neutron refraction, 557  
 Neutron scattering  
     effect of external fields, 562  
     inelastic, 404  
     very-small-angle, 563  
 Neutron scattering lengths, 275  
 Neutron spin, 558  
 Neutron topography, 564  
 Neutrons, 275  
     thermal, 275  
 Nodes of standing waves, 541  
 Non-absorbing case, 536  
 Non-absorbing crystals, 544–546  
     comparison of dynamical and geometrical theory, 547  
 Nonbonded interatomic distances, 476  
 Non-classical crystallography, 292  
 Noncrystalline fibres, 467, 469, 474  
 Noncrystallographic asymmetric unit, 244  
 Noncrystallographic rotation elements, translational components of, 248  
 Noncrystallographic rotational symmetry, 250  
 Noncrystallographic symmetry, 62, 248–249  
     apparent, 255  
     molecular averaging by, 85  
     phase improvement using, 261  
     proper, 248  
 Noncrystallographic symmetry element, position of, 259–260  
 Non-cyclic (odd) permutation of coordinates, 102–103, 107  
 Non-ideal distributions, 199, 203  
 Non-ideal probability density functions, 208  
     of  $|E|$ , 200  
 Non-independent variables, 195  
 Non-linear transformations, 254  
 Non-periodic system, 414  
 Non-primitive lattice, 66–67  
 Non-spin-flip scattering lengths, 559  
 Non-standard coordinates, 41  
 Non-standard lattice, 40  
 Non-standard *n*-torus, 41  
 Non-standard period lattice, 42  
 Norm  
     Euclidean, 26  
     on a vector space, 28  
 Normal equations, 88  
 Normal matrix, 90  
 Normal subgroup, 64–65  
  
 Normalization constant, 272, 274  
 Normalized structure factors, 215, 227, 236  
 Normalizer, 65  
 Normed space, 28  
     complete, 28  
 Notation, multi-index, 27  
 Nuclear matter, density of, 2  
 Numerical computation of discrete Fourier transform, 49  
 Numerically oriented languages, 102  
 Nussbaumer–Quandalle algorithm, 57  
  
*O*, 384  
 Oblique projections, 317  
 Observation plane, 310  
 Observational equations, 88  
 Obverse setting, 106  
 Occupancy factors, 271  
 Occupied natural spin orbitals, 18  
 Odd (non-cyclic) permutation of coordinates, 102–103, 107  
 Offset, 51  
 One-centre orbital products, 18  
 One-centre terms, 18  
 One-dimensional lattice, 454  
 One-particle potential (OPP) model, 23  
 One-phase structure seminvariants, first rank, 224  
 One-wavelength techniques, 233  
 Operational calculus, 28  
 Operations on distributions, 31  
 OPP (one-particle potential) model, 23  
 Optic modes, 402  
 Optical diffractometer, 314  
 Optical isomers, 267  
 Optical rotation, 268  
 Optical transforms, 418  
 Optimal defocus, 311  
 Orbit decomposition, 64, 67, 69–70  
     formula, 64, 68  
 Orbit exchange, 65, 72–73  
 Orbit of  $\mathbf{k}$ , 165  
 Orbital products, 17  
     one-centre, 18  
     two-centre, 18  
 Orbits, 64, 67–68  
 Order parameter, 451  
 Order–disorder, 417  
 Orientational disorder, 436  
 Origin-shift vector, 107  
 Origin-to-plane distance, 353, 356–357  
 Origin(s)  
     allowed (permissible), 210  
     definition, 227  
     molecular, 261  
     removal from a Patterson function, 236  
     selection, 238  
     specification, 210  
 Ornstein–Zernike correlation function, 425  
 ORTEP, 380  
 Orthoaxial projection, 316  
 Orthogonal matrices, 361  
 Orthogonalization, 252  
 Orthographic projection, 369–370  
 Orthorhombic groups, 82  
 Orthorhombic space groups, 102  
 Overlap between two Pattersons, 250  
  
 $P_s(\mathbf{u})$  function, 246  
 Pair probability, 415  
     conditional, 415  
 Pairwise sum, 385

