

## 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, J. P., 2.3  
Abrahams, S. C., 2.3, 2.4  
Abramowitz, M., 2.1  
Achard, M. F., 4.4  
Acharya, R., 2.3  
Adams, B. W., 5.1  
Adams, M. J., 2.3, 2.4  
Adams, P. D., 2.3, 2.5  
Adamson, R. D., 3.5  
Addison, A. W., 2.3  
Adiga, P. S., 2.5  
Adlhart, W., 4.2  
Aeppli, G., 4.2, 4.4  
Afanas'ev, A. M., 5.3  
Agard, D. A., 2.3, 2.4  
Agarwal, R. C., 1.3, 2.4  
Agrawal, R. K., 2.5  
Aguado, A., 3.5  
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  
Akishige, Y., 2.5  
Al Haddad, M., 5.3  
Alben, R., 4.4  
Albertini, G., 5.3  
Alden, R. A., 1.3  
Alexander, L. E., 4.2  
Alexeev, D. G., 4.5  
Alford, J. A., 3.5  
Al-Khayat, H. A., 4.5  
Allegra, G., 2.2  
Allen, F. H., 3.3  
Allen, L. J., 4.3  
Allen, M. P., 3.5  
Allinger, N. L., 3.3  
Almer, J., 4.2  
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  
Alzari, P. M., 5.1  
Amador, S., 4.4  
Amelinckx, S., 4.3  
Amma, E. L., 3.3  
Ammon, H. L., 3.5  
Amorós, J. L., 4.2  
Amorós, M., 4.2  
Amos, L. A., 2.5  
An, M., 1.3  
Anderson, D. C., 3.3  
Anderson, D. L., 2.3  
Anderson, P. W., 4.4  
Anderson, S., 3.3  
Andersson, B., 4.3  
Andersson, G., 4.4  
Ando, M., 5.3  
Andreeva, N. S., 2.4  
Andrews, J. W., 2.5  
Andries, K., 2.3  
Angert, I., 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, 3.5  
Argos, P., 2.2, 2.3  
Arif, M., 5.3  
Arley, N., 3.2  
Arnautova, Y. A., 3.5  
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., 1.4, 1.5, 4.2  
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  
Atwood, J. L., 3.3  
Au, A. Y., 2.5, 4.2  
Audier, M., 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  
Badasso, M. O., 2.3  
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  
Bajaj, C., 2.5  
Bak, H. J., 2.3  
Bak, P., 4.4  
Baker, D., 2.3  
Baker, E. N., 1.3, 2.3  
Baker, T. S., 2.3, 2.5  
Baldwin, J. M., 2.5  
Baldwin, P. R., 2.5  
Balibar, F., 5.1  
Ban, N., 2.5  
Banaszak, L. J., 2.3  
Bancel, P. A., 4.6  
Banerjee, K., 2.2  
Bannister, C., 2.5  
Bansal, M., 1.3  
Bantz, D., 1.3  
Bar, J., 2.5  
Barakat, R., 1.3, 2.1  
Barbour, L. J., 3.3  
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  
Baryshevskii, V. G., 5.3  
Barzaghi, M., 3.5  
Basett-Jones, D. P., 2.5  
Bash, P. A., 3.3  
Baskaran, S., 4.5  
Basokur, A. T., 2.5  
Batterman, B. W., 5.1  
Baturic-Rubicic, J., 4.4  
Bauer, G., 4.2  
Bauer, J., 3.5  
Bauer, P., 3.5  
Baumeister, W., 2.5  
Bauspiess, W., 5.3  
Baxter, W., 2.5  
Bazterra, V. E., 3.5  
Beaglehole, D., 4.4  
Bean, A. J., 2.5  
Beck, T. L., 3.5  
Becker, P. J., 1.2, 5.3  
Beckmann, E., 2.5  
Beddell, C., 3.3  
Bedzyk, M. J., 5.1  
Beer, T. de, 2.5  
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  
Bellen, H., 2.5  
Bellissent, R., 4.2  
Bellman, R., 1.3  
Belloq, A. M., 4.4  
Bellon, P. L., 2.5  
Belova, N. E., 5.3  
Belyakov, V. A., 5.3  
Benattar, J. J., 4.4  
Bender, R., 2.5  
Bendersky, L. A., 2.5  
Bengtsson, U., 2.3  
Benguigui, L., 4.4  
Bennett, D. W., 3.3  
Bennett, J. M., 1.3  
Bensimon, D., 4.4  
Bentley, J., 1.2  
Berberian, S. K., 1.3  
Berendzen, J., 2.3  
Berger, J. E., 2.5  
Bergman, G., 3.2  
Bergmann, K., 4.4  
Berkowitz, M. L., 3.5  
Berliner, R., 5.3  
Berman, H. M., 1.4  
Bern, M., 2.5  
Bernstein, F. C., 3.3  
Bernstein, H. J., 5.3  
Bernstein, J., 3.5  
Bernstein, S., 2.1  
Berry, M. V., 5.2  
Bertaut, E. F., 1.3, 1.4, 2.2, 3.4  
Berthold, T., 4.2  
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  
Bhuiya, A. K., 2.2  
Bieberbach, L., 1.3  
Biernacki, J., 2.5  
Bienenstock, A., 1.3, 1.4  
Bijvoet, J. M., 2.2, 2.3, 2.4  
Bilderback, D. H., 5.1  
Billard, J., 4.4  
Billard, L., 4.6  
Billinge, S. J. L., 4.2  
Bilz, H., 4.1  
Bing, D. H., 3.3  
Bird, D., 2.5  
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  
Blake, A. J., 3.3  
Blanc, E., 2.3  
Blaser, H., 2.3  
Blech, I., 2.5, 4.6  
Bleistein, N., 1.3  
Blessing, R. H., 2.2  
Bley, F., 4.2  
Blin, 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  
Boer, J. L. de, 4.2  
Boerrigter, S. X. M., 3.5  
Boettger, J. C., 3.5  
Boeuf, A., 5.3  
Böhm, H., 4.6  
Bohm, J., 2.5  
Böhme, R., 2.2  
Böhringer, M., 5.1  
Boisset, N., 2.5  
Boissieu, M. de, 4.2  
Bokhoven, C., 2.4  
Bokun, R. Ch., 5.3  
Bommel, A. J. van, 2.3, 2.4  
Bondot, P., 1.3  
Böni, P., 4.2  
Bonneau, P. R., 2.3  
Bonnet, M., 5.3  
Bono, P. R., 3.3  
Bonse, U., 5.1, 5.3  
Boon, M., 1.5  
Booth, A. D., 1.3  
Boots, B., 2.5  
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  
Botha, J. D., 3.3  
Böttcher, B., 2.5  
Böttcher, C. J. F., 3.5  
Boublik, M., 2.5  
Bouckaert, L. P., 1.5  
Boudard, M., 4.2  
Boulay, D. J. du, 1.4, 2.2  
Bouman, J., 2.2  
Bourne, P. E., 1.4  
Boutin, H., 4.1  
Bouwman, W. G., 4.4  
Bowen, D. K., 5.1  
Bown, M., 4.2  
Boyd, D. B., 3.3  
Boyer, L., 4.1  
Boyer, P. L., 2.3  
Boyle, L. L., 1.5  
Boysen, H., 4.2  
Bracewell, R. N., 1.3, 2.5  
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  
Braig, K., 2.5  
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

## AUTHOR INDEX

- Brisbin, D., 4.4  
 Brisse, F., 2.5, 4.5  
 Britten, P. L., 1.3, 2.2  
 Broach, R. W., 4.2  
 Brock, J. D., 4.4  
 Brockhouse, B. N., 4.1  
 Broderson, S., 3.5  
 Brooks, B. R., 3.3  
 Brooks, C. L. III, 2.5  
 Brooks, J. D., 4.4  
 Brown, C. J., 4.5  
 Brown, D., 3.5  
 Brown, F., 2.3  
 Brown, G. S., 4.4  
 Brown, H., 1.3  
 Brown, I. D., 1.4  
 Brown, M. D., 3.3  
 Brucoleri, 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  
 Brunger, A. T., 2.2, 2.3  
 Brünger, A. T., 1.3, 2.3, 4.5  
 Bruno, I. J., 3.3  
 Bryan, R. K., 1.3, 4.5  
 Bu, X., 4.2, 4.6  
 Bubeck, E., 4.2  
 Buch, K. R., 3.2  
 Budai, J., 4.4  
 Budinger, T. F., 2.5  
 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  
 Bunkóczy, G., 2.3  
 Bunn, C. W., 4.5  
 Bunshaft, A. J., 3.3  
 Burandt, B., 4.2, 4.6  
 Burch, S. F., 1.3  
 Burd, C. G., 2.5  
 Burdina, V. I., 2.3  
 Burgess, W. G., 2.5  
 Bürgi, H.-B., 3.3, 4.2  
 Burkel, E., 4.1  
 Burkert, U., 3.3  
 Burkov, S., 4.6  
 Burla, M. C., 2.2  
 Burnett, M. N., 3.3  
 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  
 Butcher, S. J., 2.5  
 Butler, B. D., 4.2  
 Buttle, K., 2.5  
 Buxton, B., 2.5, 5.2  
 Buyers, W. J. L., 4.1  
 Byerly, W. E., 1.3  
 Byler, M. A., 4.5  
 Bystroff, C., 2.3  
  
 Cael, J. J., 4.5  
 Caglioti, G., 4.2  
 Cahn, J. W., 2.5, 4.6  
 Caillé, A., 4.4  
 Calabrese, G., 2.2  
 Caliandro, R., 2.2  
 Calvayrac, Y., 4.2  
 Camalli, M., 2.2  
 Cambillau, C., 3.3  
 Campagnari, F., 4.5  
 Campbell, B. J., 4.2  
 Campbell, G. A., 1.3  
 Campbell Smith, P. J., 4.5  
 Cannillo, E., 2.4  
 Canright, G. S., 4.2  
 Cantino, M., 4.5  
 Capillas, C., 1.4, 1.5  
 Carathéodory, C., 1.3  
 Carazo, J. M., 2.5  
 Cardona, M., 4.1  
 Carlile, C. J., 4.4  
 Carlisle, C. H., 2.3  
 Carlson, J. M., 4.4  
 Carragher, B., 2.5  
 Carrascosa, J. L., 2.5  
 Carroll, C. E., 4.5  
 Carrozzi, B., 2.2  
 Carslaw, H. S., 1.3  
 Cartan, H., 1.3  
 Carter, R. E., 3.3  
 Cartwright, B. A., 3.3  
 Cascarano, G. L., 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  
 Challacombe, M., 3.5  
 Challifour, J. L., 1.3  
 Chalupa, B., 5.3  
 Champeney, D. C., 1.3  
 Champness, J. N., 1.3, 2.3, 3.3  
 Champness, N. R., 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, G., 2.3  
 Chang, S.-L., 5.1  
 Chanzy, H., 2.5, 4.5  
 Chao, Y., 2.5  
 Chao-de, Z., 2.2  
 Chaplot, S. L., 4.1  
 Chapman, D., 4.4  
 Chapman, M. S., 2.3  
 Chapon, L. C., 3.3  
 Chapuis, G., 4.6  
 Charvolin, J., 4.4  
 Chataka, T., 4.2  
 Cheetham, A. K., 4.2  
 Chemburkar, S. R., 3.5  
 Chen, H. S., 4.2  
 Chen, J., 2.5  
 Chen, J. H., 4.4  
 Chen, S., 2.5  
 Cheng, N., 2.5  
 Cheng, R. H., 2.5  
 Cheng, T. Z., 2.5  
 Cherns, D., 2.5  
 Chew, M., 4.5  
 Chiang, L. Y., 4.4  
 Chin, C., 2.5  
 Chisholm, J., 3.5  
 Chistyakov, R. R., 5.3  
 Chiu, S. N., 2.5  
 Chiu, W., 2.5  
 Chivers, R. A., 4.5  
 Choi, H.-K., 2.3  
 Choplin, F., 3.3  
 Chow, M., 2.3  
 Christensen, F., 4.4  
 Christian, P. E., 2.5  
 Chu, K. C., 4.4  
 Chukhovskii, F. N., 5.1, 5.3  
 Church, G. M., 1.3, 2.4  
 Churchill, R. V., 1.3  
 Cimmino, A., 5.3  
 Cisarova, I., 4.2, 4.6  
 Cisneros, G. A., 3.5  
 Civalleri, B., 3.5  
 Clapp, P. C., 4.3  
 Clark, A. D. Jr, 2.3  
 Clark, E. S., 4.5  
 Clark, J. J., 2.5  
 Clark, N. A., 4.4  
 Clark, P., 2.3  
 Clarke, P. J., 4.2  
 Clarke, R., 4.4  
 Clastre, J., 2.3  
 Clausen, K. N., 4.2  
 Clementi, E., 1.2  
 Clews, C. J. B., 1.3, 3.2  
 Clore, G. M., 2.3  
 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  
 Cockcroft, J. K., 3.3  
 Cockrell, P. R., 3.3  
 Cohen, D., 2.5  
 Cohen, J. B., 4.2  
 Cohen, N. C., 3.3  
 Cohen-Tannoudji, C., 1.2  
 Cole, H., 5.1  
 Cole, J. C., 3.3  
 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  
 Connell, S. R., 2.5  
 Connolly, M. L., 3.3  
 Conradi, E., 4.2  
 Convert, P., 4.2  
 Conway, J. F., 2.5  
 Cooley, J. W., 1.3  
 Cooper, M. J., 4.2  
 Coppens, P., 1.2, 3.5, 4.2, 4.6, 5.3  
 Cordes, A. W., 3.2  
 Cordingley, M. G., 2.3  
 Corey, R. B., 1.3, 2.3  
 Corfield, P. W. R., 2.3  
 Cork, J. M., 2.4  
 Coronas, J., 5.2  
 Coster, D., 2.4  
 Cotton, F. A., 3.3  
 Couch, G. S., 2.5  
 Coulson, C. A., 1.2  
 Coulter, C. L., 2.2  
 Courville, D. A., 2.3  
 Courville-Brenasin, J. de, 4.2  
 Cowan, P. L., 5.1  
 Cowan, S. W., 2.5, 3.3  
 Cowley, J. M., 2.5, 4.2, 4.3, 4.5, 5.2  
 Cowtan, K., 2.3  
 Cox, E. G., 1.3  
 Cox, J. M., 2.3, 2.4  
 Cox, S. R., 3.5  
 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  
 Craven, B. M., 3.5  
 Crick, F. H. C., 1.3, 2.2, 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  
 Crutchfield, J. P., 4.2  
 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  
 Cunningham, D., 3.3  
 Currat, R., 4.2  
 Curtis, C. W., 1.3  
 Curtis, R. J., 4.4  
 Cutfield, J. F., 2.2  
 Czaplowski, C., 3.5  
 Czaplowski, C., 3.5  
 Czerwinski, E. W., 2.3  
 Dabrowski, M., 2.5  
 Dai, J.-B., 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  
 Darby, G., 2.3  
 Darden, T. A., 3.5  
 Dark, R., 3.3  
 Darwin, C. G., 5.1  
 Das, K., 2.3  
 Dasgupta, C., 4.4  
 D'Astuto, M., 4.1  
 Daubeny, R. de P., 4.5  
 Dauter, M., 2.3  
 Dauter, Z., 2.3  
 Davey, S. C., 4.4  
 Davidov, D., 4.4  
 Davidson, E. R., 3.5  
 Davidson, J. B., 5.3  
 Davidson, W., 2.3  
 Davies, B. L., 1.5  
 Davies, D. R., 1.3  
 Davis, M. E., 2.3  
 Davis, P. J., 3.4  
 Dawson, B., 1.2, 2.5  
 Day, D., 4.5  
 Day, G. M., 3.5  
 Dayringer, H. E., 3.3  
 De Caro, L., 2.2  
 De Facio, B., 5.2  
 De Gennes, P. G., 4.4  
 De Hoff, R., 4.4  
 De Meulenaere, P., 4.3  
 De Ridder, R., 4.3  
 De Titta, G. T., 2.2, 2.5, 4.5  
 De Vries, H. L., 4.4  
 Dea, I. C. M., 4.5  
 Debaerdemaeker, T., 2.2  
 DeBoissieu, M., 4.6  
 Debreczeni, J. É., 2.3  
 Debye, P., 4.1  
 Declercq, J.-P., 2.2  
 Dederichs, P. H., 4.2  
 Deem, M. W., 3.5  
 Dehlinger, U., 4.6  
 Deimel, P., 5.3  
 Deisenhofer, J., 1.3, 2.3, 2.4  
 DeLano, W. L., 2.3  
 Delapalme, A., 5.3  
 Delaunay, B., 1.5  
 DeLeeuw, S. W., 3.5  
 Della Valle, R. G., 3.5  
 Dellby, N., 4.3  
 Deming, K., 3.5  
 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  
 Deserno, M., 3.5  
 Destrade, C., 4.4  
 Destro, R., 3.5  
 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  
 Dilanian, R. A., 3.3  
 Dimon, P., 4.4  
 Ding, D., 4.2  
 Ding, J., 2.3  
 Dintzis, H. M., 2.3  
 Dirac, P. A. M., 1.3  
 Dirl, R., 1.5  
 DiSalvo, F. J., 4.4  
 Ditchfield, R., 1.2

## AUTHOR INDEX

- Diu, B., 1.2  
 Djurek, D., 4.4  
 Dobrott, R. D., 2.3  
 Dodson, E., 2.2, 2.3, 2.4  
 Dodson, E. J., 1.3, 2.2, 2.3, 3.3  
 Dodson, G. G., 2.2, 2.3, 3.3  
 Doerschuk, P. C., 2.5  
 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  
 Dolomanov, O. V., 3.3  
 Domany, E., 4.4  
 Donabauer, J., 3.5  
 Dong, W., 2.5  
 Donohue, J., 1.3, 2.3  
 Donovan, B., 4.1  
 Dorna, V., 4.2  
 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  
 Dovesi, R., 3.5  
 Dowell, W. C. T., 2.5  
 Downing, K. H., 2.5  
 Downs, R. T., 3.3  
 Dowty, E., 1.4, 3.3  
 Doyle, P. A., 4.3, 4.5  
 Dräger, J., 4.6  
 Drenth, J., 4.5  
 Drits, V. A., 2.5  
 Dror, R. O., 3.5  
 Duan, X., 2.5  
 Duane, W., 1.3  
 Dube, P., 2.5  
 Dubernat, J., 4.2  
 Dubois, J. C., 4.4  
 Duce, D. A., 3.3  
 Duijneveldt, F. B. van, 3.5  
 Dumrongrattana, S., 4.4  
 Duncan, W. J., 5.2  
 Dunitz, J. D., 1.2, 3.5  
 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  
 Dziki, W., 3.5  
 Dzyabchenko, A., 3.5  
  