## SUBJECT INDEX

- Paley–Wiener theorem, 36, 98  
 Parabolic equation, 552  
 Parallel processing, 58  
 Parity of the *hkl* subset, 103  
 Parseval–Plancherel property, 49  
 Parseval–Plancherel theorem, 36, 45  
 Parseval's identity, 61, 63  
 Parseval's theorem, 34, 88, 386  
   with crystallographic symmetry, 69  
 Partial dislocations, 460  
 Partial net atomic charges, 385  
 Partial sum of Fourier series, 44  
 Partially bicentric arrangement, 208  
 Partially crystalline fibres, 471  
 Partially reflected wavefield, 547  
 Partially transmitted wave, 547  
 Patterson function(s), 61, 70, 235, 271, 444, 475  
   anomalous-dispersion, 248  
   constraints on interpretation of, 248  
   cylindrically averaged, 475  
   deconvolution of, 240  
   difference, 244–245  
   generalized, 409  
   interactions in, 235  
   isomorphous difference, 244  
   origin removal, 236  
   overlap between two, 250  
   second kind, 238  
   sharpened, 236  
   superposition, 241  
   symmetry of, 235  
   three-dimensional, 476  
 Patterson map, automated search, 321  
 Patterson peaks, 235  
 Patterson search, 245  
 Patterson synthesis, 265, 268–269  
 Patterson techniques, 6, 275  
 Patterson vector interactions, 239  
 Peaklist optimization, modified, 231  
*Pendellösung*, 281, 539, 543–544, 562–563  
   spherical-wave, 549  
*Pendellösung* distance, 540  
 Penetration depth, 546  
 Penrose rhomb, 505  
 Penrose tiling, 504  
 Period decimation, 47  
 Period lattice, 41, 59, 64  
   non-standard, 42  
 Period matrix, 42  
 Period subdivision, 46  
 Periodic boundary conditions, 400  
 Periodic continuation, 447  
 Periodic delta functions, 206  
 Periodic density function, 99  
 Periodic distributions, 41, 43, 59  
   and Fourier series, 40  
   Fourier transforms of, 41  
 Periodic lamellar domains, 413  
 Periodic weak phase objects, 313  
 Periodicity, 163  
   crystal, 59  
 Periodicity requirement, 8  
 Periodization, 26, 42, 51  
   and sampling, duality between, 22  
 Permissible origins, 210  
 Permissible symmetry, 99  
 Permutation of coordinates  
   cyclic (even), 102–103, 107  
   non-cyclic (odd), 102–103, 107  
 Permutation operators, 103  
 Permutation tensors, 349  
 Perpendicular (internal, complementary)  
   space, 487  
 Perspective, 368–370  
 Perturbation theory, first-order, 353  
 Phase angles, 264–265  
 Phase change, 268  
 Phase circles, 265  
 Phase determination, 265  
   *ab initio*, 261  
   direct, in electron crystallography, 320  
   statistical theory of, 96  
 Phase-determining formulae, 217  
 Phase evaluation, 264, 272, 275  
 Phase extension, 261  
 Phase-grating approximation, 556  
 Phase improvement, 261  
   using noncrystallographic symmetry, 261  
 Phase information, 274  
   from electron micrographs, 322  
 Phase invariant sums, 322  
 Phase-object approximation, 280, 445  
 Phase problem, 474  
   Bayesian statistical approach, 98  
 Phase relationships  
   quartet, 220  
   quintet, 222  
 Phase restriction, 68  
 Phase shift, 26, 51  
 Phase transformations, polytypic, 425  
 Phases  
   assignment of one or more, 227  
   best, 272  
   from multiple isomorphous replacement, 250  
   least-squares determination of, 229  
   linearly semidependent, 212  
   refinement of, 229  
 Phason flips, 507  
 Phenomenological absorption coefficients, 281  
 PHIGS (Programmers' Hierarchical Interactive Graphics System), 361  
 Phonon absorption, 404  
 Phonon dispersion relations, 405  
 Phonon emission, 404  
 Phonon scattering, 446  
 Phonons, 400  
 Physical (external, parallel) space, 487  
 Picture space, 368, 370, 376  
 Pipelining, 58  
 Pisot numbers, 491  
 Pixel, 374  
 Plancherel's theorem, 40  
 Plane of polarization, 268  
 Plane-wave dynamical theory, 538  
 Planes, 349  
   Gaussian, general, 356  
   least-squares, 353  
   least-squares, proper, 355  
 Plasmon scattering, 444  
 Plasmons  
   bulk, excitation of, 278  
   surface, 278  
*PLUTO*, 381  
 Point density, 505  
 Point groups, 163  
   average multiples for, 193  
   closed, 248  
   holohedral, 166  
 Point-group determination, 292  
 Point-group operators, 100, 108  
 Point-group symmetry of reciprocal lattice, 99  
 Point-group tables, 290  
 Poisson kernel, 45  
 Poisson summation formula, 42  
 Polar space, 253  
 Polarization, plane of, 268  
 Polarization vector, 11, 558  
 Polarizing monochromators, 560  
 Polycrystal electron-diffraction patterns, 308  
 Polycrystalline fibres, 467, 469, 474  
 Polycrystalline materials, diffuse scattering  
   from, 441  
 Polymer crystallography, 466  
 Polymer electron crystallography, 466  
 Polynomial growth  
   functions of, 40  
   locally summable function of, 39  
 Polynomial transforms, 57  
 Polynomials  
   Chinese remainder theorem for, 54, 77  
   cyclotomic, 54  
 Polyoma virus, 262  
 Polypeptide fold, chemical correctness of, 261  
 Polytype, 295  
 Polytypic phase transformations, 425  
 Population parameter, 14  
 Position of a known molecular structure, 259  
 Positional order, long-range, 449  
 Positive peaks, 243  
 Positivity criterion, 275  
 Potassium permanganate, 268  
 Potential energy of a crystal, 401  
 Potential-energy minima, 379  
 Poynting vector, 551  
 Pretransitional lengthening of correlation  
   lengths, 453  
 Prime factor algorithm, 50–51  
   multidimensional, 56  
 Primitive basis, 163  
 Primitive coefficients, 167  
 Primitive lattice, 66  
 Primitive root mod  $p$ , 53  
 Principal axes, 113  
 Principal-axis convergent-beam electron-diffraction pattern symmetries, 296  
 Principal central projections and sections, 62  
 Principal projections, 71  
 Principal sections and projections, 63  
 Probability  
   *a posteriori*, 423  
   *a priori*, 415  
 Probability densities, convolution of, 94  
 Probability density distributions, 192  
   ideal, 195  
 Probability density functions, 199  
   non-ideal, 208  
   of  $|E|$ , non-ideal, 200  
 Probability density of samples for images, 315  
 Probability theory, 94  
   analytical methods of, 94  
 Probability trees, 424  
 Processing X-ray fibre diffraction data, 472  
 Product function, 241  
 Programmers' Hierarchical Interactive Graphics System (PHIGS), 361  
 Projected charge-density approximation, 283  
 Projected glide line, 289  
 Projection approximation, 286, 553  
 Projection operator, 554  
 Projection(s), 26  
   and sections, principal central, 62  
   bounded, 63, 85  
   centrosymmetric, 242  
   oblique, 317  
   of symmetric objects, 317

## SUBJECT INDEX

- Projection(s)
  - orthoaxial, 316
  - orthographic, 369–370
  - tilt, 321
- Projector, 65
- Prolate spheroidal wavefunctions, 38
- Propagation direction, 537
- Propagation equation, 534
- Proper least-squares plane, 355
- Proper noncrystallographic symmetry, 248
- Proper rotation, 108, 113
- Protein crystallography, 268
- Protein crystals, 269
- Proteins
  - ab initio* direct phasing of, 231
  - electron crystallography of, 321
- PRXBLD*, 384
- Pseudo-distances, 28
- Pseudorotation, 379
- Pseudotranslational symmetry, 220
- Punched-card machines, 71
- Pure imaginary transforms, 80
  
- Quartet phase relationships, 220
- Quasilattice, 491
- Quasi-long-range order (QLRO), 450
- Quasimoments, 22
- Quasi-normalized structure factors, 216
- Quasiperiodic order, 498
- Quintet phase relationships, 222
  
- R* factor
  - fibre diffraction, 480
  - kinematical, 483
- Rader algorithm, 50
- Rader/Winograd algorithms, generalized, 83
- Rader/Winograd factorization, crystallographic extension of, 76
- Radial dependence of atomic electron distribution, 12
- Radial functions, 14
- Radiation damage, 278
- Radius of integration, 251
- Radon measure, 30
- Radon operator, 318
- Random copolymers, 470
- Random-start method, 229
- Random-walk problem, 96
  - exact solution, 203
- Rank of tensor, 5
- Rapidly decreasing functions, 37–38
- Raster-graphics devices, 374–375
- Rational approximant, 491
- Real antisymmetric transforms, 82
- Real crystal, 163
- Real-space averaging, 261–262
  - of electron density, 250, 261
- Real-space interpretation of extinction conditions, 291
- Real-space molecular replacement, 261
- Real-space translation functions, 260
- Real spherical harmonic functions, 14
- Real symmetric transforms, 81
- Real-valued transforms, 79
- Real waves, 548
- Reciprocal axes, 348
- Reciprocal Bravais lattice, 105
- Reciprocal cell, multiple, 106
- Reciprocal lattice, 2, 5, 42, 46, 59, 106, 164
  - point-group symmetry of, 99
  - weighted, 99–100
  - weighted, statistical properties of, 190
- Reciprocal-lattice sum, 388
- Reciprocal-lattice vectors, 386
- Reciprocal metric, 4
- Reciprocal space, 2, 386
  - symmetry in, 104
- Reciprocal-space group, 162, 165, 176
- Reciprocal-space procedures, 242
- Reciprocal-space representation of space groups, 99
- Reciprocal unit-cell parameters, 4
- Reciprocity, 36
  - property, 35
  - relationship, 282
  - theorem, 37, 40, 42, 59, 98
- Reconstruction
  - algebraic method, 318
  - back-projection method, 318
  - by Fourier transformation, 318
  - direct, methods of, 317
  - iteration method, 318
  - three-dimensional, 315
  - three-dimensional, general case, 319
- REDUCE, 106
- Reduced orbit, 69
- Reducibility of the representation, 67
- Reducible matrix group, 163
- Reference bases, choice of, 7
- Refinement
  - least-squares, 270
  - molecular-dynamics, 479
  - of phases, 229
  - restrained least-squares, 479
- Reflected intensity, 547
- Reflecting power, 543–544
- Reflection case, 539
- Reflection conditions, 68
- Reflection domain, middle of, 539
- Reflection geometry, 538, 540
- Reflection high-energy electron diffraction (RHEED), 306
- Reflections
  - main, 488
  - satellite, 488
  - substructure, 216
  - superstructure, 216
- Refraction, neutron, 557
- Refractive index, 278
- Regularization, 34
  - by convolution, 41
- Reindexing
  - additive, 57
  - multiplicative, 57
- Relationship between structure factors of symmetry-related reflections, 100
- Relationships between direct and reciprocal bases, 3
- Relatively prime integers, 350
- Relativistic effects, 279
- Representation, irreducible, 163
- Representation domain, 166
- Representation method, 218
- Representation of space groups in reciprocal space, 99
- Representation of surfaces
  - by dots, 375
  - by lines, 375
  - by shading, 375
- Representation operators, 67, 73
- Representation property, 64
- Representative operators of a space group, 108
- Repulsion energy, 385
- Residual lattice, 46
  