 Eades, J. A., 2.5  
 Eaglesham, D. J., 2.5  
 Eaker, D., 2.3  
 Eastwood, J. W., 3.5  
 Eastwood, M. P., 3.5  
 Eckold, G., 4.2  
 Edgington, P. R., 3.3  
 Edmonds, J. W., 2.2, 2.5, 4.5  
 Edwards, O. S., 4.2  
 Egami, T., 4.2  
 Egelman, E., 2.5  
 Egert, E., 2.2, 2.3  
 Eichhorn, F., 5.3  
 Eijck, B. P. van, 3.5  
 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  
 Elyutin, N. O., 5.3  
 Emery, V. J., 4.2  
 Emr, S. D., 2.5  
 Enderle, G., 3.3  
 Endoh, H., 2.5  
 Endoh, Y., 2.5  
 Endres, H., 4.2  
  
 Engel, G., 3.5  
 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  
 Erk, P., 3.5  
 Eschenbacher, P. W., 1.3  
 Esnouf, R., 2.3  
 Essmann, U., 3.5  
 Estermann, M., 4.2, 4.6  
 Etheridge, J., 5.2  
 Etherington, G., 4.4  
 Evans, A. C., 3.3  
 Evans, G., 2.3  
 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  
 Eyges, L., 3.5  
  
 Faber, T. E., 4.4  
 Facelli, J. C., 3.5  
 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  
 Farrant, G., 1.4, 2.5  
 Farrants, G. W., 3.3  
 Farrow, N. A., 2.5  
 Farrugia, L. J., 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  
 Fellmann, D., 2.5  
 Feltynowski, A., 2.5  
 Fender, B. E. F., 4.2  
 Fernandez, J.-J., 2.5  
 Ferrara, J. D., 2.3  
 Ferraris, G., 2.5  
 Ferraro, M. B., 3.5  
 Ferrel, R. A., 4.3  
 Ferrin, T. E., 2.5, 3.3  
 Fewster, P. F., 5.1  
 Feynman, R., 5.2  
 Fields, P. M., 4.3  
 Fillipini, G., 3.5  
 Filman, D. J., 2.3  
 Finch, J. T., 2.5  
 Finger, L. W., 3.3  
 Fingerland, A., 5.1  
 Finkelstein, K. D., 5.3  
 Finkenstadt, V. L., 4.5  
 Finn, R., 2.5  
 Fischer, J., 2.3  
 Fischer, K., 1.2  
 Fischer, R. X., 3.3  
 Fischer, W., 1.4  
 Fisher, J., 2.2  
 Fisher, P. M. J., 4.3  
 Fishman, G., 2.5  
 Fiske, S. J., 2.2  
 Fitzgerald, P. M. D., 1.4, 2.3  
 Flack, H. D., 4.2  
 Flaute, T. J., 4.4  
 Fleming, R. M., 4.4  
 Flensburg, C., 2.3  
 Fletterick, R. J., 2.3, 3.3  
 Flook, R. J., 2.4  
  
 Foadi, J., 2.2  
 Fock, R., 5.2  
 Fogel, D. B., 2.3  
 Foley, J. D., 3.3  
 Folkhard, W., 1.3  
 Fontaine, D. de, 4.2  
 Fontell, K., 4.4  
 Fontes, E., 4.4, 5.1  
 Ford, G. C., 2.3  
 Ford, L. O., 3.3  
 Fornberg, A., 1.3  
 Forst, R., 4.2  
 Förster, E., 5.1  
 Forster, F., 2.5  
 Forsyth, J. B., 1.3, 4.2  
 Forsyth, V. T., 4.5  
 Fortier, S., 2.2  
 Fortuin, C. M., 3.4  
 Forwood, C. T., 2.5  
 Foster, R. M., 1.3  
 Foucher, P., 4.4  
 Fouret, P., 4.2  
 Fouret, R., 4.2  
 Fourme, R., 2.3  
 Fout, G. S., 2.3  
 Fowler, R. H., 1.3  
 Fowweather, F., 1.3  
 Fox, G., 2.3  
 Frampton, C. S., 3.5  
 Francis, N., 2.5  
 Frangakis, A. S., 2.5  
 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, D., 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  
 Frenkel, D., 3.5  
 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., 4.2, 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, A., 2.5  
 Fujiwara, K., 2.5, 5.2  
 Fujiyoshi, Y., 2.5  
 Fukuhara, A., 2.5, 5.2  
 Fukuyama, K., 2.3  
 Fuller, S. D., 2.5  
 Fuller, W., 4.5  
 Fultz, B., 4.2  
 Fung, K. K., 2.5  
 Furey, W., 2.3  
 Furie, B., 3.3  
 Furie, B. C., 3.3  
 Furusaka, M., 4.2  
 Fusti-Molnar, L., 3.5  
  
 Gabashvili, I. S., 2.5  
 Gabor, D., 2.5  
 Gähler, R., 5.3  
 Galerne, Y., 4.4  
  
 Gallo, L., 3.3  
 Gallo, S. M., 2.2  
 Gallop, J. R., 3.3  
 Gallwitz, U., 4.5  
 Gane, P. A. C., 4.4  
 Gannon, M. G. J., 4.4  
 Garcia, A. E., 3.5  
 Garcia-Golding, F., 4.4  
 Garcia-Granda, S., 2.2  
 Garcia-Rodriguez, L., 2.2  
 Gardner, K. H., 4.5  
 Garland, C. W., 4.4  
 Garland, Z. G., 4.4  
 Garman, E., 2.3  
 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  
 Gavezzotti, A., 3.5  
 Gavrilov, V. N., 5.3  
 Gay, R., 2.3  
 Gaykema, W. P. J., 2.3  
 Gayle, F. W., 4.2  
 Gebhard, W., 4.5  
 Geddes, A. J., 3.3  
 Gehlen, P., 4.2  
 Gehlhaar, D. K., 2.3  
 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  
 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  
 Giacobozzo, C., 2.1, 2.2  
 Giarrusso, F. F., 3.3  
 Gibbons, P. C., 4.2  
 Gibbs, J. W., 2.3  
 Gibson, M. A., 2.5  
 Giegé, R., 2.3  
 Giesebrecht, J., 2.5  
 Gilbert, P. F. C., 2.5  
 Gill, P. E., 3.3  
 Gill, P. M. W., 3.5  
 Gillan, B. E., 4.2  
 Gilli, G., 2.4  
 Gilligan, K., 3.3  
 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  
 Girling, R. L., 3.3  
 Gjønnnes, J., 2.5, 4.3, 5.2  
 Gjønnnes, 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  
 Glosli, J., 3.5  
 Glück, M., 1.5  
 Glucksman, M. J., 4.5  
 Glykos, N. M., 2.3  
 Go, N., 3.3  
 Goddard, T. D., 2.5  
 Godréche, C., 4.6  
 Goedkoop, J. A., 1.3, 2.2  
 Goff, J. P., 4.2  
 Golas, M. M., 2.5  
 Goldman, A. I., 4.2, 4.6  
 Goldstine, H. H., 1.3  
 Golovchenko, J. A., 5.1  
 Golub, G. H., 2.5  
 Goncharov, A. B., 2.5  
 Gonzalez, A., 4.5

## AUTHOR INDEX

- Gonzalez, R. F., 2.5  
 Good, I. J., 1.3  
 Goodby, J. W., 4.4  
 Goodman, P., 2.5, 5.2  
 Goodyear, G., 2.5  
 Goossens, D. J., 4.2  
 Gordon, R., 2.5  
 Gosling, R. G., 4.5  
 Gossling, T. H., 3.3  
 Gould, R. O., 2.2  
 Gouyet, J. F., 4.6  
 Gowen, B., 2.5  
 Graaf, H. de, 4.5  
 Graaff, R. A. G. de, 2.2  
 Graeff, W., 5.1, 5.3  
 Gragg, J. E., 4.2  
 Gramlich, V., 2.2  
 Gransbergen, E. F., 4.4  
 Grant, D. F., 2.2  
 Grassucci, R. A., 2.5  
 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  
 Greenberg, W. L., 2.5  
 Greenblatt, D. M., 2.5  
 Greenhalgh, D. M. S., 1.3  
 Greer, J., 3.3  
 Grems, M. D., 1.3  
 Grenander, U., 1.3  
 Griffith, J. P., 2.3  
 Grigorieff, N., 2.5  
 Grimm, H., 1.3, 4.2  
 Grindley, J., 3.5  
 Grinstein, G., 4.4  
 Gronsky, R., 2.5  
 Gros, P., 2.3  
 Gross, L., 1.3  
 Grosse-Kunstleve, R. W., 1.4, 2.2, 2.3  
 Grubb, D. T., 4.5  
 Grzegory, I., 4.1  
 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  
 Gullberg, G. T., 2.5  
 Gunther, L., 4.4  
 Gur, Y., 1.5  
 Gurskaya, G. V., 2.5  
 Guru Row, T. N., 1.2  
 Guryan, C. A., 4.2  
 Gutierrez, G. A., 4.5  
 Guyot-Sionnest, P., 4.4  
  
 Haas, F. de, 2.5  
 Hadamard, J., 1.3  
 Haefner, D. R., 4.2  
 Haefner, K., 4.2  
 Haibach, T., 4.6  
 Hall, I. H., 4.5  
 Hall, M., 1.3  
 Hall, R. J., 2.5  
 Hall, S. R., 1.4, 2.2  
 Halla, F., 4.2  
 Hall-Wallace, M., 3.3  
 Halperin, B. I., 4.4  
 Hamaker, C., 2.5  
 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, J., 2.5  
 Hansen, N. K., 1.2  
 Hao, Q., 2.2  
 Harada, J., 4.2  
 Harada, Y., 2.3, 2.5, 4.3  
 Harauz, G., 2.5  
 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, G. W., 4.2  
 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  
 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  
 Hashimoto, T., 2.5  
 Hass, B. S., 3.3  
 Hastings, C. Jr., 3.4  
 Hastings, J. B., 5.3  
 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  
 Hauser, J., 3.3  
 Havelka, W., 2.5  
 Havighurst, R. J., 1.3  
 Hayakawa, M., 4.2  
 Hayes, W., 4.2  
 Hazen, E. E., 3.3  
 He, L. X., 2.5  
 He, Y., 2.3  
 Head-Gordon, M., 3.5  
 Heagle, A. B., 2.5  
 Heap, B. R., 3.3  
 Hearmon, R. F. S., 4.1  
 Hearn, A. C., 1.4  
 Hecht, H. J., 2.3  
 Heel, M. van, 2.5  
 Hegerl, R., 2.5  
 Hehre, W. J., 1.2  
 Heideman, M. T., 1.3  
 Heil, P. D., 4.5  
 Heinemann, J. J. L., 2.2  
 Heiney, P. A., 4.4, 4.6  
 Helfrich, W., 4.4  
 Helgaker, T., 3.5  
 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  
 Hennion, M., 4.2  
 Henry, R., 3.5  
 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  
 Hewat, A., 3.3  
 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  
 Hirabayashi, M., 2.5  
 Hiraga, K., 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  
 Hlinka, J., 4.2  
 Ho, M.-H., 2.5  
 Ho, M.-S., 2.5  
 Hockney, R. W., 3.5  
 Hodgkin, D. C., 2.2, 2.3, 2.4  
 Hodgson, K. O., 2.4  
 Hodgson, M. L., 1.3  
 Hoffmann, J.-U., 4.2  
 Hofmann, D., 4.5  
 Hofmann, D. W. M., 3.5  
 Hogle, J., 2.3, 3.3  
 Hohlwein, D., 4.2  
 Hohn, M., 2.5  
 Høier, R., 2.5, 4.3, 5.2  
 Hol, W. G. J., 2.3, 3.3  
 Holbrook, S. R., 1.3, 2.4  
 Hollenberg, J., 2.5  
 Holm, C., 3.5  
 Holmes, K. C., 2.5, 4.5  
 Honegger, A., 3.3  
 Hong, H., 4.2  
 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  
 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  
 Howe, J. M., 2.5, 4.2  
 Howells, E. R., 2.1  
 Howells, R. G., 2.2  
 Howie, A., 2.5, 4.3, 4.5, 5.2  
 Hradil, K., 4.2  
 Hrdlička, Z., 5.3  
 Hsiou, Y., 2.3  
 Hsiung, H., 4.4  
 Hu, Ch., 4.2  
 Hu, H., 4.5  
 Hu, H. H., 2.5  
 Huang, C., 3.3  
 Huang, C. C., 2.5, 4.4  
 Huang, K., 1.3, 4.1  
 Huang, Z., 2.5  
 Hubbard, R. E., 3.3  
 Huber, R., 1.3, 2.3, 2.4  
 Hudson, L., 4.5  
 Hudson, P. J., 3.3  
 Huesman, R. H., 2.5  
 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  
 Hughes, S. H., 2.3  
 Hull, S., 4.2  
 Hull, S. E., 2.2  
 Hüller, A., 4.2  
 Hummel, W., 3.3  
 Hummelink, T., 3.3  
 Hummelink-Peters, B. G., 3.3  
 Hummer, G., 3.5  
 Hümmer, K., 5.1  
 Humphreys, C. J., 2.5, 4.3, 5.2  
 Hunsmann, N., 2.5  
 Hunt, J. F., 2.3  
 Huntingdon, H. B., 4.1  
 Hurley, A. C., 1.2, 2.5, 5.2  
 Huse, D. A., 4.4  
 Hutching, M. T., 4.2  
 Iannelli, P., 4.5  
 Ibers, J. A., 2.4, 4.2  
 Iijima, S., 4.3  
 Iizumi, M., 4.2  
 Ilag, L. L., 2.3  
 Imamov, R. M., 2.5  
 Immirzi, A., 1.3  
 Imry, Y., 4.4  
 Indenbom, V. L., 5.3  
 Ingram, V. M., 2.3, 2.4  
 Inoue, A., 2.5  
 Iolin, E. M., 5.3  
 Irwin, M. J., 2.2  
 Isaacs, N. W., 1.3, 2.2, 2.4, 3.3  
 Ishida, M., 2.5  
 Ishihara, K. N., 2.5, 4.6  
 Ishii, T., 4.2  
 Ishikawa, I., 5.3  
 Ishikawa, T., 5.1  
 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  
 Ivantchev, S., 1.5  
 Iwata, H., 4.2  
 Izumi, F., 3.3  
  
 Jach, T., 5.1  
 Jack, A., 1.3, 2.4  
 Jackson, J. I., 2.5  
 Jacobson, R. A., 2.2, 2.3  
 Jacques, J., 4.4  
 Jaeger, J. C., 1.3  
 Jagodzinski, H., 4.2  
 Jahn, W., 2.5  
 Jakana, J., 2.5  
 James, R. W., 1.2, 1.3, 2.3, 4.2, 5.1  
 Jan, J.-P., 1.5  
 Janiak, M. J., 4.4  
 Janner, A., 1.3, 2.5, 4.2, 4.6  
 Janot, C., 4.2  
 Janot, Chr., 4.6  
 Jansen, L., 1.5  
 Janssen, P. A. J., 2.3  
 Janssen, T., 1.3, 1.5, 2.5, 4.2, 4.6  
 Jap, B. K., 2.5  
 Jaric, M. V., 4.2, 4.6  
 Jarić, M. Y., 2.5  
 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  
 Jenni, S., 2.5  
 Jensen, L. H., 1.3, 2.3, 2.4  
 Jeu, W. H. de, 4.4  
 Jiang, J.-S., 2.3  
 Jia-xing, Y., 2.2  
 Jih, J. H., 2.3  
 Jogl, G., 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, 2.5, 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, R., 4.2, 4.5  
 Jones, R. C., 4.2  
 Jones, T. A., 2.3, 2.5, 3.3  
 Jones, W., 3.5  
 Jones, Y., 2.3  
 Jorgensen, P., 3.5  
 Josefsson, T. W., 4.3  
 Joyeux, L., 2.5  
 Joyez, G., 4.2  
 Jürgen, H., 1.3  
 Just, W., 4.2