- Resolution
  - image, 284
  - instrumental, 285
- Restacking, 461
- Restrained least-squares refinement, 479
- RHEED (reflection high-energy electron diffraction), 306
- Rhombohedral lattice, 83
- Riemann integral, 27
- Riemann–Lebesgue lemma, 35
- Right action, 64–65
- Right cosets, 64
- Right representation, 64
- Rigid-body motion, 19
- Rigid-body superposition, 364
- Rigid rotation, 8
- Ring systems
  - condensed, 379
  - fused, 384
- Rings*, 384
- Robertson's sorting board, 71
- Rocking curve, 541, 545, 562
  - width at half-height, 544
  - width of, 540
- Rocking microbeam diffraction (RMBD), 306
- Root-mean-square error, 273
- Rotation, 368, 371
  - improper, 108, 113
  - molecular, 460
  - optical, 268
  - proper, 108, 113
  - rigid, 8
  - screw, 19
  - X*-fold, 288
- Rotation axes, improper, 248
- Rotation functions, 250
  - fast, 255
  - locked, 255
- Rotation-function Eulerian space groups, 256
- Rotation matrix, 255, 361
  - trace of, 253
- Rotation operator, 6
  - inverse, 99
- Rotation part of space-group operation, 100
- Rotation vector, 363
- Rotational filtering, 314
- Rotational structure (form) factor, 437
- Rotational symmetry, noncrystallographic, 250
- Roto-inversionary axes, 288
- Row–column method, 55
  
- Saddlepoint
  - approximation, 94–95
  - equation, 97
  - expansion, 96
  - method, 36, 97
- SAED (selected-area electron diffraction), 285, 482
- Sampling, 26, 42
  - and periodization, duality between, 42
  - considerations, 92
  - theorems, 61
- Satellite reflections, 414, 488
- Satellite tobacco necrosis virus, 250
- Sayre's equation, 84, 225
- Sayre's squaring method, 87
- Scalar products, 5, 348
  - mixed, matrices of, 8
- Scale, 368
- Scale factors, 269
- Scaling of heavy-atom-derivative data sets, 246
- Scaling symmetry, 498