## AUTHOR INDEX

- Kabsch, W., 3.3, 4.5  
 Kac, M., 1.3  
 Kaczmarz, S., 2.5  
 Kadečková, S., 5.3  
 Kaenel, R. A., 1.3  
 Kagan, Yu., 5.3  
 Kainuma, Y., 4.3, 5.2  
 Kaiser, H., 5.3  
 Kaiser-Bischoff, I., 4.2  
 Kakinoki, J., 4.2  
 Kalantar, A. H., 3.2  
 Kaldor, U., 2.1  
 Kalning, M., 4.2, 4.6  
 Kamada, K., 5.3  
 Kambe, K., 2.5, 5.2  
 Kamer, G., 2.3  
 Kamper, J., 2.3  
 Kaneko, K., 2.5  
 Kaneyama, T., 2.5  
 Kang, S. J., 3.3  
 Kannan, K. K., 2.3  
 Kansy, K., 3.3  
 Kaplan, D. R., 5.1  
 Kaplan, M., 4.4  
 Kara, M., 1.2  
 Karamertzanis, P. G., 3.5  
 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  
 Kaufman, M. J., 2.5  
 Kawaguchi, A., 4.5  
 Ke, E. Y., 2.5  
 Kearsley, S. K., 3.3  
 Keeling, J., 2.3  
 Keen, D. A., 4.2  
 Kek, S., 4.2, 4.6  
 Keller, A., 4.5  
 Keller, E., 3.3  
 Keller, J., 4.2  
 Kelley, B., 4.4  
 Kelly, B. A., 4.4  
 Kelton, K. F., 4.2, 4.6  
 Kendall, M., 1.2, 2.1  
 Kendrew, J. C., 1.3, 2.3, 2.4  
 Kennard, O., 3.1, 3.3  
 Kessel, M., 2.5  
 Kessler, M., 3.3  
 Ketelaar, J. A. A., 2.3  
 Khalak, H. G., 2.2  
 Khinchin, A. I., 1.3  
 Kiefer, J. E., 1.3, 2.1  
 Kiely, C. J., 2.5  
 Kikuta, S., 5.1, 5.3  
 Kim, M., 2.5  
 Kim, S.-H., 1.3, 2.3, 2.4  
 Kirby, I., 2.3  
 Kirichuk, V. S., 2.5  
 Kirkland, E. J., 2.5  
 Kirov, A., 1.4, 1.5  
 Kiselev, N. A., 2.5  
 Kissinger, C. R., 2.3  
 Kitagaku, M., 4.3  
 Kitagawa, Y., 2.4  
 Kitaigorodskii, A. J., 4.1  
 Kitaigorodsky, A. I., 4.2  
 Kitamura, N., 4.3  
 Kittel, C., 3.5, 4.4  
 Kitz, N., 1.3  
 Kjeldgaard, M., 2.5, 3.3  
 Klapperstück, M., 4.4  
 Klar, B., 5.3  
 Klechkovskaya, V. V., 2.5  
 Klei, H. E., 2.3  
 Klein, A. G., 5.3  
 Klein, M. L., 3.5  
 Kleinstück, K., 5.3  
 Kleman, M., 4.6  
 Klepeis, J. L., 3.5  
 Kleywegt, G. J., 2.3  
 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  
 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  
 Kokkinidis, M., 2.3  
 Kolar, H., 2.5  
 Kolba, D. P., 1.3  
 Kolodziej, S., 2.5  
 Komada, T., 2.5  
 Komorek, M., 4.2  
 Komura, Y., 4.2  
 Komura, Y., 4.2  
 Kong, Y. F., 2.5  
 Konner, J. H., 1.3, 2.4  
 Kopka, M. L., 2.3  
 Kopp, S., 2.5, 4.5  
 Kopperschläger, G., 2.5  
 Korekawa, M., 4.2, 4.6  
 Koritsansky, T., 3.5  
 Korn, D. G., 1.3  
 Körner, T. W., 3.5  
 Korpiun, P., 5.3  
 Kortan, A. R., 4.4  
 Kossel, W., 2.5  
 Koster, A. J., 2.5  
 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  
 Koymans, L., 2.3  
 Krabbendam, H., 2.2  
 Krahl, D., 2.5, 4.3  
 Krämer, S., 2.5  
 Kraus, W., 3.3  
 Kraut, J., 1.3, 2.3, 2.4  
 Kress, W., 4.1  
 Kreuger, R. J., 5.2  
 Kriegman, D. J., 2.5  
 Krisch, M., 4.1  
 Krishna, P., 4.2  
 Krivanek, O. L., 4.3  
 Krivoglaz, M. A., 4.2, 4.3  
 Kroeker, M., 3.3  
 Kroon, J., 2.2, 3.5  
 Kroumova, E., 1.5  
 Kruse, F. H., 1.3  
 Kuchta, L., 2.2  
 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  
 Kull, F. J., 2.5  
 Kuntz, I. D., 3.3  
 Kuo, K. H., 2.5  
 Kurihara, K., 4.2  
 Kuriyan, J., 1.3  
 Kurki-Suonio, K., 1.2  
 Kuszewski, J., 2.3  
 Kutateladze, T. G., 2.5  
 Kutznetsov, P. I., 1.2  
 Kuvdaldin, B. V., 5.3  
 Kuwabara, S., 2.5  
 Kvardakov, V. V., 5.3  
 Kycia, S., 4.2  
 Kyriakidis, C. E., 2.2  
 Lacour, T. F. M., 1.3  
 Ladbroke, B. D., 4.4  
 Ladisa, M., 2.2  
 Ladjadj, M., 2.5  
 Lagacé, L., 2.3  
 Lagendijk, R. L., 2.5  
 Lagomarsino, S., 5.1, 5.3  
 Lajzerowicz, J., 4.4  
 Lajzerowicz, J., 2.2  
 Laloe, F., 1.2  
 Lambert, D., 5.3  
 Lambert, M., 4.4  
 Lambert, M. A., 2.5  
 Lambiotte, J. J. Jr., 1.3  
 Lamfers, H.-J., 4.2  
 Lamy, J., 2.5  
 Lamzin, V. S., 2.3  
 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  
 Lanzavecchia, S., 2.5  
 Larine, M., 1.4  
 Larmor, J., 1.3  
 Lata, K. R., 2.5  
 Lattman, E. E., 2.3, 2.4  
 Laue, M., 1.1  
 Laue, M. von, 1.3, 5.1  
 Laurette, I., 2.5  
 Laval, J., 4.1  
 Laves, R., 4.2  
 Lavoine, J., 1.3  
 Lawrence, M. C., 2.5  
 Lawrence, P. D., 2.5  
 Lawson, K. D., 4.4  
 Lawton, J. A., 2.5  
 Le Bail, A., 3.3  
 Le Guillou, J. C., 4.4  
 Lea, S. M., 2.3  
 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, H., 3.5  
 Lee, J. C., 2.5  
 Lee, P. L., 4.2  
 Lee, S. D., 4.4  
 Lee, Y.-R., 5.1  
 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., 2.5, 4.3  
 Lei, J., 4.2  
 Leiman, P. G., 2.3  
 Leith, A., 2.5  
 Lele, S., 4.2  
 Lemoine, G., 3.3  
 Lentz, P. J. Jr., 2.3  
 Lepault, J., 2.5  
 Lerch, M., 4.2  
 Lerner, F. Ya., 2.5  
 Lescar, J., 5.1  
 Lescoute, A., 2.5  
 Lesk, A. M., 3.3  
 Leslie, A. G. W., 1.3, 2.3, 3.3  
 Lessinger, L., 2.2  
 Leszczynski, M., 4.1  
 Leung, P., 1.2  
 Leusen, F. J. J., 3.5  
 Leusen, F. J. L., 3.5  
 Levanyuk, A. P., 4.4  
 Levelut, A. M., 4.4  
 Levens, S. A., 1.3  
 Levine, D., 2.5, 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  
 Lewis, M., 2.3  
 Lewis, T. C., 3.5  
 Lewitt, R. M., 2.5  
 Li, D. X., 2.5  
 Li, F. H., 2.5  
 Li, J. Q., 2.5  
 Li, Y., 2.5  
 Liang, C., 3.5  
 Liang, K. S., 4.4  
 Liang, Y. Y., 2.5  
 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., 2.3  
 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, W., 2.5  
 Liu, Y.-W., 2.5  
 Livanova, N. B., 2.5  
 Livesey, A. K., 1.3  
 Lloyd, T. E., 2.5  
 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  
 Loris, R., 5.1  
 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  
 Lövgren, S., 2.3  
 Lowde, R. D., 5.3  
 Lu, C., 1.3  
 Lu, G., 2.3  
 Luban, M., 4.4  
 Lubensky, T. C., 4.4  
 Lucas, B. W., 4.2  
 Luck, J. M., 4.6  
 Ludewig, J., 5.1  
 Ludtke, S. C., 2.5

## AUTHOR INDEX

- Ludtke, S. J., 2.5  
 Luenberger, D. G., 3.3  
 Luić, M., 2.2  
 Lunin, V. Y., 2.3  
 Lunin, V. Yu., 1.3  
 Lunina, N. L., 2.3  
 Luo, M., 2.3  
 Lurie, N. A., 4.1  
 Lurz, R., 2.5  
 Lushington, K. J., 4.4  
 Luther, P., 4.5  
 Luty, T., 4.1  
 Luzzati, V., 2.3, 4.4  
 Lybanon, M., 3.2  
 Lyman, P. F., 5.1  
 Lynch, D. F., 2.5, 5.2  
 Lynch, R. E., 2.3
- Ma, J. P., 2.5  
 Ma, Q., 2.3  
 Ma, S. K., 4.4  
 MacGillavry, C. H., 1.3, 4.5  
 Machin, P. A., 3.3  
 Mackay, A. L., 2.2, 2.5, 3.3  
 MacKay, M., 2.3  
 MacLane, S., 1.3  
 MacNicol, D. D., 2.5  
 Macovski, A., 2.5  
 Macrae, C. F., 3.3  
 MacRae, T. P., 4.5  
 Mada, H., 4.4  
 Madariaga, G., 1.5  
 Madden, P. A., 3.5  
 Madelung, E., 3.4  
 Madhav Rao, L., 5.3  
 Magdoff, B. S., 2.3  
 Magnus, W., 1.3  
 Mahendrasingam, A., 4.5  
 Mahon, M., 3.3  
 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  
 Malladi, R., 2.5  
 Mallick, S. P., 2.5  
 Mallikarjunan, M., 3.3  
 Malthête, J., 4.4  
 Maly, K., 4.2, 4.6  
 Mandelkern, L., 4.5  
 Mandelkow, E., 4.5  
 Mani, N. V., 2.4  
 Manley, R. St. J., 2.5  
 Mannami, M., 2.5  
 Mao, Y., 2.5  
 Marabini, R., 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  
 Marko, M., 2.5  
 Marks, L. D., 4.3  
 Marsh, R. E., 3.2, 3.5  
 Marson, F., 4.4  
 Martin, C., 2.3  
 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  
 Massariol, M.-J., 2.3  
 Massidda, V., 3.4  
 Mastryukov, V. S., 2.5  
 Masumoto, K., 2.5
- Masumoto, T., 2.5  
 Matadeen, R., 2.5  
 Matej, S., 2.5  
 Materlik, G., 1.2, 5.1  
 Mathews, F. S., 3.3  
 Mathiesen, R. H., 5.1  
 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, J., 2.5  
 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  
 McArdle, P., 3.3  
 McCabe, P., 3.3  
 McCall, M. J., 3.3  
 McClellan, J. H., 1.3  
 McCourt, M. P., 2.5, 4.5  
 McCoy, A. J., 2.3  
 McDonald, W. S., 2.4  
 Mcewen, B., 2.5  
 McFarland, K., 3.5  
 McGreevy, R. L., 4.2  
 McIntyre, G. J., 1.2  
 McKean, H. P., 1.3  
 McKenna, R., 2.3  
 Mckernen, S., 2.5  
 McLachlan, A. D., 3.3  
 McLachlan, D., 2.3, 2.5  
 McMahan, B., 1.4  
 McMillan, W. L., 4.4  
 McMullan, R. K., 3.3  
 McMurchie, L. E., 3.5  
 McPherson, A., 2.4  
 McQueen, J. E., 3.3  
 McWhan, D. B., 4.4  
 Mechin, I., 2.5  
 Meiboom, S., 4.4  
 Meichle, M., 4.4  
 Melone, S., 5.3  
 Mendiratta, S. K., 5.3  
 Meng, E. C., 2.5  
 Menzer, G., 2.3  
 Mermin, N. D., 1.1, 4.6  
 Mersereau, R. M., 1.3, 2.5  
 Merwe, J. H. van der, 4.4  
 Messiah, A., 5.2  
 Metropolis, N., 4.2  
 Meyer, C. E., 4.3  
 Meyer, C. H., 2.5  
 Meyer, E. F., 3.3  
 Meyer, G., 2.5  
 Meyer, L. B., 2.5  
 Meyer, R. B., 4.4  
 Michalec, R., 5.3  
 Michejda, C. J., 2.3  
 Micu, A. M., 4.2  
 Midgley, P. A., 2.5  
 Mielke, T., 2.5  
 Mierzewski, 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, J. S., 4.2  
 Miller, R., 2.2, 4.5  
 Miller, S. C., 1.5  
 Miller, S. T., 2.3  
 Mills, D. M., 5.1  
 Mimori-Kiyosue, Y., 4.5  
 Minakawa, N., 5.3  
 Mindell, J. A., 2.5
- Ming, D. M., 2.5  
 Mitra, A. K., 4.5  
 Mitra, K., 2.5  
 Mitsui, T., 4.5  
 Miyake, S., 2.5  
 Miyano, K., 4.4  
 Miyazaki, M., 2.5  
 Mo, F., 5.1  
 Mo, Y. D., 2.5  
 Moereels, H., 2.3  
 Moliere, G., 4.3  
 Moliterni, A. G. G., 2.2  
 Möllenstedt, G., 2.5  
 Moncrief, J. W., 2.3  
 Moncton, D. E., 4.4  
 Montroll, E. W., 1.3  
 Moodie, A. F., 2.5, 5.2  
 Mooji, W. T. M., 3.5  
 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  
 Morgenroth, W., 4.2  
 Mori, M., 4.3  
 Moriguchi, S., 2.5  
 Morimoto, C. N., 3.3  
 Morinaga, M., 4.2  
 Moring, I., 2.3  
 Moritz, W., 4.2  
 Morniroli, J. P., 2.5  
 Morris, E. P., 2.5  
 Morris, J., 3.5  
 Morris, R. L., 1.3  
 Moser, W. O. J., 1.3  
 Mosley, A., 4.4  
 Moss, B., 2.5  
 Moss, D. S., 4.2  
 Moss, G., 1.2  
 Moss, S. C., 4.2, 4.3  
 Mosser, A. G., 2.3  
 Motherwell, W. D. S., 3.3, 3.5  
 Motohashi, H., 5.3  
 Mouche, F., 2.5  
 Moussa, F., 4.4  
 Moustiakimov, M., 2.2  
 Muirhead, H., 2.3, 2.4  
 Mukamel, D., 4.4  
 Mukherjee, A. K., 2.2  
 Mullapudi, S., 2.5  
 Müller, H., 4.2  
 Müller, R., 5.1  
 Müller, U., 4.2  
 Munn, R. W., 3.4  
 Murakami, W. T., 2.3  
 Murdock, W. L., 1.3  
 Murray, W., 3.3  
 Murshudov, G. N., 2.3  
 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  
 Nagem, R. A. P., 2.3  
 Naiki, T., 2.5  
 Nakatsu, K., 2.3  
 Namba, K., 4.5  
 Nambudripad, R., 4.5  
 Narayan, R., 1.3, 2.2, 2.4  
 Narayanan, B. A., 3.5  
 Natarajan, P., 2.5  
 Nathans, R., 4.2  
 Natterer, F., 1.3, 2.5  
 Navaza, J., 1.3, 2.2, 2.3  
 Nave, C., 1.3, 4.5  
 Navia, M. A., 2.4  
 Nawab, H., 1.3  
 Naya, S., 2.2, 4.5  
 Neder, R. B., 4.2  
 Neisser, J. Z., 4.5  
 Nelson, D. E., 1.3
- Nelson, D. R., 4.2, 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  
 Newsam, J. M., 3.5  
 Neyertz, S., 3.5  
 Ng, E. G., 2.5  
 Niall, H. D., 3.3  
 Nicastro, D., 2.5  
 Nicholson, P. B., 4.5  
 Nicholson, R. B., 2.5, 5.2  
 Nickell, S., 2.5  
 Nickitenko, A., 2.5  
 Nieh, Y.-P., 2.3  
 Nield, V. M., 4.2  
 Nierhaus, K. H., 2.5  
 Nigam, G. D., 2.1  
 Niggli, A., 1.3  
 Niimura, N., 4.2  
 Nijboer, B. R. A., 3.4, 3.5  
 Nilges, M., 2.3  
 Nishimura, D. G., 2.5  
 Nissen, P., 2.5  
 Nitsch, M., 2.5  
 Nitta, I., 2.2  
 Nityananda, R., 1.3, 2.2  
 Nixon, P. E., 2.3  
 Nolze, G., 3.3  
 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  
 Nosé, S., 3.5  
 Nowacki, W., 2.5  
 Nowell, H., 3.5  
 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, Y., 2.5  
 Ogawa, T., 2.5  
 Ogburn, K. D., 2.5  
 Ohara, M., 4.5  
 Ohshima, K., 4.2, 4.3  
 Ohtsuki, Y. H., 4.3, 5.1  
 Oikawa, T., 4.3  
 Okabe, A., 2.5  
 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, J., 3.5  
 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  
 Ord, K., 2.1  
 Orlando, R., 3.5  
 Orlov, S. S., 2.5  
 Orlova, E. V., 2.5  
 Ørmen, P.-J., 1.2  
 Ostermann, A., 4.2  
 O'Sullivan, J. D., 2.5  
 Oszlányi, G., 2.2  
 Ott, H., 2.2  
 Ottensmeyer, F. P., 2.5  
 Overduin, M., 2.5  
 Overhauser, A. W., 4.2, 5.3  
 Ozawa, T. C., 3.3

## AUTHOR INDEX

- Pabst, M., 4.1  
 Paciorek, W. A., 4.6  
 Pähler, A., 2.2  
 Paley, R. E. A. C., 1.3  
 Palleschi, V., 4.4  
 Palmer, M. R., 2.5  
 Palmer, R. A., 2.3, 2.4  
 Palmer, S. B., 5.3  
 Pan, M., 2.5  
 Pan, Q., 2.5  
 Pandey, D., 4.2  
 Panepucci, E. H., 2.3  
 Pannu, N. S., 2.3  
 Pantelides, C. C., 3.5  
 Paoletti, A., 4.2  
 Pape, T., 2.5  
 Paradossi, G., 4.5  
 Park, H., 4.5  
 Parks, T. W., 1.3  
 Parlett, B. N., 2.5  
 Parmon, V. S., 2.5  
 Parodi, O., 4.4  
 Parsey, J. M. Jr., 4.2  
 Parthé, E., 4.3  
 Parthasarathy, R., 2.3, 2.4  
 Parthasarathy, S., 2.1, 2.2, 2.4  
 Pascual-Montano, A., 2.5  
 Pashley, D. W., 2.5, 4.5, 5.2  
 Pastore, A., 3.3  
 Patel, J. R., 5.1  
 Patel, K., 3.5  
 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  
 Patwardhan, A., 2.5  
 Pätzold, H., 4.3  
 Paul, D., 2.5  
 Pauling, L., 1.3, 2.3  
 Paulmann, C., 4.2  
 Pauwels, R., 2.3  
 Pavelčík, F., 2.2  
 Pavlovitch, A., 4.6  
 Pavone, P., 4.1  
 Pawley, G. S., 4.1  
 Pearce, L. J., 3.3  
 Pearl, L. H., 3.3  
 Pearlman, D. A., 3.5  
 Pearson, J., 3.3  
 Pearson, K., 1.3  
 Pease, M. C., 1.3  
 Pedersen, B., 4.2  
 Pedersen, L., 3.5  
 Peerdeman, A. F., 2.2, 2.3, 2.4  
 Peierls, R. E., 4.4  
 Peisl, J., 4.2  
 Penczek, P. A., 2.5  
 Penning, P., 5.1  
 Penrose, R., 2.5, 4.6  
 Penzkofer, B., 4.2  
 Pepinsky, R., 1.3, 2.2, 2.3, 2.4  
 Perera, L., 3.5  
 Perez, S., 4.5  
 Pérez, S., 2.5  
 Perez-Mato, J. M., 1.4, 1.5, 4.2  
 Perham, R. N., 4.5  
 Perrakis, A., 2.3  
 Perram, J. W., 3.5  
 Perrier de la Bathie, R., 5.3  
 Pershan, P. S., 4.4  
 Perutz, M. F., 2.2, 2.3, 2.4  
 Peschar, R., 2.2  
 Petef, G., 2.3  
 Peters, C., 1.3  
 Petersen, H. G., 3.5  
 Petrascheck, D., 5.3  
 Petricek, V., 4.2, 4.6  
 Pétrouff, J. F., 5.3  
 Petrov, V. V., 1.3  
 Petrova, T. E., 2.3  
 Petržílka, V., 5.3  
 Petsko, G. A., 1.3, 3.3  
 Pettersen, E. F., 2.5  
 Pezerat, H., 4.2  
 Pfaff, G., 3.3  
 Pflanz, S., 4.2  
 Pflugrath, J. W., 2.3  
 Phillips, D. C., 2.1, 2.2, 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  
 Pillardy, J., 3.5  
 Pilling, D. E., 1.3  
 Pindak, R., 4.4  
 Pink, M. G., 3.3  
 Pinsker, Z. G., 2.5, 5.1  
 Piquemal, J. P., 3.5  
 Pirie, J. D., 4.1  
 Piro, O. E., 2.2  
 Plano, R. J., 4.4  
 Plotnikov, A. P., 2.5  
 Plotnikov, V. P., 2.5  
 Pochon, F., 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  
 Polikarpov, I., 2.3  
 Poljak, R. J., 2.3  
 Pollack, H. O., 1.3  
 Pollock, E. L., 3.5  
 Ponder, J. W., 3.5  
 Poole, C. P., 3.3  
 Popa, N. C., 4.1  
 Pople, J. A., 1.2  
 Popp, D., 4.5  
 Porter, T. K., 3.3  
 Porter, W., 3.5  
 Portier, R., 2.5, 5.2  
 Potenzzone, R., 3.3  
 Potter, C. S., 2.5  
 Potterton, E. A., 3.3  
 Potts, R. B., 1.3  
 Pouget, J. P., 4.2  
 Powell, B. M., 4.2  
 Powell, M. J. D., 2.5  
 Prandl, W., 4.2  
 Prange, T., 2.3  
 Prasad, B. V. V., 2.5  
 Pratt, L. R., 3.5  
 Press, W., 4.2, 4.6  
 Preston, A. R., 2.5  
 Price, L. S., 3.5  
 Price, S. L., 3.5  
 Prick, A. J., 2.2  
 Prins, J. A., 2.4, 4.2, 5.1  
 Proffen, Th., 4.2  
 Prosen, R. J., 1.3, 2.3  
 Prost, J., 4.4  
 Prout, C. K., 3.3  
 Provencher, S. W., 2.5  
 Pryor, A. W., 4.1, 4.6  
 Pulay, P., 3.5  
 Puliti, P., 5.3  
 Pullan, L., 2.5  
 Purisima, E. O., 3.3  
 Pustovskikh, A. I., 2.5  
 Pusztai, L., 4.2  
 Pynn, R., 4.1  
 Qian, C., 2.3  
 Quandalle, P., 1.3  
 Quick, J., 3.5  
 Quilichini, M., 4.2  
 Quiocho, F. A., 2.5, 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  
 Radons, W., 4.2  
 Rae, A. D., 2.2, 2.3  
 Raghavacharyulu, I. V. V., 1.5  
 Raghavan, N. V., 2.4  
 Raghavan, R. S., 2.4  
 Rahman, S. H., 4.2  
 Raimondi, D. L., 1.2  
 Raïtman, E. A., 5.3  
 Raiz, V. Sh., 2.4  
 Raja, V. N., 4.4  
 Rajagopal, H., 2.4  
 Rajashankar, K. R., 2.3  
 Ramachandran, G. N., 2.2, 2.3, 2.4, 5.1  
 Ramagopal, U. A., 2.3  
 Raman, C. V., 4.1  
 Raman, S., 2.2, 2.3, 2.4  
 Ramaseshan, S., 2.3, 2.4  
 Ramaswamy, S., 4.4  
 Rango, C. de, 2.2, 2.4  
 Rao, R. R., 1.3  
 Rao, S. N., 2.3  
 Rao, S. T., 3.3  
 Raselli, A., 3.3  
 Rasmussen, B., 5.1  
 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  
 Redlack, A., 3.5  
 Rees, A. L. G., 2.5  
 Rees, D. C., 2.3  
 Refaat, L. S., 2.3  
 Reid, T. J. III, 2.3  
 Reif, F., 1.3  
 Reijnen, L. L. van, 1.3  
 Reiner, I., 1.3  
 Reiss-Husson, F., 4.4  
 Reman, F. C., 4.4  
 Remillard, B., 4.5  
 Ren, J., 2.3  
 Ren, P. Y., 3.5  
 Renka, R., 2.5  
 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, L. M., 2.3  
 Rice, S. O., 1.3  
 Richardson, J. S., 3.3  
 Richardson, J. W., 2.2  
 Richardson, R. M., 4.4  
 Rickert, S. E., 4.5  
 Riddle, A. C., 2.5  
 Rieckel, C., 4.2  
 Riesz, M., 1.3  
 Rietveld, H. M., 4.2  
 Riley, D., 3.5  
 Rimmer, B., 2.3  
 Rini, J. M., 2.3  
 Rivard, G. E., 1.3  
 Rixon, F. J., 2.5  
 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  
 Rodriguez-Carvajal, J., 3.3  
 Roetti, C., 1.2, 3.5  
 Rogers, D., 2.1, 2.2, 2.3  
 Rokhsar, D. S., 4.6  
 Rollett, J. S., 1.3, 3.3  
 Roseman, A. M., 2.5  
 Rosen, J., 1.5  
 Rosenbluth, A. W., 4.2  
 Rosenbluth, M. N., 4.2  
 Rosenstein, R. D., 2.3  
 Ross, C., 2.3  
 Rosshirt, E., 4.2  
 Rossmann, M. G., 1.3, 2.2, 2.3, 2.4, 3.3  
 Rossouw, C. J., 2.5, 4.3  
 Rouiller, I., 2.5  
 Roux, D., 4.4  
 Roversi, P., 2.3, 3.5  
 Rowlands, D., 2.3  
 Rowlands, R. J., 4.5  
 Rozenfeld, A., 2.5  
 Rueckert, R. R., 2.3  
 Ruedenberg, K., 1.2  
 Ruf, T., 4.1  
 Rugman, M., 4.4  
 Rühle, M., 2.5  
 Ruijgrok, Th. W., 3.5  
 Ruiz, T., 2.5  
 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  
 Rypniewski, W., 2.5  
 Ryskin, A. I., 2.5  
 Saad, A., 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  
 Sagui, C., 3.5  
 Sahni, V. C., 4.1  
 Saibil, H. R., 2.5  
 Saito, M., 2.5  
 Saito, P., 2.5  
 Saito, R., 2.5  
 Saito, Y., 2.2, 2.3  
 Saitoh, K., 2.5  
 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., 2.5, 5.3  
 Sandonis, J., 5.3  
 Sands, D. E., 1.1, 3.1  
 Sanjurjo, J. R., 2.5  
 Sansom, C., 4.2  
 Sarikaya, M., 2.5  
 Sarko, A., 4.5  
 Sasada, Y., 2.3, 3.3  
 Sato, H., 4.2  
 Satow, Y., 2.4  
 Saunders, M., 2.5  
 Saunders, V. R., 3.5  
 Saube, A., 4.4  
 Sauvage, M., 4.3, 5.3  
 Saxton, W. O., 2.5  
 Sayre, D., 1.3, 2.2, 2.3, 2.4, 2.5, 4.5  
 Scaringe, P. R., 4.2  
 Scaringe, R. P., 2.5  
 Scatturin, V., 2.5  
 Schacher, G. E., 3.4  
 Schaeftzling, R., 4.4  
 Schaffitzel, C., 2.5  
 Schärpf, O., 4.2  
 Schatz, M., 2.5  
 Schenk, H., 2.2  
 Scheraga, H. A., 3.3, 3.5

## AUTHOR INDEX

- Scheres, S. H. W., 2.5  
 Scheringer, C., 1.2  
 Scherm, R., 5.3  
 Scherzer, O., 2.5  
 Schevitz, R. W., 2.2, 2.3, 2.4  
 Schilling, J. W., 2.3  
 Schiltz, M., 2.3  
 Schiske, P., 2.5  
 Schlenker, M., 5.3  
 Schmatz, W., 4.2  
 Schmidt, H. H., 5.3  
 Schmidt, M. U., 3.5  
 Schmidt, R., 2.5  
 Schmidt, T., 2.3  
 Schmidt, W. C. Jr., 3.3  
 Schnabel, W., 4.2  
 Schneider, A. I., 4.5  
 Schneider, T. R., 2.2, 2.3  
 Schoenberg, I. J., 3.5  
 Schoenborn, B. P., 2.4  
 Schofield, P., 4.1  
 Schomaker, V., 1.1, 1.2, 1.3, 2.3, 2.5, 3.2  
 Schomberg, H., 2.5  
 Schoone, J. C., 2.4  
 Schrader, H., 4.2  
 Schramm, H. J., 2.5  
 Schröder, M., 3.3  
 Schröder, R., 2.5  
 Schroder, R. R., 2.5  
 Schroeder, M. R., 1.3  
 Schroeer, B., 2.5  
 Schuessler, H. W., 1.3  
 Schüler, M., 2.5  
 Schuller, D. J., 2.3  
 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  
 Schwarzenbach, D., 1.2  
 Schwarzenberger, R. L. E., 1.3  
 Schweika, W., 4.2  
 Schweizer, B., 3.5  
 Schweizer, J., 5.3  
 Scott, W. R., 1.3  
 Scudder, M. L., 2.4  
 Sears, V. F., 4.2, 5.3  
 Secomb, T. W., 2.5  
 Sedláková, L., 5.3  
 Seidl, E., 5.3  
 Seitz, E., 4.2  
 Seitz, F., 1.4  
 Sekii, H., 2.5, 5.2  
 Selinger, J. V., 4.4  
 Sellar, J. R., 5.2  
 Semiletov, S. A., 2.5  
 Senechal, M., 4.6  
 Serrano, J., 4.1  
 Sethna, J. P., 4.4  
 Sezan, M. I., 2.5  
 Sha, B. D., 2.5  
 Shaffer, P. A. Jr., 1.3  
 Shaikh, T., 2.5  
 Shakked, Z., 2.1, 2.3  
 Shan, N., 3.5  
 Shan, Y. B., 3.5  
 Shankland, K., 2.5, 4.5  
 Shannon, C. E., 1.3, 2.5  
 Shannon, M. D., 2.5  
 Shao-Hui, Z., 2.2  
 Shapiro, A., 3.3  
 Shappell, M. D., 2.3  
 Shashidhar, R., 4.4  
 Shashua, R., 2.1  
 Shastri, S. D., 5.1  
 Shaw, D. E., 3.5  
 Sheat, S., 2.3  
 Shechtman, D., 2.5, 4.6  
 Sheldrick, G. M., 2.2, 2.3  
 Shen, Q., 5.1  
 Shen, Y. R., 4.4  
 Shenefelt, M., 1.3  
 Sheriff, S., 2.3, 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, G. G., 4.4  
 Shirane, G., 4.1, 4.2  
 Shmueli, U., 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  
 Siegrist, T., 3.3  
 Sieker, L. C., 2.4  
 Sigaud, G., 4.4  
 Sigler, P. B., 2.2, 2.3, 2.4  
 Sigworth, F. J., 2.5  
 Sikka, S. K., 2.4  
 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  
 Simonson, T., 2.3  
 Simpson, A. A., 2.3  
 Simpson, P. G., 2.3  
 Singh, A. K., 2.3, 2.4  
 Singleton, R. C., 1.3  
 Sinha, S. K., 3.5, 4.4  
 Sint, L., 2.2  
 Sippel, D., 5.3  
 Siripitayananon, J., 4.2  
 Sirota, E. B., 4.4  
 Sirota, M. I., 2.5  
 Sivardière, J., 5.3  
 Sivý, J., 2.2  
 Sixma, T. K., 2.3  
 Sjögren, A., 2.5  
 Skehel, J. J., 2.3  
 Skilling, J., 1.3  
 Skoglund, U., 2.3  
 Skoulios, A., 4.4  
 Skovoroda, T. P., 2.3  
 Skuratovskii, I. Y., 4.5  
 Slater, L. S., 1.5  
 Sleight, M. E., 2.5  
 Slepian, D., 1.3  
 Sluckin, T. J., 4.4  
 Sly, W. G., 1.3  
 Smaalen, S. van, 4.2, 4.6  
 Small, D., 4.4  
 Smit, B., 3.5  
 Smith, A. B. III, 4.4  
 Smith, D. J., 2.5  
 Smith, E. R., 3.5  
 Smith, G., 3.3  
 Smith, G. D., 2.2  
 Smith, G. S., 4.4  
 Smith, G. W., 4.4  
 Smith, J. C., 4.2  
 Smith, J. L., 2.2, 2.3  
 Smith, J. V., 1.5  
 Smith, M. B. K., 2.3  
 Smith, R. H. Jr., 2.3  
 Smith, T., 4.1  
 Smith, W., 3.5  
 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  
 Soldani, M., 3.5  
 Solitar, D., 1.3  
 Solmon, D. C., 2.5  
 Solomon, L., 4.4  
 Somenkov, V. A., 5.3  
 Somers, D., 2.3  
 Sondhauss, P., 5.1  
 Soni, R. P., 1.3  
 Sorensen, L. B., 4.4  
 Sorzano, C. O. S., 2.5  
 Soyer, A., 3.3  
 Spackman, M. A., 3.5  
 Spagna, R., 2.2  
 Spahn, C. M. T., 2.5  
 Spanton, S., 3.5  
 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, 3.3  
 Spellward, P., 2.5  
 Spence, J. C. H., 2.5, 4.3  
 Spiegel, M. R., 2.1  
 Spink, J. A., 2.5  
 Spiwek, H., 3.5  
 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., 2.5, 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  
 Stahl, S. J., 2.5  
 Stammers, D., 2.3  
 Stanley, E., 2.2, 4.5  
 Stark, H., 2.5  
 Stark, W., 4.5  
 Stasiak, A., 2.5  
 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., 2.5, 4.6  
 Steinkilberg, M., 2.5  
 Steinrauf, L. K., 2.3  
 Steitz, T. A., 2.3, 2.5  
 Stence, C. N., 2.3  
 Stephanik, H., 5.1  
 Stephen, M. J., 4.4  
 Stephens, P. W., 4.2, 4.4, 4.6  
 Stephenson, G. B., 4.4  
 Stephenson, R., 3.3  
 Stetsko, Yu. P., 5.1  
 Steurer, W., 2.5, 4.2, 4.6  
 Steven, A. C., 2.5  
 Stevens, E. D., 1.2  
 Stewart, A. T., 4.1  
 Stewart, R. F., 1.2  
 Stokes, H. T., 1.5  
 Stone, A. J., 3.5  
 Stoops, J. K., 2.5  
 Storke, K. H., 4.5  
 Storoni, L. C., 2.3  
 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, L., 5.2  
 Sturtevant, J. M., 4.5  
 Su, Z., 1.2  
 Suck, D., 2.3, 3.3  
 Sugihara, K., 2.5  
 Sun, W., 2.5  
 Sundaralingam, M., 3.3  
 Sundaram, K., 3.3  
 Sundberg, M., 2.5  
 Suresh, K. A., 4.4  
 Suryan, G., 1.3  
 Suski, T., 4.1  
 Sussman, J. L., 1.3, 2.4  
 Sutcliffe, D. C., 3.3  
 Sutherland, I. E., 3.3  
 Suito, A., 2.2  
 Suzuki, E., 4.5  
 Suzuki, H., 4.5  
 Suzuki, S., 2.5  
 Svergun, D. I., 2.5  
 Swaminathan, S., 2.3, 3.3  
 Swanson, S. M., 3.3  
 Swartzrauber, P. N., 1.3  
 Swoboda, M., 4.3  
 Symmons, M. F., 4.5  
 Szegö, G., 1.3  
 Szillard, L., 2.4  
 Tadokoro, H., 4.5  
 Taftø, J., 4.3  
 Taftø, T., 2.5  
 Taguchi, I., 2.2  
 Tajbakhsh, A. R., 4.4  
 Takagi, K., 2.5  
 Takagi, S., 2.5, 5.1, 5.3  
 Takahashi, H., 5.2  
 Takahashi, M., 2.5  
 Takahashi, T., 5.3  
 Takaki, Y., 4.2  
 Takano, T., 1.3  
 Takayoshi, H., 2.5  
 Takana, A., 3.3  
 Takeuchi, Y., 2.3, 2.4  
 Talapov, A. L., 4.4  
 Tama, F., 2.5  
 Tamarkin, J. D., 1.3  
 Tanaka, I., 4.2  
 Tanaka, K., 1.2  
 Tanaka, M., 2.5, 5.2  
 Tanaka, N., 2.3, 2.4, 4.3  
 Tanaka, S., 4.5  
 Tang, G., 2.5  
 Tanji, T., 2.5  
 Tanner, B. K., 5.1  
 Tao, X., 2.3  
 Tao, Y., 2.3  
 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, 2.3  
 Taupin, D., 5.3  
 Tavares, P., 2.5  
 Taveau, J. C., 2.5  
 Taylor, C. A., 1.3, 1.4, 4.2  
 Taylor, D. J., 2.2  
 Taylor, G. H., 4.4  
 Taylor, R., 3.1, 3.3  
 Taylor, W. J., 2.3  
 Tchoubar, D., 4.2  
 Teeter, M. M., 2.3, 2.4  
 Teller, A. H., 4.2  
 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, 2.3  
 Teplyakov, A., 2.3  
 Terauchi, M., 2.5