## SUBJECT INDEX

- Scanning microbeam diffraction (SMBD), 306
- Scanning transmission electron microscope (STEM), 282
- Scattering
- classical Thomson, 10
  - coherent, 404
  - Compton, 405
  - critical, 453
  - diffuse, 443
  - forward, 552
  - from mesomorphic structures, 449
  - incoherent, 404
  - incoherent inelastic, 404
  - inelastic, 278, 443
  - inelastic neutron, 404
  - kinematical, 279
  - Laue, 432
  - low-angle, 419
  - magnetic, 11, 559
  - multiple, 443
  - of neutrons by thermal vibrations, 404
  - of X-rays by thermal vibrations, 402
  - phonon, 446
  - plasmon, 444
  - thermal diffuse, 278
  - X-ray, 58
  - X-ray, elastic component of, 10
  - X-ray, inelastic component of, 10
- Scattering cross sections, 557
- Scattering diagrams, 556
- Scattering factors
- atomic, 10, 265
  - complex, 246
  - dynamical, 446
  - spherical atomic, 10
- Scattering lengths, 557
- atomic, 11
  - neutron, 275
  - non-spin-flip, 559
  - spin-flip, 559
- Scattering matrix method, 312
- Scattering operator, 15
- Scattering power, 267
- Scherzer defocus, 283
- conditions, 311
- Scherzer phase function, 311
- Schrödinger equation, 278
- Schur's lemma, 67, 73
- Scrambling, 51
- Screen coordinates, 368, 370
- Screw correlations, 21
- Screw rotation, 19
- Screw shifts, 429
- Script*, 384
- Search directions, 87
- Second Bethe approximation, 280
- Second-order Born approximation, 11
- SECS*, 384
- Section, 26
- Sections and projections, 26, 62
- duality between, 40
  - principal, 63
- Selected-area electron diffraction (SAED), 285, 482
- Selection rules, 93
- Self-energy terms, 385
- Self-Patterson, 92
- vectors, 251
- Self-rotation function, 92
- Self-seeding, 482
- Self-vectors, 242
- Semi-direct product, 65
- Semi-norm on a vector space, 28
- Semi-reciprocal space, 553
- Series-termination errors, 60, 84, 92
- Seven-beam approximation, 556
- Shadows, 376
- Shake and Bake*, 231
- Shannon interpolation, 26, 48
- Shannon interpolation formula, 46, 85
- Shannon interpolation theorem, 61
- Shannon sampling criterion, 46, 63, 85
- Shannon sampling theorem, 45, 61, 262
- Sharpened Patterson functions, 236
- Shift of space-group origin, 104
- Shift property, 49, 61
- Short cyclic convolutions, 54
- Short-range order (SRO), 415, 450
- correlation functions, 429
  - in multi-component systems, 432
  - parameters, 444, 447
  - Warren parameters, 431
- Sign conventions for electron diffraction, 279–280
- Simulated annealing, 474
- Sine strips, 71
- Single-crystal electron-diffraction patterns, 306
- Single isomorphous replacement (SIR), 244, 265
- difference electron density, 244
  - phasing, 244
- Single isomorphous replacement with anomalous scattering (SIRAS), 233
- SIR (single isomorphous replacement), 244
- difference electron density, 244
  - phasing, 244
- SIRAS (single isomorphous replacement with anomalous scattering), 233
- Site-symmetry group, 167
- Site-symmetry restrictions, 14
- Size distribution, 415
- Size effect, 432
- Skew-circulant matrix, 53
- Sliding filter, 378
- Small-angle scattering approximation, 278
- Small values of  $\mu_{\sigma f}$ , 548
- SMBD (scanning microbeam diffraction), 306
- Smectic films, 456
- Smectic-A phase, 449, 452–453
- modulated, 455
- Smectic-B phase, 449
- Smectic-C phase, 453
- modulated, 455
- Smectic-D phase, 464
- Smectic-F phase, 458
- Smectic-I phase, 458
- Sobolev space, 40
- Software, Hall symbols in, 107
- Solids
- electron band theory, 537
  - theory of, 9
- Solution of dynamical theory, 540
- Solvable space groups, 66
- Solvent flattening, 84
- Solvent regions, 62
- Sound velocities, 406
- Southern bean mosaic virus, 250, 262
- Space groups, 66, 163, 264
- cubic, 102
  - Eulerian, 254
  - finite, 164
  - hexagonal, 103
  - holosymmetric, 166
  - in reciprocal space, 150
- Space groups
- monoclinic, 103
  - orthorhombic, 102
  - reciprocal-space representation of, 99
  - representative operators of, 108
  - rotation-function, 254
  - solvable, 66
  - symmorphic, 66, 163
  - tetragonal, 103
  - triclinic, 102
  - trigonal, 103
- Space-group algorithm, 104
- Space-group analyses of single crystals, 291
- Space-group determination by convergent-beam electron diffraction, 285
- Space-group notation, explicit-origin, 112
- Space-group operation, 100
- intrinsic and location-dependent components of translation part, 100
  - rotation part, 100
  - translation part, 100
- Space-group origin, shift of, 104
- Space-group-specific Fourier summations, 101
- Space-group-specific structure-factor formulae, 101
- Space-group-specific symmetry factors, 99
- Space-group symbols
- computer-adapted, 102, 106, 112
  - explicit, 107–109
  - Hall, 107, 112, 115
  - Hermann–Mauguin, 103
- Space-group symmetry, 475
- Space-group tables, 104
- Space-group types, 66
- affine, 163
  - crystallographic, 163
- Special Harker planes, 240
- Special  $\mathbf{k}$  vector, 165
- Special position, 67
- condition, 67
- Special reflection, 68
- Spectrometer, triple-axis, 405
- Specular reflection, 456
- Spherical angles, 252
- Spherical atomic scattering factor, 10
- Spherical atoms, 101
- Spherical Dirichlet kernel, 60, 84
- Spherical Fejér kernel, 60
- Spherical harmonic expansion, atom-centred, 14
- Spherical harmonic functions, real, 14
- Spherical harmonics, 258
- Spherical interference function, 251
- Spherical polar coordinates, 252
- Spherical viruses, 317
- Spherical-wave *Pendellösung*, 549
- Spin-flip scattering lengths, 559
- Spin orbitals, occupied natural, 18
- Spiro links, 384
- Spot boundaries, 474
- Squarability criterion, 275
- Square-integrable functions, 40
- Square-summable sequences, 45
- Squaring method equation, 84
- SRO (short-range order), 415, 450
- correlation functions, 429
  - in multi-component systems, 432
  - parameters, 444, 447
  - Warren parameters, 431
- Stacked transformations, 373
- Standard basis of  $\mathbb{R}^n$ , 40
- Standard coordinates, 41, 59, 67
- Standard Gaussian function, 37, 39