## AUTHOR INDEX

- Terwilliger, T. C., 2.2, 2.3, 2.4  
Teworte, R., 5.1  
Thierry, J. C., 2.3  
Thoen, J., 4.4  
Thomas, D. J., 3.3  
Thomas, K. M., 4.4  
Thomsen, K., 3.3  
Thon, F., 2.5  
Thorpe, M. F., 4.2  
Thouless, D. G., 4.4  
Thuman, P., 2.2  
Tibbals, J. E., 4.2  
Tikhonov, V. I., 1.2  
Tildesley, D. J., 3.5  
Timmer, J., 2.5  
Tinh, N. H., 4.4  
Tinnappel, A., 2.5  
Tirion, M., 4.5  
Titchmarsh, E. C., 1.3  
Tivol, W. F., 2.5  
Tivol, W. T., 4.5  
Tjian, R., 3.3  
Toby, B. H., 3.3  
Toepflich, 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  
Torrise, A., 3.5  
Tosoni, L., 2.5  
Toukmaji, A., 3.5  
Toupin, R., 2.2  
Tournaire, M., 2.5  
Tournarie, M., 5.2  
Tramontano, A., 3.3  
Traub, W., 2.2  
Trèves, F., 1.3  
Trickey, S. B., 3.5  
Trommer, W. E., 2.3  
Tronrud, D. E., 1.3, 2.3  
Trueblood, K. N., 1.1, 1.2, 1.3, 2.3  
Trus, B. L., 2.5  
Truter, M. R., 1.3  
Tsai, A. P., 2.5  
Tsao, J., 2.3  
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  
Tsujiyama, S., 2.5  
Tsukihara, T., 2.3, 3.3  
Tsuprun, V. L., 2.5  
Tsuruta, H., 2.5  
Tukey, J. W., 1.3  
Tulinsky, A., 2.4  
Turberfield, K. C., 4.2  
Turkenburg, M. G., 2.3  
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  
Unser, M., 2.5  
Unwin, P. N. T., 2.5  
Uragami, T., 5.1  
Urzhumtsev, A., 2.3  
Usha, R., 2.3  
Ushigami, Y., 5.3  
Uson, I., 2.3  
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., 2.3, 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 Hove, L., 4.1, 4.3  
Van Loan, C. F., 2.5  
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  
Varn, D. P., 4.2  
Varnum, J. C., 2.3  
Vartanyants, I. A., 5.1  
Vaucher, C., 4.4  
Vaughan, P. A., 2.2  
Vedani, A., 3.3  
Velazquez-Muriel, J., 2.5  
Venkataraman, G., 4.1  
Venkatesan, K., 2.4  
Venuti, E., 3.5  
Vereijken, J. M., 2.3  
Vermin, W. J., 2.2  
Vernoslova, E., 2.3  
Verschoor, A., 2.5  
Verwer, P., 3.5  
Vibert, P. J., 4.5  
Vicković, I., 2.2  
Vijayan, M., 2.2, 2.3, 2.4  
Vilkov, L. V., 2.5  
Villain, J., 4.4  
Vincent, R., 2.5  
Vine, W. J., 2.5  
Viterbo, D., 2.2  
Vogel, R. H., 2.5  
Volbeda, A., 2.3  
Volkman, N., 2.5  
Volkov, A., 3.5  
Von der Lage, F. C., 1.2  
Vonderviszt, F., 4.5  
Vonnrhein, C., 2.3  
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  
Wagenknecht, T., 2.5  
Wagner, E. H., 5.1  
Waho, T., 4.3  
Waite, J., 3.5  
Wakabayashi, K., 4.5  
Walian, P. J., 2.5  
Walker, C. B., 4.1  
Waller, I., 1.2  
Walsh, G. R., 3.3  
Walz, J., 2.5  
Wang, B. C., 1.3, 2.3, 2.4  
Wang, D. N., 2.5  
Wang, H., 4.5  
Wang, J., 4.4, 5.1  
Wang, R., 4.2  
Wang, X. J., 4.4  
Wang, Z. L., 4.3  
Ward, J. C., 1.3  
Ward, K. B., 2.3  
Wark, J. S., 5.1  
Warme, P. K., 3.3  
Warren, B., 1.3  
Warren, B. E., 1.3, 4.2, 4.4  
Warren, G. L., 2.3  
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  
Watkin, D. J., 3.3  
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  
Watson, W. T., 2.5  
Wawak, R. J., 3.5  
Waxham, M. N., 2.5  
Webb, H., 2.5  
Weber, H. J., 3.5  
Weber, H. P., 3.5  
Weber, T., 4.2  
Weber, Th., 4.2  
Weckert, E., 5.1  
Wedemeyer, W. J., 3.5  
Weeks, C. M., 2.2, 2.3, 4.5  
Weidner, E., 4.2  
Weikenmeier, A., 2.5  
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, A., 2.5  
Welch, P. D., 1.3, 2.5  
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  
Westhof, E., 2.5  
Weyl, H., 1.3  
Weymouth, J. W., 4.1  
Whelan, M., 4.3  
Whelan, M. J., 2.5, 4.3, 5.2  
White, C., 3.5  
White, H., 2.5  
White, J. G., 2.3  
White, P., 2.2  
Whitfield, H. J., 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, S., 3.5  
Wilke, W., 4.2  
Wilkins, M. H. F., 4.5  
Wilkins, S. W., 1.3, 2.2  
Williams, D. E., 3.4, 3.5, 4.1  
Williams, G. J. B., 3.3  
Williams, R. M., 4.4  
Williams, T. V., 3.3  
Willingmann, P., 2.3  
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, 4.2, 4.5  
Wilson, E. B., 1.1  
Wilson, I. A., 2.3  
Wilson, K. S., 2.1, 2.2, 2.3  
Wilson, S. A., 5.3  
Windsor, C. G., 4.2  
Wingfield, P. T., 2.5  
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  
Witt, C., 2.5  
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, 1.4, 1.5, 2.2  
Wong, H. C., 2.5  
Wong, S. F., 4.2  
Woods, R. E., 2.5  
Woodward, I., 2.3, 2.4  
Woolfson, M. M., 1.3, 2.1, 2.2, 2.3, 2.5  
Wooster, W. A., 4.2  
Wostrack, A., 4.2  
Wright, D. C., 4.6  
Wright, M. H., 3.3  
Wrighton, P. G., 4.4  
Wrinch, D. M., 2.3  
Wu, H., 2.3  
Wu, M. N., 2.5  
Wu, T. B., 4.2  
Wu, X.-J., 2.5  
Wu, Y. K., 2.5  
Wübbeling, F., 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  
Wynne, S. A., 2.5  
Xia, D., 2.3  
Xiang, S.-B., 2.5  
Xiaodong, Z., 1.4  
Xu, H., 2.2  
Xu, P. R., 4.3  
Xu, Y., 2.3  
Yagi, N., 4.5  
Yamamoto, A., 2.5, 3.3, 4.6  
Yamamoto, N., 2.5  
Yamashita, I., 4.5  
Yamazaki, H., 5.1  
Yang, C., 2.3, 2.5  
Yang, W., 3.5  
Yang, Y. W., 1.2  
Yao, J.-X., 2.2, 2.5  
Yeates, T. O., 2.3  
Yelon, W. B., 5.3  
Yessik, M., 4.2  
Yin, Z. H., 2.5  
Yin, Z. Y., 2.5  
Yip, S., 4.1  
Yonath, A., 2.2  
York, D. M., 3.5  
Yoshioka, H., 4.3  
Yosida, K., 1.3  
Youla, D. C., 2.5  
Young, A. P., 4.4  
Young, C. Y., 4.4  
Young, R. A., 4.2  
Yu, L. J., 4.4  
Yuan, B.-L., 4.5  
Yuen, C. K., 2.5  
Zachariasen, W. H., 1.3, 1.4, 2.4, 5.1, 5.3  
Zak, J., 1.5  
Zalkin, A., 2.4  
Zaluzec, N. J., 2.5  
Zambianchi, P., 5.1  
Zarka, A., 5.3  
Zaschke, H., 4.4  
Zassenhaus, H., 1.3  
Zechmeister, K., 1.3, 2.5  
Zegenhagen, J., 5.1  
Zegers, I., 5.1  
Zeilinger, A., 5.3  
Zeitler, E., 2.5  
Zelenka, J., 5.3  
Zelepukhin, M. V., 5.3  
Zellner, J., 5.1  
Zelwer, C., 2.2  
Zemanian, A. H., 1.3  
Zemlin, F., 2.5  
Zenetti, R., 4.2  
Zeng, G. L., 2.5  
Zernike, F., 4.2  
Zeyen, C., 4.2, 5.3

## AUTHOR INDEX

Zhang, K. Y. J., 2.3  
Zhang, W. P., 2.5  
Zhao, Z. X., 2.5  
Zheng, C.-D., 2.2, 2.5  
Zheng, Y. L., 2.5  
Zhong, Z.-Y., 2.5

Zhou, Z. H., 2.5  
Zhu, J., 2.5  
Zhu, Y., 2.5  
Zhukhlistov, A. P., 2.5  
Zicovich-Wilson, C. M., 3.5  
Ziman, J. M., 1.1

Zinn-Justin, J., 4.4  
Zlotnick, A., 2.5  
Zobetz, E., 4.6  
Zolotoyabko, E., 5.3  
Zou, J.-Y., 2.5, 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, 512  
*A priori* probability, 504  
*Ab initio* phase determination, 273  
Abbe theory, 303  
Abel summation procedure, 46  
Abelian groups, 42, 79  
Aberrations, 303  
Absolute configuration, 282, 285  
Absolutely integrable functions, 27  
Absorbing crystals, 629, 637–638, 640  
Absorption coefficient, 634, 639  
    effective, 628  
    linear, 628  
    phenomenological, 303  
Absorption edge, 284  
Absorption function, 542  
Absorption in electron diffraction, 362  
Accelerated convergence, 449  
    formula *via* Patterson function, 454  
Acceptance domain, 596  
Acentric reflections, 74  
Acoustic modes, 486  
Action, 68  
Additive reindexing, 61  
Adiabatic approximation, 484  
Adjusted coefficients, 180  
Affine change of coordinates, 35  
Affine change of variables, 40  
Affine space-group type, 177  
Affine transformation, 120  
Agarwal's FFT implementation of the Fourier method, 98  
Alfalfa mosaic virus, 259  
Algebra of functions, 75  
Algebraic integers, 78, 82  
Algebraic number theory, 82  
Algebraic reconstruction technique (ART), 370  
Aliasing, 47, 49, 93  
Alignment of electron-microscopy images, 379  
Allowed origins, 215  
'Almost everywhere', 26  
Analytical methods of probability theory, 102  
Angle between two vectors, 404  
Angles  
    Eulerian, 262, 420  
    spherical, 262  
Anisotropic displacement parameters, 443  
Anisotropic displacement tensors, 6  
Anisotropic fluid, 547  
Anisotropic Gaussian atoms, 63  
Anisotropic temperature factors, 73  
Anisotropic weights, 413  
Annular dark-field detector, 305  
Anomalous absorption, 633, 659  
Anomalous difference, 288, 291  
Anomalous dispersion (scattering), 255–256, 282, 284  
    integration with direct methods, 237  
    Patterson function, 257  
Anomalous scatterers, 64, 74, 256, 284, 286  
Anomalous transmission effect, 633  
Antiferromagnetic domains, 661  
Anti-nodes of standing waves, 633  
Antisymmetric tensor, 6  
Aperiodic crystals, 590  
    disorder diffuse scattering from, 526  
    ideal, 590  
Aperiodic structure, 590  
Apparent noncrystallographic symmetry, 267  
Approximate helix symmetry, 570  
Approximations  
    adiabatic, 484  
    Bethe, second, 302  
    Born, first-order, 10, 300  
    Born, second-order, 11  
    Born–Oppenheimer, 17  
    Edgeworth, 21  
    forward-scattering, 301  
    harmonic, 484  
    kinematical, 62, 300–301, 359, 394, 583, 658  
    phase-grating, 652  
    phase-object, 301, 542  
    projected charge-density, 305  
    projection, 648  
    saddlepoint, 102–103  
    seven-beam, 652  
    small-angle-scattering, 300  
    three-beam, 652  
    two-beam, 302, 649  
    two-beam dynamical, 394  
    weak-phase-object, 304  
Area detector, 294  
Argand diagram, 283  
Arithmetic classes, 71  
    of representations, 71  
Arithmetic crystal class, 177  
Arms of star, 178  
ART (algebraic reconstruction technique), 370  
Artificial temperature factor, 94, 100  
Aspherical-atom form factor, 14  
Aspherical multipole refinement, 459  
Associated actions in function spaces, 69  
Associativity properties of convolution, 100  
Assumption of independence, 209  
Assumption of uniformity, 203, 209  
Astigmatism, 378  
Asymmetric carbon atom, 285  
Asymmetric images, 365  
Asymmetric unit, 69, 72, 180  
    noncrystallographic, 253  
Asymmetry ratio, 631  
Asymptotic crystal shape, 470  
Asymptotic distribution of eigenvalues of Toeplitz forms, 45, 68  
Asymptotic expansions  
    and limit theorems, 103  
    of Gram–Charlier and Edgeworth, 105  
Atom-centred spherical harmonic expansion, 12  
Atomic characteristic functions, 211  
Atomic electron densities, 75  
Atomic error matrix, 416  
Atomic force-constant matrix, 485  
Atomic form factor, 10  
    X-ray, 293  
Atomic scattering factor, 10, 284  
    spherical, 10  
Atomic scattering length, 11  
Atomic surface, 590, 596  
Atomic temperature factor, 17  
ATOMS, 443–445  
Autocorrelation, 65  
Autocorrelation function, 388  
Automated Patterson-map search, 389  
Automorphism, 69, 71  
Auxiliary basis set expansion, 479  
Auxiliary basis set fitting, 459  
Average difference cluster method, 518  
Average intensity  
    of general reflections, 195  
    of zones and rows, 196  
Average multiples for point groups, 197  
Averaged electron density, 274  
Axial disorder, 517  
B-splines, 476  
    approximation to trigonometric functions, 477  
    derivatives of, 477  
    Fourier transforms of, 477  
    recursion for, 477  
    tensor product, 480  
B3LYP basis set, 479  
Back-shift correction, 96  
Back surface, 639  
Background diffraction, accurate subtraction of, 575  
Backprojection, 367  
    filtered, 371  
Backward convolution theorem, 44, 75  
Bacterial rhodopsin, 274  
*Balls&Sticks*, 443–444  
*BALSAC*, 443–445  
Banach spaces, 28  
Band-limited function, 49  
Base-centred lattices, 90  
Bases  
    Cartesian, 7  
    contravariant, 5–6  
    covariant, 5–6  
    direct and reciprocal, relationships between, 3  
    mutually reciprocal, 2–3  
    primitive, 177  
    reference, choice of, 7  
Basic crystallographic computations, 91  
Basic domain, 180  
Basic structure, 591  
Basis vectors, contravariant, 405  
Bayesian statistical approach to the phase problem, 106  
Beavers–Lipson factorization, 58, 76–77  
Beavers–Lipson strips, 76, 93  
Bessel's inequality, 47  
Best Fourier, 91, 290  
Best phase, 290  
Best plane, 410  
Beta distribution  
    first kind, 201  
    second kind, 201  
Bethe approximation, second, 302  
Biaxial nematic order, 549  
Bieberbach theorem, 68  
Bijvoet differences, 257  
Bijvoet equivalents, 286–287  
Bijvoet pair, 285–286  
*Bilder*, 440  
Binary systems, distortions in, 522  
Binding energy, 284  
Bloch-wave formulation, 650  
Bloch waves, 300, 628  
Bloch's theorem, 9, 486  
    alternative form of, 9  
Blow and Crick formulation, 290  
Body-centred lattices, 90  
Body-diagonal axes, 128  
Bond angles, 437  
Bond orientational order, 547  
Booth's differential Fourier syntheses, 96  
Booth's method of steepest descents, 96  
Bootstrap technique, 388  
Borie–Sparks method, 523  
Born approximation  
    first-order, 10, 300  
    second-order, 11  
Born–Oppenheimer approximation, 17  
Born series, 300, 651  
    expansion, 543  
Born–von Karman boundary conditions, 177  
Born–von Kármán theory, 484  
Borrmann effect, 303, 633  
Borrmann triangle, 641  
Boundary conditions, 628, 639  
    at exit surface, 635  
    periodic, 479  
Bounded projections, 67, 92  
Bounded subset, 25  
Boy's function, 471  
BP (bright-field pattern), 310  
Bragg case, 631  
Bragg's law, departure of incident wave from, 630  
Bragg–Lipson charts, 93  
Branch, 485  
Bravais lattices  
    centred, 121  
    direct and reciprocal, 121  
Bright-field image intensity, 362  
Bright-field pattern (BP), 310  
Brillouin zone, 9, 485  
    first, 178  
Bulk plasmon excitation, 300  
Burg entropy, 68  
Burnside's theorem, 71  
Butterfly loop, 53