## SUBJECT INDEX

- Standard lattice, 40  
 Standard  $n$ -torus, 40  
 Standard uncertainty of distance from an atom to a plane, 355  
 Standing waves, 541  
   anti-nodes of, 541  
   nodes of, 541  
 Star  
   arms of, 165  
   of  $\mathbf{k}$ , 165  
 Starting models, 476  
 Statistical properties of the weighted reciprocal lattice, 190  
 Statistical theory of communication, 96  
 Statistical theory of phase determination, 96  
 Statistics  
   crystallographic, 199  
   structure-factor, 102  
 Status of centrosymmetry, 108  
 Steepest descents, Booth's method, 89  
 STEM (scanning transmission electron microscope), 282  
 Stereochemical information, 474  
 Stereoviews, 370  
 Stirling's formula, 97  
 Structural connectivity, 377  
 Structure amplitude, 10  
 Structure determination by X-ray fibre diffraction analysis, 474  
 Structure factors, 6, 8, 10, 59, 264  
   calculation of, 68  
   for one-phonon scattering, 403  
   Fourier-Bessel, 468  
   from model atomic parameters, 86  
   geometric, 101, 120  
   in terms of form factors, 60  
   inequalities among, 217  
   joint probability distribution of, 97  
   normalized, 215, 227, 236  
   quasi-normalized, 216  
   tables of, 102, 120  
   trigonometric, 101, 120  
   trigonometric, even absolute moments of, 201  
   trigonometric, moment of, 200  
   unitary, 216  
   *via* model electron-density maps, 86  
 Structure-factor algebra, 70, 97–98  
 Structure-factor formalism, generalized, 23  
 Structure-factor formulae, space-group-specific, 101  
 Structure-factor statistics, 102  
 Structure invariants, 210  
 Structure seminvariants, 211  
   algebraic relationships, 224  
   one-phase, 224, 227  
   two-phase, 225  
 Structure theorem, 34  
   for distributions with compact support, 41, 45  
 Sturkey's solution, 553  
 Subcentric arrangement, 208  
 Subdivision and decimation of period lattices, duality between, 46  
 Sublattice, 46  
 Subspace sectioning, 379, 383  
 Substitutional disorder, 447, 471  
 Substitutional order, 446  
 Substructure reflections, 216  
 Sum function, 241  
 Sum of images, 240  
 Summable functions, 27  
 Summation convention, 5  
 Summation problem in crystallography, 45  
 Superposition methods, 240  
 Superposition of Patterson functions, 241  
 Superstructure, 417  
 Superstructure reflections, 216  
 Support, 26  
   compact, 26, 36, 43  
   of a distribution, 31  
   of a tensor product, 33  
 Support condition, 34, 43  
   generalized, 34  
 Surface effects, 455  
 Surface phase, 459  
 Surface plasmons, 278  
 Surfaces  
   atomic, 486, 492  
   dispersion, 537, 555, 560  
   fractal atomic, 493  
   representation by dots, 375  
   representation by lines, 375  
   representation by shading, 375  
   van der Waals, 375, 381  
 Sybyl, 384  
 Symbolic programming techniques, 99  
 Symbolically oriented languages, 102  
 Symmetric Bragg condition, 287  
 Symmetric objects, projections of, 317  
 Symmetric rectangular density modulation, 497  
 Symmetry, 162, 253, 373  
   conjugate, 35, 39  
   conjugate and parity-related, 79  
   crystal, 64  
   crystallographic, 248  
   cyclic, 77  
   dihedral, 77  
   effects on Fourier image, 99  
   helical, 93, 317, 467, 475  
   helical, approximate, 469  
   Hermitian, 60, 69, 79  
   in Fourier space, 105  
   in reciprocal space, 104  
   noncrystallographic, 62, 248–249  
   noncrystallographic, molecular averaging by, 85  
   noncrystallographic, proper, 248  
   noncrystallographic, rotational, 250  
   of Patterson function, 235  
   permissible, 99  
   pseudotranslational, 220  
   scaling, 498  
 Symmetry elements  
   extinction rules for, 291  
   individual, observation in CBED patterns, 288  
 Symmetry factors, 101  
   space-group-specific, 99  
   tables of, 99  
 Symmetry-generating algorithm, 107  
 Symmetry group, 162  
 Symmetry operation, 162  
 Symmetry property, 38  
 Symmetry-related reflections, relationship between structure factors of, 100  
 Symmorphic space groups, 66, 163  
 Synchrotron radiation, 264, 274  
 Systematic absences, 68, 105  
 Systematic errors, 351  
 Szegő's theorem, 43, 63, 98  
 Tangent formula, 218, 274  
   application of, 227  
   modified, 229  
   weighted, 220  
 TDS (thermal diffuse scattering), 278, 400, 407, 443  
 TEM (transmission electron microscope), 282  
 Temperature factors, 68, 269  
   anisotropic, 69  
   artificial, 87, 92  
   atomic, 18  
   isotropic, 68  
 Tempered distributions, 36, 38, 40, 45, 68  
   definition and examples of, 39  
   Fourier transforms of, 38–39  
 Tensor formulation of vector product, 6  
 Tensor-algebraic formulation, 2, 5  
 Tensor product, 27, 33, 50  
   of distributions, 33  
   of matrices, 49, 55–56  
   structure of, 72  
   support of, 33  
 Tensor product property, 35, 63, 93  
   of a Fourier transform, 71  
 Tensors, 5  
   anisotropic displacement, 6  
   antisymmetric, 6  
   libration, 19  
   metric, 4–5  
   permutation, 349  
   rank of, 5  
   translation, 19  
   translation, libration and screw-motion, 6  
 Test-function spaces, 29  
 Test functions, 38  
 Tetragonal family, 103  
 Tetragonal groups, 83  
 Tetragonal space groups, 103  
 Text processing, 106  
 Texture electron-diffraction patterns, 307, 326  
 THEED (transmission high-energy electron diffraction), 306  
 Theory of distributions, 25, 28  
 Theory of solids, 9  
 Thermal diffuse scattering (TDS), 278, 400, 407, 443  
 Thermal fluctuations, 452  
 Thermal neutrons, 275  
 Thermal streaks, 447  
 Thermotropic phase, 451  
 Thick crystals, 312, 545  
 Thin crystals, 546  
   comparison of geometrical and dynamical theory, 545  
 Thin films, 457  
   crystal defects in, 445  
 Thomson scattering, classical, 10  
 Three-beam approximation, 556  
 Three-beam inversion, 556  
 Three-dimensional electron-diffraction data, 324  
   from a single crystal orientation, 484  
   from two crystal orientations, 484  
 Three-dimensional Hermite polynomials, 22  
 Three-dimensional isotropic harmonic oscillator, 18  
 Three-dimensional Patterson function, 476  
 Three-dimensional reconstruction, 315  
   general case, 319  
 Three-dimensional structure determination by electron crystallography, 323