## SUBJECT INDEX

- Calculus
  - of asymmetric units, 79
  - operational, 28
- Cameron*, 443–444
- CaRIne*, 443–444
- Carpet of cross-vectors, 260
- Cartesian basis, 7
- Cartesian coordinate system, 404
- Cartesian coordinates, 418, 445
- Cartesian frames of reference, 5
- Cartesian product, 25, 42
- Cartesian system, transformation to, 3
- Cauchy kernel, 46
- Cauchy–Schwarz inequality, 27, 47
- Cauchy sequence, 26
- Cauchy's theorem, 104
- CBED (convergent-beam electron diffraction), 307
  - coherent, 323, 333
- CCP14 (Collaborative Computational Project Number 14), 443
- Cell constants, 576
- Central-limit theorem, 103, 198
  - Lindeberg–Lévy version, 204
- Central section theorem, 367
- Centre-of-mass translational displacements, 525
- Centre of symmetry, false, 115
- Centred Bravais lattice, 121
- Centred lattices, 73
- Centric reflections, 73
- Centring
  - effect of, 196
  - translations, 121
  - type, 121
- Centrosymmetric projections, 251–252
- Centrosymmetry, status of, 123
- Cesàro sum, 46
- Chain rule, 99
- Chain trace, 441
- Chains, flexible, 436
- Change-of-basis matrix, 123
- Change of crystal axes, 120
- Channelling pattern, 544
- Characteristic functions, 102, 197, 208
  - atomic, 211
- Charge densities, Coulomb energy of, 474
- Charge distributions, Gaussian, 461, 471–472
- CHARMM*, 442
- CHEMGRAF*, 439
- Chemical correctness of polypeptide fold, 273
- Chem-X*, 442
- Chinese remainder theorem (CRT), 54, 61, 82
  - for polynomials, 57, 84
  - reconstruction, 54
  - reconstruction formula, 57
- Chirality, 285
- Choice of reference bases, 7
- Cholesteryl iodide, 249
- $\alpha$ -Chymotrypsin, 271
- Circular harmonic expansions, 100
- Classical Thomson scattering, 10
- Classification of crystallographic groups, 70
- Classification of electron-microscopy images, 381
- Clebsch–Gordan coefficients, 17
- Closed point group, 258
- Closed subset, 25
- Cluster model, 545
- Clustering, 518
- Clustering algorithms, 380
- Clusters, 500
- Cochran's Fourier method, 96
- Cocycle, 85
- Coherence, 434
- Coherence length, 568
- Coherent convergent-beam electron diffraction, 323, 333
- Coherent scattering, 488
- Collaborative Computational Project Number 14 (CCP14), 443
- Column part, 177
- Common line, 382
- Communication, statistical theory of, 104
- Commutative ring, 54
- Compact Gaussians, 472
- Compact subset, 25
- Compact support, 25, 36, 44
  - distributions with, 30, 40, 43–44, 47
- Complement of the incomplete gamma function, 450–451
- Complete normed space, 28
- Complete vector spaces, 26
- Completely reducible matrix group, 176
- Complex antisymmetric transforms, 87
- Complex scattering factor, 255
- Complex symmetric transforms, 87
- Components of vector products, 405
- Components of vectors, 5
- Composite lattice, 449, 452
- Composite structure, 593
- Compound nucleus, 11
- Compound transformations, 429
- Compton scattering, 489
- Computational and algebraic aspects of mutually reciprocal bases, 4
- Computational cost of Ewald direct sum, linear scaling of, 474
- Computer-adapted space-group symbols, 117, 122, 127
- Computer-algebraic languages, 122
- Computer architecture, 52, 61
- Computer simulations of diffuse scattering, 528
- Condensed ring systems, 437
- Conditional convergence, 460
- Conditional pair probability, 504
- Conformational variability, 388
- Conforming/nonconforming disorder, 518
- Conformons, 431
- Conjugacy classes of subgroups, 69
- Conjugate and parity-related symmetry, 85
- Conjugate distribution, 104–105
- Conjugate families of distributions, 106
- Conjugate gradient method, 436
- Conjugate symmetry, 35, 40
- Conjugation, 69
- Connectivity
  - drawing, 435
  - implied, 435
  - logical, 435
  - structural, 435
- Connectivity tables, 435
- Connectivity tree, 439
- Consistency condition, 39
- Constant **Q** mode, 490
- Constraints, 436, 440–441
  - on interpretation of Patterson functions, 258
- Continuous diffraction on layer lines, 575
- Continuum dielectric medium, 467
- Contragredient, 40
  - of a matrix, 35
- Contrast transfer function, 370, 376
- Contravariant bases, 5–6
- Contravariant basis vectors, 405
- Contravariant components, 5
- Conventional coefficients, 180
- Convergence
  - accelerated, 449
  - accelerated, formula *via* Patterson function, 454
  - conditional, 460
  - of distributions, 30
  - of Fourier series, 45
- Convergence-accelerated direct sum, 452
- Convergence method, 231
- Convergent-beam electron diffraction (CBED), 307
  - coherent, 323, 333
- Conversion of translations to phase shifts, 35
- Convolution, 64, 244
  - associativity properties of, 100
  - cyclic, 51, 55
  - of distributions, 34
  - of Fourier series, 44
  - of probability densities, 102
  - of two distributions, 34
- Convolution property, 35, 51
- Convolution techniques, 392
- Convolution theorem, 37, 42, 44, 46, 67, 102, 106
  - backward version, 44, 75
  - forward version, 44, 64–65, 75
- Convolution theorems with crystallographic symmetry, 75
- Cooley–Tukey algorithm, 52, 61, 77
  - vector-radix version, 58
- Cooley–Tukey factorization, multidimensional, 58–59, 79
- Coordinate systems, 177
  - Cartesian, 404
  - natural, 404
- Coordinates
  - affine change of, 35
  - Cartesian, 418, 445
  - crystallographic, 418
  - fractional, 42, 63, 262
  - homogeneous, 418, 421
  - nonstandard, 42
  - positional, 437
  - screen, 426, 428
  - spherical, 467
  - spherical polar, 263
  - standard, 42, 63, 71–72
  - transformation of, 5, 7, 33
  - world, 426
- Copolymers, random, 571
- Core of discrete Fourier transform matrix, 83
- Correction-factor approach, 203, 212
- Correlated lattice disorder, 573
- Correlation, 64
- Correlation functions, 75, 100, 252, 489, 505, 541
  - Ornstein–Zernike, 514
  - short-range-order, 518
- Correlation length, 550
  - pretransitional lengthening of, 551
- Correlations
  - intermolecular, 525
  - librational–librational, 525
  - vibrational–librational, 525
- Coset averaging, 48–49
- Coset decomposition, 48, 58
- Coset reversal, 59
- Cosets, 48, 71
  - left, 68
  - right, 69
- Cosine strips, 76
- Coulomb energy, 449
  - of charge densities, 474
- Coulomb interactions, 458
  - between Gaussians, 459
  - damped, 471
  - direct, 472
- Coulombic lattice energy, 449, 453
- Covariance, 407
  - interatomic, 411
- Covariances, 411
- Covariant bases, 5–6
- Covariant components, 5
- Cowpea mosaic virus, 259
- Critical angle, 554
- Critical scattering, 551
- Cross correlation, 76, 388
- Cross-correlation function, 365
- Cross-Patterson vectors, 260
- Cross-rotation function, 100
- Cross-vectors, 251
  - carpet of, 260
- CRT (Chinese remainder theorem), 54, 61, 82
  - for polynomials, 57, 84
  - reconstruction, 54
  - reconstruction formula, 57
- Cruikshank's modified Fourier method, 97
- Cryo-electron microscopy (cryo-EM), 375
- Cryscon*, 443
- Crystal axes, change of, 120
- Crystal class, arithmetic, 177
- Crystal defects in thin films, 542
- Crystal periodicity, 62
- Crystal-structure imaging, 306
- Crystal-structure prediction, 458
- Crystal structures
  - display of, 443
  - incommensurate, 445
  - magnetic, 445
  - polyhedral display of, 443
  - root-mean-square differences between, 445
- Crystal Studio*, 443–444
- Crystal symmetry, 68

## SUBJECT INDEX

- Crystal systems, 71, 123
- Crystal-B phase, 558
- Crystal-E phase, 560
- Crystal-G phase, 560
- Crystal-H phase, 560
- Crystal-J phase, 560
- Crystal-K phase, 560
- Crystalline approximant, 590
- Crystallographic applications of Fourier transforms, 62
- Crystallographic coordinates, 418
- Crystallographic discrete Fourier transform, 77
  - algorithms, 76
- Crystallographic extension of the Rader/Winograd factorization, 82
- Crystallographic Fourier transform theory, 62
- Crystallographic group action, 79
  - in real space, 71
  - in reciprocal space, 72
- Crystallographic groups, 68
  - classification of, 70
- Crystallographic statistics, 204
- Crystallographic symmetry, 258
- Crystallographica*, 443–444
- CrystalMaker*, 443–445
- CrystMol*, 443–445
- Cubic space groups, 90, 118
- Cumulant expansion, 21
- Cumulant-generating functions, 103, 198
- Cumulative distribution functions, 201
- Cuprous chloride azomethane complex, 247
- Cyclic convolution, 51, 55
- Cyclic (even) permutation of coordinates, 118, 122
- Cyclic groups, 71
- Cyclic symmetry, 83
- Cyclotomic polynomials, 57
- Cylindrically averaged diffraction patterns, 572
- Cylindrically averaged Patterson function, 577
  
- Damped Coulomb interaction, 471
- Dark-field pattern (DP), 309
- Data flow, 61
- Data handling, Hall symbols in, 123
- Data space, 426–427, 429–430
- de la Vallée Poussin kernel, 46
- Debye model, 486
- Debye theory, 484
- Debye–Waller factor, 551, 634
- Decagonal phase, 607
- Decagonal point groups, 354
- Decagonal quasicrystals, 354
- Decimation, 25, 49, 53
  - and subdivision of period lattices, duality between, 48
  - in frequency, 54, 59, 86
  - in time, 53, 85
  - period, 48
- Decimation matrix, 58–59, 78
- Decomposition, 78
  - coset, 48, 58
  - orbit, 69, 72, 74–75
- Deconvolution of a Patterson function, 249
- Defects, 299, 518
- Defocus, 366
  - optimal, 361
  - Scherzer, 305
  - Scherzer, conditions, 362
- Deformed crystal, 632
- Delta functions, 25
  - Dirac, 28, 450
  - periodic, 211
  - three-dimensional Dirac, 464
  - transforms of, 40
- Density modification, 91, 392
- Density modulation, 601
  - harmonic, 601
  - symmetric rectangular, 601
- Density of nuclear matter, 2
- Deoxyhaemoglobin, 273
- Depth cueing, 429, 439
- Derivatives
  - for model refinement, 95
  - for variational phasing techniques, 94
  - of B-splines, 477
- Detectors
  - annular dark-field, 305
  - area, 294
- Determinantal formulae, 227
- Determinantal inequalities, 67
- Deviation parameter, 631, 633
- Diamond*, 443–445
- Diamond's real-space refinement method, 99
- Dielectric response, 468
- Dielectric susceptibility, 627, 642
  - Fourier expansion of, 627
- Difference Fourier analysis, 576
- Difference Fourier synthesis, 288, 579
- Difference Fourier technique, 288
- Difference Patterson functions, 253–254
  - isomorphous, 253
- Differential syntheses, 36, 67, 97
- Differentiation, 25, 36
  - and multiplication by a monomial, 40
  - of distributions, 31
  - under the duality bracket, 31
- Differentiation identities, 51
- Differentiation property, 106
- Diffraction, dynamical, 393
- Diffraction beams, intensities of, 358
- Diffraction by helical structures, 100, 568
- Diffraction conditions, 63
- Diffraction groups, 308–311, 313
- Diffraction imaging techniques, 661
- Diffraction patterns, cylindrically averaged, 572
- Diffraction relations, 2
- Diffraction vector, 2
- Diffraction meters, optical, 364
- Diffuse Gaussians, 472
- Diffuse scattering, 540
  - computer simulations of, 528
  - elastic, 492
  - from aperiodic crystals, 526
  - from polycrystalline materials, 534
  - from quasicrystals, 527
  - modelling of, 528
  - of X-rays, 492
- Digit reversal, 53, 59, 62
- Digital electronic computation of Fourier series, 76
- Dihedral symmetry, 84
- Dimension of a representation, 176
- Dipalmitoylphosphatidylcholine, 562
- Dipole moment, 454
  - of unit cell, 461
- Dirac delta function, 28, 450
  - three-dimensional, 464
- Direct Bravais lattice, 121
- Direct Coulomb interaction, 472
- Direct Fourier inversion, 370
- Direct inspection of structure-factor equation, 116
- Direct lattice, 2, 5, 42, 121, 177
- Direct-lattice sum, 453
- Direct methods, 102, 117, 215, 288
  - in macromolecular crystallography, 235
  - integration with anomalous-dispersion techniques, 237
  - integration with isomorphous replacement techniques, 236
- Direct-methods packages, 234
- Direct metric, 4
- Direct phase determination, 36
  - in electron crystallography, 388
- Direct space, 176
- Direct-space crystal lattice, 450
- Direct-space sum, 449
- Direct-space transformations, 120
- Direct sum potential, 462
- Direct unit-cell parameters, 4
- Direction cosines of plane normal, 414
- Dirichlet kernel, 46
  - spherical, 64, 91
- Discotic phases, 561
- Discrete Fourier transform matrix, core of, 83
- Discrete Fourier transformation, 47
- Discrete Fourier transforms, 24, 77
  - algorithms, 76
  - matrix representation of, 51
  - numerical computation of, 52
  - properties of, 51
- Discretization, 368
- Dislocations, 555
- Disorder, 540
  - axial, 517
  - conforming/nonconforming, 518
  - from turns, twists and torsions of chains, 517
  - lattice, 572
  - lattice, correlated, 573
  - longitudinal, 516
  - orientational, 524
  - substitutional, 545, 572
  - two-dimensional, 514
- Disordered fibres, 568
- Dispersion corrections, 284, 286, 627
- Dispersion effects, 284
- Dispersion energy, 449
- Dispersion equations, 300
- Dispersion interactions, 459
- Dispersion surface, 629, 650, 657
- Displacive modulation, 600
  - harmonic, 601
- Display space, 426–427, 429–431, 434
- Displaying crystal structures, 443
- Distance function, 27
- Distribution function, 509
  - cumulative, 201
- Distributions
  - associated with locally integrable functions, 30
  - beta, first kind, 201
  - beta, second kind, 201
  - conjugate, 104–105
  - conjugate families of, 106
  - convergence of, 30
  - convolution of, 34
  - definition of, 30
  - differentiation of, 31
  - division of, 32
  - electron-magnetization, 11
  - equal, 45
  - Fourier transforms of, 39
  - gamma, 201
  - Gaussian, 290
  - hypersymmetric, 201
  - ideal acentric, 200
  - ideal centric, 200
  - integration of, 32
  - lattice, 43–44, 47–48
  - maximum-entropy, 36, 106
  - moments of, 102
  - motif, 63
  - multiplication of, 32
  - non-ideal, 203, 207
  - of finite order, 30
  - of random atoms, 104
  - of sums, averages and ratios, 202
  - operations on, 31
  - periodic, 42, 44, 62
  - probability density, 197
  - probability density, ideal, 200
  - support of, 30
  - $T$  on  $\Omega$ , 30
  - tempered, 36, 39, 41, 47, 72
  - tensor products of, 33
  - theory of, 25, 28
  - with compact support, 30, 40, 43–44, 47
- Divided differences, 651
- Division of distributions, 32
- Division problem, 32
- Docking, 387, 441
- Domain
  - basic, 180
  - minimal, 179
  - of influence, 178
  - representation, 179
- Domain structure, 441
- Double-phased synthesis, 283
- Double-sorting technique, 273
- DP (dark-field pattern), 309
- Drawing connectivity, 435
- DrawXTL*, 443–445
- Dual, topological, 30, 39–40
- Dual relationships, 2

## SUBJECT INDEX

- Duality  
 between differentiation and multiplication by a monomial, 67  
 between periodization and sampling, 44  
 between sections and projections, 41  
 between subdivision and decimation of period lattices, 48
- Duality bracket, 39
- Duality product, 31
- Dummy indices, 5
- Dynamic parallax, 427, 441
- Dynamical approximation, two-beam, 394
- Dynamical diffraction, 393, 542  
 theory, 301, 626  
 two-beam, formulae, 303
- Dynamical extinction, 319, 323–324, 333, 335
- Dynamical matrix, 486
- Dynamical scattering effects, 388
- Dynamical scattering factor, 543
- Dynamical shape function, 651
- Dynamical theory, 301, 626  
 fundamental equations, 628  
 of neutron diffraction, 654  
 plane-wave, 630  
 solution of, 633
- Dynamics, 9  
 of three-dimensional crystals, 484
- E* maps, interpretation of, 232
- Edgeworth approximation, 21
- Edgeworth series, 103
- EDSA (electron-diffraction structure analysis), 356
- Effect of centring, 196
- Effective absorption coefficient, 628
- Effective potential-energy function, 581
- Effects of symmetry on the Fourier image, 114
- Eigenspace decomposition of  $L^2$ , 37
- Eigenvalue, 649
- Eigenvalue decomposition, 436
- Eigenvalues and eigenvectors of orthogonal matrices, 425
- Einstein model, 486
- Elastic component of X-ray scattering, 10
- Elastic constants, measurement of, 490
- Elastic diffuse scattering, 492
- Electromagnetic electron lenses, 299, 303
- Electron band theory of solids, 629
- Electron crystallography, 388  
 direct phase determination, 388  
 of polymers, 583  
 of proteins, 389  
 three-dimensional structure determination by, 391
- Electron density, 2, 8, 15, 115, 290  
 averaged, 274  
 real-space averaging of, 259, 273
- Electron-density calculations, 74
- Electron-density maps, Fourier synthesis of, 91
- Electron diffraction, 540  
 absorption in, 362  
 sign conventions, 301–302
- Electron-diffraction data  
 for crystal-structure determination, 583  
 three-dimensional, 391, 585
- Electron-diffraction patterns  
 geometric theory of, 359  
 polycrystal, 358  
 single-crystal, 356  
 texture, 357, 394
- Electron-diffraction structure analysis (EDSA), 356
- Electron distribution, atomic, radial dependence of, 12
- Electron lenses, electromagnetic, 299, 303
- Electron-magnetization distribution, 11
- Electron micrographs  
 Fourier transform of, 393, 584  
 phase information from, 390
- Electron-microscope image contrast, 542
- Electron-microscope imaging, 541
- Electron tomography, 377, 382
- Electronic analogue computer X-RAC, 76
- Electronic structure, 9
- Electrons, interaction with matter, 299
- Electrostatic energy, 449, 463
- Electrostatic potential, 2, 461
- Electrostatic properties of molecular surfaces, 438
- Embedding method, *n*-dimensional, 591
- Enantiomer, 286
- Enantiomeric ambiguity, 247
- Enantiomorph definition, 231
- Enantiomorphic images, weak, 247
- Enantiomorphic solutions, 246
- Energy minimization, 437, 440, 442
- Entire functions, 36
- Entrance surface, 639
- Entropy, 94
- Envelope, 258
- Envelope functions, 305
- Epitaxial orientation techniques, 583
- Equal-amplitude assumption, 580
- Equal distribution, 45
- Equivalent matrix groups, 176
- Equivalent reflections, 285
- Error matrix, atomic, 416
- Error propagation, 411
- Errors, 289  
 root-mean-square, 291  
 systematic, 408
- Essential bounds, 45
- Essentially bounded function, 27
- Euclidean algorithm, 48, 56, 66
- Euclidean norm, 25
- Euclidean space, 25
- Euler gamma function, 463
- Euler spline, 477
- Eulerian angles, 262, 420
- Eulerian space, 263
- Eulerian space groups, 263  
 rotation-function, 265
- Eulerian symmetry elements, 264
- Even (cyclic) permutation of coordinates, 118, 122
- Ewald method, 458
- Ewald potential, 466
- Ewald result, 449
- Ewald sum surface term, 467
- Ewald wave, 628
- Exchange between differentiation and multiplication by monomials, 102
- Exchange between multiplication and convolution, 25
- Excitation error, 647
- Excitations  
 bulk plasmon, 300  
 inner-shell, 300  
 interband, 300  
 intraband, 300
- Explicit-origin space-group notation, 127
- Explicit space-group symbols, 123–124
- Exploration of parameter space by molecular model building, 576
- Exponential coefficient, 13
- Exsolution, 505
- Extended resolution, 274
- Extended structures, 445
- External fields, effect on neutron scattering, 659
- External modes, 486
- Extinction, 638  
 dynamical, 319, 323–324, 333, 335
- Extinction distance, 632–633
- Extinction factors, 658
- $F_{\text{HLE}}$ , 288
- $F_{\text{HUE}}$ , 288
- Face-centred lattices, 90
- Face-diagonal axes, 128
- Factor group, 69, 71
- Factorization, 78
- False centre of symmetry, 115
- Fast Fourier Poisson method, 475, 478
- Fast Fourier transform (FFT), 77  
 three-dimensional (3DFFT), 475–476
- Fast rotation function, 268
- Feedback method, 253
- Fejér kernel, 46, 464  
 spherical, 64
- Fermi pseudo-potential, 654
- Fermi surface, 545
- FFT (fast Fourier transform), 77  
 three-dimensional (3DFFT), 475–476
- Fibonacci chain, 595
- Fibonacci sequence, 594
- Fibre axis, 568
- Fibre diffraction, 41, 576  
*R* factor, 582  
 specimens for, 568  
 X-ray, 567
- Fibres  
 axially periodic, transform of, 101  
 disordered, 568  
 macromolecular, 581  
 noncrystalline, 568, 570, 576  
 partially crystalline, 572  
 polycrystalline, 568, 570, 576
- Field emission gun, 307
- Figures of merit, 232, 290
- Films  
 freely suspended, 554  
 smectic, 554
- Filtered backprojection, 371
- Filtered image, 364
- Filtering  
 iterative low-pass, 575  
 rotational, 365
- Finite crystal of point charges, 465
- Finite field, 55
- Finite space group, 177
- Finite spherical crystal, 469
- First Brillouin zone, 178
- First-order Born approximation, 10, 300
- First-order perturbation theory, 411
- Flagpole, 183
- Flexible chains, 436
- Flexible rings, 436
- Flight time, neutron, 660
- Flipping ratio, 658
- Focusing of neutron beams, 660
- Force-constant matrix, atomic, 485
- Form factor, 63  
 aspherical-atom, 14  
 atomic, 10  
 atomic, X-ray, 293  
 geometric, 605  
 Kikuchi-line, 543
- FORTRAN, 122
- FORTRAN interface, 122
- FORTRAN interpreter, 122
- Forward convolution theorem, 44, 64–65, 75
- Forward scattering, 647
- Forward-scattering approximation, 301
- Four-dimensional vector, 424
- Fourier analysis, 63  
 and filtration in reciprocal space, 364
- Fourier approach, 212
- Fourier–Bessel series, 209
- Fourier–Bessel structure factors, 569
- Fourier coefficients, 46, 283, 464
- Fourier convolution theorem, 10
- Fourier cotransform, 35
- Fourier cotransformation, 41
- Fourier expansion, 2  
 of dielectric susceptibility, 627
- Fourier images, 114, 306  
 effects of symmetry on, 114
- Fourier inversion, direct, 370
- Fourier map, 283
- Fourier method, 207  
 Agarwal's FFT implementation of, 98  
 Cochran's, 96  
 Cruickshank's modified, 97
- Fourier representation, 293
- Fourier series, 24  
 convergence of, 45  
 convolution of, 44  
 digital electronic computation of, 76  
 electron density and its summation, 63  
 partial sum of, 46
- Fourier shell correlation (FSC), 384–385
- Fourier space, 116  
 symmetry in, 120
- Fourier summations, 116  
 space-group-specific, 116