## SUBJECT INDEX

- Three-generator symbol, 108  
 Through-focus series method, 312  
 Tie point, 536  
 Tilt projections, 321  
 Tilted hexatic phase, 458  
 Toeplitz determinants, 43, 63  
 Toeplitz forms, 43, 63  
   asymptotic distribution of eigenvalues of, 43, 63  
 Toeplitz matrices, 44  
 Toeplitz–Carathéodory–Herglotz theorem, 43  
 Topography, neutron, 564  
 Topological dual, 30–31, 38–39  
 Topological vector spaces, 28  
 Topology, 28, 38  
   general, 28  
   in function spaces, 28  
   metrizable, 28  
   not metrizable, 30  
   on  $\mathcal{G}(\Omega)$ , 30  
   on  $\mathcal{G}_k(\Omega)$ , 30  
   on  $\mathcal{E}(\Omega)$ , 29  
 Torsion angles, 350  
 Total cross section, 11  
 Total-reflection domain, 546  
   width of, 541, 546  
 Trace of rotation matrix, 253  
 Transfer function, 49  
   of lens, 282  
 Transformation properties of direct and reciprocal base vectors and lattice-point coordinates, 100  
 Transformations  
   affine, 105  
   compound, 371  
   direct-space, 104  
   linear, 7  
   non-linear, 254  
   of coordinates, 5, 7, 33  
   stacked, 373  
   to a Cartesian system, 3  
   viewing, 368–369, 371–372, 374  
   viewport, 368, 370  
   windowing, 368  
 Transformed variance–covariance matrix, 351  
 Transforms  
   complex antisymmetric, 80  
   complex symmetric, 80  
   Hermitian-antisymmetric, 80  
   of an axially periodic fibre, 93  
   of delta functions, 39  
   optical, 418  
   polynomial, 57  
   pure imaginary, 80  
   real antisymmetric, 82  
   real symmetric, 81  
   real-valued, 79  
 Translate, 26  
 Translation, 19, 26, 368, 371  
   part of space-group operation, 100  
   part of space-group operation, intrinsic and location-dependent components of, 100  
 Translation, libration and screw-motion tensors, 6  
 Translation functions, 92, 258  
   general, 258  
   real-space, 260  
 Translation lattice, 163  
 Translation tensor, 19  
 Translation vector, 249  
 Translational components of noncrystallographic rotation elements, 248  
 Translational displacement, 19  
 Translational invariance, 554  
 Translations, conversion to phase shifts, 35  
 Transmission case, 538  
 Transmission electron microscope (TEM), 282  
 Transmission geometry, 538–540  
   intensities of plane waves in, 541  
 Transmission high-energy electron diffraction (THEED), 306  
 Transposition formula, 75  
   for intermediate results, 72  
 Triads, mutually reciprocal, 2  
 Triangular inequality, 28  
 Triclinic groups, 82  
 Triclinic space groups, 102  
 Trigonal groups, 83  
 Trigonal space groups, 103  
 Trigonometric moment problem, 43  
 Trigonometric structure factors, 101, 120  
   even absolute moments of, 201  
   moment of, 200  
 Trigonometric structure-factor expressions, vectors of, 96  
 Triple-axis spectrometer, 405  
 Triple point, 455  
 Triplet relationships using structural information, 219  
 Triplets, search of, 227  
 Triply periodic, 535  
 Tunability, 275  
 Twiddle factors, 51, 55–56, 58, 75  
 Twins, 292  
 Two-beam approximation, 280, 553  
 Two-beam case, 536  
 Two-beam dynamical approximation, 326  
 Two-beam dynamical diffraction formulae, 281  
 Two-centre orbital products, 18  
 Two-centre terms, 18  
 Two-dimensional disorder, 425  
 Two-dimensional hexatic phase, 457  
 Two-phase structure seminvariants, first rank, 225  
 Two-wavelength method, 275  
 Type of rotation (proper or improper), 108  
  