## SUBJECT INDEX

- Fourier synthesis, 63, 286, 290  
     best, 290  
     of electron-density maps, 91  
 Fourier-transform space, 450  
 Fourier transformation  
     discrete, 47  
     inverse, 36, 41  
     mathematical theory of, 24  
 Fourier transforms, 24, 35, 450  
     crystallographic applications, 62  
     crystallographic, discrete, 77  
     crystallographic, theory of, 62  
     discrete, 24  
     discrete, core of matrix, 83  
     discrete, matrix representation of, 51  
     discrete, numerical computation of, 52  
     discrete, properties of, 51  
     exchange of subdivision and decimation, 49  
     in  $L^1$ , 35  
     in  $L^2$ , 37  
     in polar coordinates, 101  
     in  $\mathcal{F}$ , 37  
     inverse, 8  
     kernels of, 35  
     of a distribution, 39  
     of a Gaussian, 463  
     of B-splines, 477  
     of density, 478  
     of electron micrographs, 393, 584  
     of periodic distributions, 42  
     of tempered distributions, 39–40  
     tables of, 39  
     tensor product property of, 76  
     various writings of, 39  
*FpStudio*, 443–445  
 Fractal atomic surface, 597  
 Fractal sequence, 598  
 Fractional coordinates, 42, 63, 262  
 Fréchet space, 28  
 Freely suspended films, 554  
 Fresnel reflection law, 554  
 Friedel equivalent, 282, 285  
 Friedel pair, 285  
 Friedel's law, 64, 73, 75, 255, 299  
 Frobenius congruences, 71, 73  
*Frodo*, 441  
 FSC (Fourier shell correlation), 384–385  
 Fubini's theorem, 27, 35, 39  
 Function spaces  
     associated actions in, 69  
     topology in, 27  
 Functional derivative, 99  
 Functions of polynomial growth, 41  
 Fundamental domain, 68–70, 72  
 Fundamental equations of dynamical theory, 628  
 Fundamental region, 178  
 Fundamental relationships, 3  
 Fused-ring systems, 442  
  
*G*-invariant function, 70  
 Gamma distribution, 201  
 Gamma functions, 450  
     Euler, 463  
     incomplete, 450, 454  
 Gamma radiation, 293  
 Gauss' law, 461  
 Gaussian atomic densities, 39  
 Gaussian atoms, 72–73, 93  
     anisotropic, 63  
 Gaussian charge distributions, 461, 471–472  
 Gaussian density, sampling of, 479  
 Gaussian distribution, 290  
 Gaussian function, 39  
     standard, 38, 41  
 Gaussian plane, general, 413  
 Gaussian weights, 413  
 Gaussians, 99  
     compact, 472  
     Coulombic interactions between, 459  
     diffuse, 472  
     Fourier transform of, 463  
     interacting spherical, lattice sums of, 471  
     normalized, 472  
 General conditions for possible reflections, 115  
 General Gaussian plane, 413  
 General  $\mathbf{k}$  vector, 178  
 General linear change of variable, 35  
 General multivariate Gaussians, 38  
 General reflections, average intensity of, 195  
 General superposition, 422  
 General topology, 27  
 General transformation, 423  
 General translation function, 269  
 Generalized multiplexing, 88  
 Generalized Patterson function, 494  
 Generalized Rader/Winograd algorithms, 90  
 Generalized structure-factor formalism, 22  
 Generalized support condition, 34  
 Geometric form factor, 605  
 Geometric redundancies, 66  
 Geometric structure factors, 116–117, 135  
 Geometric theory of electron-diffraction patterns, 359  
 Gibbs phenomenon, 46, 64  
 GKS (Graphical Kernel System), 419  
 GKS-3D (Graphical Kernel System for Three Dimensions), 419  
 Global crystallographic algorithms, 89  
 Global minimum, 437–438  
 Glyceraldehyde-3-phosphate dehydrogenase, 259, 273–274  
 Good algorithm, 54  
 Good factorization, multidimensional, 82  
 Goodness of fit, 416  
 Gram–Charlier series, 20, 103  
 Gram–Schmidt process, 425, 437  
*GRAMPS*, 439  
 Graphical Kernel System (GKS), 419  
 Graphical Kernel System for Three Dimensions (GKS-3D), 419  
 Graphics, 418  
     standards for, 419  
 Gravity, 660–661  
 Green's theorem, 32, 93  
*GRETEP*, 443–445  
 Gridding method, 373  
*GRIP*, 440  
 Group actions, 68, 77  
     crystallographic, 79  
     crystallographic, real space, 71  
     crystallographic, reciprocal space, 72  
 Group characters, 89  
 Group cohomology, 80  
 Group extensions, 71  
 Group of units, 52  
 Group ring  
     integral, 79  
     module over, 24  
 Group–subgroup relationship, 118  
 Groups, 68  
*Guide*, 441  
  
 Haemoglobin, 251–252, 282, 287  
     horse, 252  
 Hall symbols, 123, 127, 130  
     in data handling, 123  
     in software, 123  
 Handedness, 333  
 Hankel transform, 101  
 Hardy's theorem, 39  
 Harker diagram, 257, 283, 290  
 Harker lines, 249  
 Harker peaks, 76  
 Harker planes, 249  
     special, 249  
 Harker sections, 248–249  
 Harmonic approximation, 484  
 Harmonic density modulation, 601  
 Harmonic displacive modulation, 601  
 HDD (high-dispersion diffraction), 356  
 Heavy-atom-derivative data sets, scaling of, 255  
 Heavy-atom derivatives, 287  
 Heavy-atom distribution, 288  
 Heavy-atom location, 249  
     three-dimensional methods, 252  
 Heavy-atom lower estimate, 257  
 Heavy-atom parameters, 289  
 Heavy-atom sites, 251  
  
 Heavy-atom substitution, 255  
 Heavy atoms, 286  
 HEED (high-energy electron diffraction), 356  
 Heisenberg's inequality, 39, 91  
 Helical structures, 518  
     diffraction by, 100, 568  
 Helical symmetry, 101, 375, 569, 576  
     approximate, 570  
 Helix repeat units, 569  
 Hermann–Mauguin space-group symbol, 119  
 Hermite coefficients, 476  
 Hermite function, 38, 103  
     multivariate, 38, 99  
 Hermite Gaussians, 473  
     normalized, 473  
 Hermite polynomials, three-dimensional, 21  
 Hermitian-antisymmetric transforms, 87  
 Hermitian form, 44  
 Hermitian symmetry, 64, 74, 85  
 Herringbone packing, 560  
 Hexagonal axes, 118  
 Hexagonal family, 118  
 Hexagonal space groups, 90, 119  
 Hexatic phase, 555–556  
     in two dimensions, 555  
     tilted, 556  
 Hexatic-B phase, 558  
 Hexokinase, 273  
 Hidden-line algorithms, 434  
 Hidden-surface algorithms, 434  
 High-dispersion diffraction (HDD), 356  
 High-energy electron diffraction (HEED), 356  
 High-resolution electron diffraction (HRED), 356  
 High-resolution electron microscopy (HREM), 360  
 High-voltage limit, 652  
 Higher angular momentum charge distributions, 473  
 Higher-order Laue zone (HOLZ) reflections, 308, 335  
 Highlighting, 434  
 Hilbert space, 27, 35, 47  
 Hologram, in-line, 307  
 Holohedral point group, 179  
 Holosymmetric space group, 180  
 HOLZ (higher-order Laue zone) reflections, 308, 335  
 Homogeneous coordinates, 418, 421  
 Homogeneous symmetric polynomial, 652  
 Homometric pair, 246  
 Homometric structures, 246  
 Homomorphism, 176  
 Horse haemoglobin, 252  
 HRED (high-resolution electron diffraction), 356  
 HREM (high-resolution electron microscopy), 360  
 Hybridization, 442  
*HYDRA*, 441  
 Hydrogen bonding, 439, 441–442  
 Hydrophobic properties of molecular surfaces, 438  
 Hyperatoms, 592  
 Hypercrystal, 590, 592  
 Hypersymmetric distributions, 201  
 Hypothetical atoms, 94  
  
 Icosahedral phase, 613  
 Icosahedral point groups, 353  
 Icosahedral quasicrystals, 352  
 Ideal acentric distributions, 200  
 Ideal aperiodic crystal, 590  
 Ideal centric distributions, 200  
 Ideal crystal, 176, 590  
 Ideal probability density distributions, 200  
 Idempotents, 54  
 Image averaging in real space, 364  
 Image contrast, electron-microscope, 542  
 Image detection, 249  
 Image enhancement, 361, 363  
 Image intensity, bright-field, 362  
 Image of a function by a geometric operation, 26  
 Image processing in transmission electron microscopy, 361  
 Image reconstruction, 361  
 Image resolution, 306  
 Image restoration, 361–362  
 Images  
     asymmetric, 365  
     filtered, 364  
     Fourier, 306

## SUBJECT INDEX

- with point symmetry, 365
- Immunoglobulin, 271
- Implication theory, 248
- Implicit function theorem, 33
- Implied connectivity, 435
- Improper rotation axes, 258
- Improper rotations, 123, 128
- In-line hologram, 307
- Incident wave, departure from Bragg's law, 630
- Incoherent inelastic scattering, 488
- Incoherent scattering, 488
- Incommensurability, 550
- Incommensurate crystal structures, display of, 445
- Incommensurate intergrowth structure, 593
- Incommensurately modulated structures, 344, 591
- Incomplete gamma function, 450, 454
  - complement of, 450–451
  - evaluation of, 454
- Independence, assumption of, 209
- Index, 68
- Index of refraction, 628
- Indicator functions, 32, 42, 47, 65, 91–92
- Induction formula, 105
- Inductive limit, 30
- Inelastic component of X-ray scattering, 10
- Inelastic scattering, 300, 540
  - neutron, 488
  - X-ray, 490
- Inequalities among structure factors, 221
- Inner-shell excitations, 300, 542
- Insight*, 439
- Insight II*, 442
- Instrumental resolution, 307
- Integral group ring, 79
- Integral representation, 68
  - theory, 71
- Integrals
  - Lebesgue, 26
  - Riemann, 26
- Integrated intensity, 637–638, 640
- Integration
  - by parts, 31
  - Lebesgue's theory of, 28
  - of anomalous-dispersion techniques with direct methods, 237
  - of distributions, 32
  - of isomorphous replacement techniques with direct methods, 236
- Intensities of diffraction beams, 358
- Intensities of plane waves
  - in reflection geometry, 638
  - in transmission geometry, 634
- Intensities of reflected and refracted waves, 634
- Intensity differences, 285
- Intensity statistics, 105
- Interaction between symmetry and decomposition, 78
- Interaction between symmetry and factorization, 79
- Interaction matrix, 249
- Interaction of electrons with matter, 299
- Interaction of X-rays with matter, 626
- Interatomic covariance, 411
- Interatomic vectors, 65
- Interband excitation, 300
- Interference function, 65
  - spherical, 261
- Interferometry, neutron, 660
- Intermolecular correlations, 525
- Intermolecular force fields, 458
- Internal modes, 486
- Interpolation, 368
- Interpolation formula, 47
- Interpolation kernel, 92
- Interpolation of trigonometric functions, 478
- Interpretation of  $E$  maps, 232
- Intraband excitation, 300
- Intramolecular energy terms, 455
- Intrinsic component of translation part of space-group operation, 116
- Invariance of  $L^2$ , 37
- Inverse Fourier transform, 8
- Inverse Fourier transformation, 36, 41
- Inverse rotation operator, 114
- Ionic crystal, electrostatic energy of, 449
- Irreducible matrix group, 176
- Irreducible representations (irreps), 175
  - type of, 181
- Ising model, 68
- Isometry, 37
- Isometry property, 37
- Isomorphism, 176, 290–291
  - lack of, 255
- Isomorphous addition, 283
- Isomorphous crystals, 283
- Isomorphous differences, 288, 291
- Isomorphous heavy-atom derivatives, 580
- Isomorphous replacement, 251, 282
  - difference Patterson functions, 251, 253
  - multiple, 290
  - single, 252, 283
  - techniques, integration of direct methods with, 236
- Isomorphous synthesis, 283
- Isotropic harmonic oscillator, three-dimensional, 17
- Isotropic temperature factors, 73
- Isotropy subgroups, 68, 72
- Iterative low-pass filtering, 575
- Jacobians, 33, 51
- Joint probability distribution of structure factors, 105
- Juxtaposition of chains, 578
- k** vector
  - general, 178
  - special, 178
  - uni-arm, 181
- k**-vector type, 180
- Kernels, 58
  - Cauchy, 46
  - de la Vallée Poussin, 46
  - Dirichlet, 46
  - Fejér, 46, 464
  - interpolation, 92
  - of Fourier transformations, 35
  - Poisson, 46
  - spherical Dirichlet, 64, 91
  - spherical Fejér, 64
- Kikuchi-line contrast, 543
- Kikuchi-line form factor, 543
- Kinematical approximation, 62, 300–301, 359, 394, 583, 658
- Kinematical diffraction formulae, 302
- Kinematical diffraction intensities, 302
- Kinematical  $R$  factor, 584
- Kinematical scattering, 300
- Klug peaks, 267
- Known structural fragment, use of, 272, 389
- Kronecker symbol, 5
- '*Kubic harmonics*', 12
- $L^p$  spaces, 26
- LACBED (large-angle convergent-beam electron diffraction), 345
- Lack of isomorphism, 255
- Lagrange multiplier, 95, 106, 414
- Lagrange's theorem, 68
- LALS*, 578
- Lamellar domains with long-range order, 505–506
- Landau–Peierls effect, 551–552
- Langmuir troughs, 583
- Languages
  - computer-algebraic, 122
  - numerically and symbolically oriented, 117
- Laplace's equation, 468
- Large-angle convergent-beam electron diffraction (LACBED), 345
- Large values of  $\mu_{ot}$ , 641
- Larmor precession, 655
- Lattice, 42
  - base-centred, 90
  - body-centred, 90
  - centred, 73
  - composite, 449, 452
  - direct, 2, 5, 42, 121, 177, 450
  - face-centred, 90
  - nonprimitive, 71
  - nonstandard, 42
  - nonstandard period, 43
  - one-dimensional, 552
  - period, 42, 62, 68
  - primitive, 71
  - reciprocal, 2, 5, 43, 48, 62, 121, 177
  - residual, 48
  - rhombohedral, 90
  - standard, 42
- Lattice disorder, 572
  - correlated, 573
- Lattice distributions, 43–44, 47–48
- Lattice-dynamical model, 484
- Lattice energy, 458
  - Coulombic, 449, 453
- Lattice mode, 71
- Lattice-parameter mapping, 626
- Lattice plane, 2, 406
- Lattice sums, 44, 460
  - of interacting spherical Gaussians, 471
- Lattice transform, 450
- Lattice-translation subgroup, 123
- Lattice type, 123
- Laue case, 631
- Laue equations, 2
- Laue groups, 115
- Laue point, 630
- Laue scattering, 520
- Layer lines, continuous diffraction on, 575
- Lead, 287
- Least resolvable distance, 306
- Least-squares adjustment of observed positions, 413
- Least-squares approximation of trigonometric functions, 478
- Least-squares determination of phases, 233
- Least-squares method, multivariate, 95
- Least-squares plane, 410
  - proper, 413
- Least-squares refinement, 289
- Lebesgue integral, 26
- Lebesgue's theory of integration, 28
- LEED (low-energy electron diffraction), 356
- Left action, 68, 70, 72, 79
- Left cosets, 68
- Left representation, 72
- Legendre polynomials, 468
- Leibnitz's formula, 451
- Length of a function, 26
- Length of a vector, 404
- Lennard–Jones potential, 490
- L'Hospital's rule, 451
- Libration, 18
- Libration tensor, 18
- Librational–librational correlations, 525
- Lifshitz point, 553
- Lifshitz's reformulation, 98
- Lindeberg–Lévy version of the central-limit theorem, 204
- Line drawings, 433
- Linear absorption coefficient, 628
- Linear change of variable, general, 35
- Linear forms, 30
- Linear functionals, 28
- Linear scaling of computational cost of Ewald direct sum, 474
- Linear transformation, 7
- Linearity, 35, 51
- Linearization formulae, 75
- Linearly semidependent phases, 216
- Linked-atom least-squares (*LALS*) system, 578
- Liouville's theorem, 37
- Liquid crystals, 547
- Lissajous curve, 105
- Little co-group, 178, 180
- Little group, 178
- Local ordering, 518
- Locally integrable functions, 30
  - distributions associated with, 30
- Locally summable function of polynomial growth, 40
- Location-dependent component of translation part of space-group operation, 116
- Locked rotation function, 267–268
- Locked translation function, 271
- Logical connectivity, 435
- London dispersion interactions, 475
- Lone pairs, 442