 Uni-arm  $\mathbf{k}$  vector, 167  
 Uniaxial nematic order, 452  
 Uniformity, assumption of, 199, 205  
 Uniformizable space, 28  
 Unit cell, 165–166  
 Unit-cell parameters  
   direct, 4  
   reciprocal, 4  
 Unit cube, 41  
 Unitary matrix group, 163  
 Unitary structure factors, 216  
 Unitary transformations, 36  
 Unscrambling, 75  
 Uranium, 269  
  
 Valence density, 13  
 van der Waals surfaces, 375, 381  
 Van Hove correlation functions, 405  
 Variance, 350  
 Variance–covariance matrix, 350  
   transformed, 351  
 Variances, 354  
 Vector interactions in a Patterson map, 239  
 Vector lattice, 163  
  
 Vector machines, 375  
 Vector map, 235  
 Vector overlap, 242  
 Vector processing, 58  
 Vector product, 349  
   components of, 349  
   tensor formulation of, 6  
 Vector radix Cooley–Tukey algorithm, 55  
 Vector radix FFT algorithms, 56  
 Vector relationships, 349  
 Vector-search procedures, 241  
 Vector space  
   complete, 27  
   norm on, 28  
   semi-norm on, 28  
   topological, 28  
 Vectors  
   angle between two, 348  
   components of, 5  
   cross-Patterson, 251  
   four-dimensional, 366  
   interatomic, 61  
   length of, 348  
   of trigonometric structure-factor expressions, 96  
   origin-shift, 107  
   polarization, 11, 558  
   Poynting, 551  
   rotation, 363  
   self-Patterson, 251  
   translation, 249  
 Vertical mirror plane, 289  
 Very-small-angle neutron scattering, 563  
 Vibrating crystals, 562  
 Vibrational–librational correlations, 437  
 Viewing transformation, 368–369, 371–372, 374  
 Viewport, 368, 370  
 Viewport transformation, 368, 370  
 Viruses, spherical, 317  
 Vitamin B<sub>12</sub>, 268  
  
 Waller–Hartree formula, 444, 446  
 Warren short-range-order parameters, 431  
 Wavefield, 535, 537  
 Wavefunctions, prolate spheroidal, 38  
 Wavelengths, 277  
 Wavevectors, 542  
 Weak enantiomorphic images, 238  
 Weak phase objects, 311, 481  
   periodic, 313  
 Weak-phase-object approximation, 283  
 Weighted difference map, 90–91  
 Weighted lattice distribution, 42  
 Weighted reciprocal lattice, 99–100  
   statistical properties of, 190  
 Weighted reciprocal-lattice distribution, 59  
 Weighted tangent formula, 220  
 Weighting factor, 271  
 Weights  
   anisotropic, 355  
   Gaussian, 355  
 Width of rocking curve, 540  
   at half-height, 544  
 Width of total-reflection domain, 541, 546  
 Wigner–Seitz cell, 165  
 Wilson plot, 269  
 Window, 368, 371, 376  
 Windowing, 368, 370  
 Windowing transformation, 368  
 Winograd algorithms, 50, 54

## SUBJECT INDEX

- Winograd small FFT(s)
  - algorithms, 54
  - nesting of, 56
- Wintgen letter, 167
- Wintgen position, 167
- Wintgen symbol, 167
- World coordinates, 368
- Wyckoff letter, 167
- Wyckoff position, 100, 167
- Wyckoff symbols, 67
- X-ray analysis, 269
- X-ray fibre diffraction analysis, 466
  - data processing, 472
  - structure determination by, 474
- X-ray scattering, 275
  - cross section, 452
- X-ray topographs, 534
- X-rays, 275
  - diffuse scattering of, 407
  - interaction with matter, 534
- z buffer, 376
- Zero-absorption case, 540
- Zonal data sets
  - view down the chain axis, 483
  - view onto the chain axes, 483
- Zone-axis patterns, 286, 291
- Zones and rows, average intensity of, 191