## SUBJECT INDEX

- Long-range order (LRO), 505, 548  
   positional, 547  
 Longitudinal disorder, 516  
 Lorentz point, 630  
 Low-angle scattering, 508  
 Low-energy conformational changes, 582  
 Low-energy electron diffraction (LEED), 356  
 LRO (long-range order), 548  
   positional, 547  
 Lyotropic phase, 548  
 Lysozyme, 252
- MACCS*, 442  
 Macromolecular crystallography, 282  
   direct methods in, 235  
 Macromolecular fibre structures, 581  
 Macromolecular refinement techniques, 99  
 Macromolecular structures, direct determination of, 583  
 Macroscopically spherical crystal, 467  
 Madelung constant, 449  
 Magic-integer methods, 233  
 Magnetic crystal structures, display of, 445  
 Magnetic domains, 661  
 Magnetic scattering, 11, 656  
 Main reflections, 592  
 Manganese, 286  
 Many-beam case, 629  
 Mapping, 25  
 Maschke, theorem of, 176  
 Mathematical theory of Fourier transformation, 24  
 Matrices of mixed scalar products, 8  
 Matrix algebra, 262  
 Matrix-column pair, 177  
 Matrix groups, 176  
   completely reducible, 176  
   equivalent, 176  
   irreducible, 176  
   reducible, 176  
   unitary, 176  
 Matrix part, 177  
 Matrix representation, 114  
   of discrete Fourier transform, 51  
 Maximum determinant rule, 228  
 Maximum entropy, 106, 392  
 Maximum-entropy distributions, 36  
   of atoms, 106  
 Maximum-entropy methods, 102, 234  
 Maximum-entropy theory, 106  
 Maximum function, 250  
 Maximum likelihood, 392  
 Maxwell's equations, 627, 643  
 MBD (microbeam diffraction), 356  
 McMurchie–Davidson recursion, 475  
 MDIR (multidimensional isomorphous replacement), 579  
*MDKINO*, 439  
 Mean-field theory, 549  
 Mean-square displacement amplitude, 443  
 Mean values, 408  
 Mechanical pressure tensor, 470  
 Meijer's *G* function, 201  
 Mercury, 287  
*Mercury*, 443–444  
 Mesomorphic structures, scattering from, 547  
 Metric  
   direct, 4  
   reciprocal, 4  
 Metric space, 25, 27  
 Metric tensors, 4–5  
 Metrizable topology, 25  
 Metrizable topology, 28  
 Micelle, 547  
 Microanalysis, 298–299  
 Microbeam diffraction (MBD), 356  
 Microdiffraction, 544–545  
*MIDAS*, 439  
 Middle of reflection domain, 631  
 Minima  
   global, 437–438  
   multiple, 437  
   potential-energy, 437  
 Minimal domain, 179  
 Minimization function, 289
- Minimum function, 250  
 MIR (multiple isomorphous replacement), 290  
   phases, 259  
 Mirror image, 285  
*MM2/MMP2*, 442  
*MMS-X*, 440  
 Modelling of diffuse scattering, 528  
 Modelling transformations, 431  
 Modified tangent formula, 233  
 Modulated phases, 550  
 Modulated smectic-A phase, 553  
 Modulated smectic-C phase, 553  
 Modulated structure, 591  
 Modulation function, 591  
 Module, 79  
   over a group ring, 24  
*Molbuild*, 442  
 Molecular averaging by noncrystallographic symmetry, 92  
 Molecular axis, 568  
 Molecular dynamics, 442  
 Molecular-dynamics refinement, 581  
 Molecular envelope, 32, 65, 92–93  
 Molecular mechanics, 437  
 Molecular model building, 577  
 Molecular modelling, 6, 418  
 Molecular orientational order, 547  
 Molecular origin, 273  
 Molecular replacement, 244, 258, 272, 274, 292  
   real-space, 273  
 Molecular rotation, 558  
 Molecular structure, position of a known, 270  
 Molecular surfaces, hydrophobic and electrostatic properties of, 438  
*MolXtl*, 443–444  
 Moment-generating functions, 36, 102  
 Moment-generating properties, 102  
   of  $\mathcal{F}$ , 67  
 Moments of a distribution, 102  
 Monochromators, 660  
   polarizing, 658  
 Monoclinic family, 118  
 Monoclinic space groups, 89, 118  
 Mosaic crystals, 626  
 Mosaic model, 659  
 Mosaicity, 356  
 Motif, 42–44  
 Motif distribution, 63  
 Multicritical point, 553  
 Multidimensional algorithms, 58  
 Multidimensional Cooley–Tukey factorization, 58–59, 79  
 Multidimensional factorization, 58  
 Multidimensional Good factorization, 82  
 Multidimensional isomorphous replacement (MDIR), 579  
 Multidimensional prime factor algorithm, 59  
 Multidimensional structure, 437  
 Multigrid method, 480  
 Multi-index, 26, 36, 38  
 Multi-index notation, 26  
 Multiple diffuse scattering, 542  
 Multiple isomorphous replacement (MIR), 290  
   phases, 259  
 Multiple minima, 437  
 Multiple reciprocal cell, 121  
 Multiple scattering, 540  
 Multiple simultaneous superposition, 425  
 Multiple-wavelength method, 293  
 Multiplexing, generalized, 88  
 Multiplexing–demultiplexing, 85  
 Multiplication by a monomial, 25  
 Multiplication of distributions, 32  
 Multiplicative group of units, 56  
 Multiplicative reindexing, 61  
 Multiplicity, 116, 180  
 Multiplicity corrections, 251  
 Multiplier functions, 41  
 Multipliers, 44  
   Lagrange, 95, 106, 414  
 Multipoles, rotation of, 475  
 Multireference alignment, 382  
 Multi-Slater determinant wavefunction, 15  
 Multislice, 306, 651
- calculations, 544  
   computer programs, 544  
   recurrence relation, 651  
 Multivariate Gaussian, 44  
 Multivariate Hermite functions, 38, 99  
 Multivariate least-squares method, 95  
 Mutually reciprocal bases, 2–3  
   computational and algebraic aspects of, 4  
 Mutually reciprocal triads, 2  
 Myoglobin, 252, 282, 287
- n*-dimensional embedding method, 591  
*n*-shift rule, 98  
*n*-torus  
   nonstandard, 42  
   standard, 42  
 Natural coordinate system, 404  
 Negative peaks, 252  
 Nematic order  
   biaxial, 549  
   uniaxial, 549  
 Nematic phase, 547, 549  
 Nested algorithms, 62  
 Nested neighbourhood principle, 223  
 Nesting, 61  
   of Winograd small FFTs, 60  
 Net distortions, 517  
 Neutral unit cell, 461  
 Neutron absorption, 655  
 Neutron beams, focusing of, 660  
 Neutron crystallography, 293  
 Neutron diffraction, 560  
   dynamical theory of, 654  
 Neutron flight time, 660  
 Neutron interferometry, 660  
 Neutron refraction, 654  
 Neutron scattering  
   effect of external fields, 659  
   inelastic, 488  
   very small angle, 660  
 Neutron scattering lengths, 293  
 Neutron spin, 655  
 Neutron topography, 661  
 Neutrons, 293  
   thermal, 293  
 Nodes of standing waves, 633  
 Non-absorbing case, 629  
 Non-absorbing crystals, 637–639  
   comparison of dynamical and geometrical theory, 640  
 Nonbonded interatomic distances, 578  
 Noncrystalline fibres, 568, 570, 576  
 Noncrystallographic asymmetric unit, 253  
 Noncrystallographic rotation elements, translational components of, 258  
 Noncrystallographic symmetry, 66, 258  
   apparent, 267  
   molecular averaging by, 92  
   phase improvement using, 273  
   proper, 258  
   rotational, 260  
 Noncrystallographic symmetry element, position of, 270–271  
 Non-cyclic (odd) permutation of coordinates, 118, 122  
 Non-ideal distributions, 203, 207  
 Non-ideal probability density functions, 212  
   of  $|E|$ , 205  
 Non-independent variables, 199  
 Nonlinear transformations, 264  
 Nonperiodic system, 503  
 Nonprimitive lattice, 71  
 Non-spin-flip scattering lengths, 657  
 Nonstandard coordinates, 42  
 Nonstandard lattice, 42  
 Nonstandard *n*-torus, 42  
 Nonstandard period lattice, 43  
 Norm  
   Euclidean, 25  
   on a vector space, 28  
 Normal equations, 95  
 Normal matrix, 98  
 Normal subgroup, 68–69  
 Normalization constant, 290, 293

## SUBJECT INDEX

- Normalized Gaussians, 472  
 Normalized Hermite Gaussians, 473  
 Normalized structure factors, 216, 231, 246  
 Normalizer, 69  
 Normed space, 28  
   complete, 28  
 Notation, multi-index, 26  
 Nuclear matter, density of, 2  
 Numerical computation of discrete Fourier transform, 52  
 Numerically oriented languages, 117  
 Nussbaumer–Quandalle algorithm, 60
- O*, 441  
 Observation plane, 361  
 Observational equations, 95  
 Obverse setting, 121  
 Occupancy factors, 289  
 Occupied natural spin orbitals, 15  
 Odd (non-cyclic) permutation of coordinates, 118, 122  
 Offset, 53  
 OLEX, 443–445  
 One-centre orbital products, 15  
 One-centre terms, 15  
 One-dimensional lattice, 552  
 One-particle potential (OPP) model, 22  
 One-phase structure seminvariants, 231  
   first rank, 229  
 Operational calculus, 28  
 Operations on distributions, 31  
 OPP (one-particle potential) model, 22  
 Optic modes, 486  
 Optical diffractometer, 364  
 Optical isomers, 286  
 Optical rotation, 286  
 Optimal defocus, 361  
 Optimization, 436  
 Orbit decomposition, 69, 72, 74–75  
   formula, 69, 73  
 Orbit exchange, 70, 77–78  
 Orbit of  $\mathbf{k}$ , 178  
 Orbital products, 15  
   one-centre, 15  
   two-centre, 17  
 Orbits, 68, 72–73  
 Order–disorder, 507  
 Order parameter, 549  
 Orientational disorder, 524  
 Origin-shift vector, 123  
 Origin-to-plane distance, 410, 414  
 Origin(s)  
   allowed (permissible), 215  
   definition, 231  
   molecular, 273  
   removal from a Patterson function, 245  
   selection, 247  
   specification, 215  
 Ornstein–Zernike correlation function, 514  
 ORTEP, 438  
 ORTEP-3 for Windows, 443–444  
 ORTEP-III, 443–444  
 ORTEX, 443–444  
 Orthogonal matrices, 419  
   eigenvalues and eigenvectors of, 425  
 Orthogonalization, 262  
 Orthographic projection, 427–428  
 Orthorhombic space groups, 89, 118  
*Oscail X*, 443–444  
 Overlap between two Pattersons, 260
- $P_s(\mathbf{u})$  function, 256  
 Pair probability, 504  
   conditional, 504  
 Pairwise sum, 449  
 Paley–Wiener theorem, 36, 106  
 Parabolic equation, 648  
 Parallel processing, 61  
 Parity of the  $hkl$  subset, 119  
 Parseval–Plancherel property, 52  
 Parseval–Plancherel theorem, 37, 47  
 Parseval’s identity, 64, 67  
 Parseval’s theorem, 35, 95, 450  
   with crystallographic symmetry, 74
- Partial dislocations, 558  
 Partial net atomic charges, 449  
 Partial sum of Fourier series, 46  
 Partially bicentric arrangement, 212  
 Partially crystalline fibres, 572  
 Partially reflected wavefield, 639  
 Partially transmitted wave, 639  
 Particle–particle particle–mesh method, 475  
 Patterson function(s), 64–65, 75, 244, 289, 541, 577  
   anomalous-dispersion, 257  
   constraints on interpretation of, 258  
   cylindrically averaged, 577  
   deconvolution of, 249  
   difference, 253–254  
   generalized, 494  
   interactions in, 244  
   isomorphous difference, 253  
   origin removal, 245  
   overlap between two, 260  
   second kind, 247  
   sharpened, 245–246  
   superposition, 250  
   symmetry of, 244  
   three-dimensional, 577  
 Patterson map, automated search, 389  
 Patterson peaks, 244  
 Patterson search, 254  
 Patterson synthesis, 283, 286–287  
 Patterson techniques, 6, 293  
 Patterson vector interactions, 248  
 PEANUT, 443–444  
*Pendellösung*, 303, 632, 635–636, 659–660  
   spherical-wave, 641  
*Pendellösung* distance, 632–633  
 Penetration depth, 638  
 Penrose rhomb, 610  
 Penrose tiling, 609  
 Pentagonal point groups, 354  
 Period decimation, 48  
 Period lattice, 42, 62, 68  
   nonstandard, 43  
 Period matrix, 43  
 Period subdivision, 48  
 Periodic boundary conditions, 479, 485  
 Periodic continuation, 544  
 Periodic delta functions, 211  
 Periodic density function, 114  
 Periodic distributions, 42, 44, 62  
   and Fourier series, 42  
   Fourier transforms of, 42  
 Periodic images, 460  
 Periodic lamellar domains, 502  
 Periodic weak phase objects, 364  
 Periodicity, 176  
   crystal, 62  
 Periodicity requirement, 9  
   and sampling, duality between, 44  
 Periodograms, 378  
 Permissible origins, 215  
 Permissible symmetry, 114  
 Permutation of coordinates  
   cyclic (even), 118, 122  
   non-cyclic (odd), 118, 122  
 Permutation operators, 118  
 Permutation tensors, 405  
 Perpendicular (internal, complementary) space, 592  
 Perspective, 418, 426–428, 434  
 Perturbation theory, first-order, 411  
 Phase angles, 282–283  
 Phase change, 286  
 Phase circles, 283  
 Phase determination, 283  
   *ab initio*, 273  
   direct, 36  
   direct, in electron crystallography, 388  
   statistical theory of, 104  
 Phase-determining formulae, 221  
 Phase evaluation, 282, 291, 293  
 Phase extension, 274  
 Phase-grating approximation, 652  
 Phase improvement, 274  
   using noncrystallographic symmetry, 273
- Phase information, 292  
   from electron micrographs, 390  
 Phase invariant sums, 389  
 Phase-object approximation, 301, 542  
 Phase problem, 576  
   Bayesian statistical approach, 106  
 Phase relationships  
   quartet, 225  
   quintet, 227  
 Phase restriction, 73  
 Phase shift, 25, 53  
 Phase transformations, polytypic, 514  
 Phases  
   assignment of one or more, 231  
   best, 290  
   from multiple isomorphous replacement, 259  
   from single isomorphous replacement, 253  
   least-squares determination of, 233  
   linearly semidependent, 216  
   refinement of, 233  
 Phason flips, 611  
 Phasons, 527  
 Phenomenological absorption coefficients, 303  
 PHIGS (Programmers’ Hierarchical Interactive Graphics System), 419  
 Phonon absorption, 488  
 Phonon dispersion relations, 489  
 Phonon emission, 488  
 Phonon scattering, 543  
 Phonons, 484  
 Physical (external, parallel) space, 592  
 Picture space, 426–428, 434  
 Pipelining, 61  
 Pisot numbers, 595  
 Pixel, 432  
 Plancherel’s theorem, 41  
 Plane of polarization, 286  
 Plane-wave dynamical theory, 630  
 Planes, 406  
   Gaussian, general, 413  
   least-squares, 410  
   least-squares, proper, 413  
 Plasmon scattering, 541  
 Plasmons  
   bulk, excitation of, 300  
   surface, 300  
*Platon*, 443–444  
*PLUTO*, 439  
*Pluton*, 444  
 Point charges, finite crystal of, 465  
 Point density, 610  
 Point-group determination by convergent-beam electron diffraction, 307  
 Point-group operators, 115, 123  
 Point-group symmetry of reciprocal lattice, 114  
 Point groups, 177  
   average multiples for, 197  
   closed, 258  
   decagonal, 354  
   holohedral, 179  
   icosahedral, 353  
   pentagonal, 354  
 Point multipoles, 459  
 Point-spread function, 366  
 Poisson kernel, 46  
 Poisson summation formula, 44  
 Poisson’s equation, 462  
 Polar space, 263  
 Polarization, plane of, 286  
 Polarization response, 467  
 Polarization vector, 11, 655  
 Polarizing monochromators, 658  
 Polycrystal electron-diffraction patterns, 358  
 Polycrystalline fibres, 568, 570, 576  
 Polycrystalline materials, diffuse scattering from, 534  
 Polyhedral display of crystal structures, 443  
 Polymer crystallography, 567  
 Polymer electron crystallography, 567  
 Polynomial growth  
   functions of, 41  
   locally summable function of, 40  
 Polynomial transforms, 61

## SUBJECT INDEX

- Polynomials  
 Chinese remainder theorem for, 57, 84  
 cyclotomic, 57
- Polyoma virus, 274
- Polypeptide fold, chemical correctness of, 273
- Polytypic phase transformations, 514
- Population parameter, 12
- Position of a known molecular structure, 270
- Positional coordinates, 437
- Positional order, long-range, 547
- Positive peaks, 252
- Positivity criterion, 293
- Potassium permanganate, 286
- Potential energy of a crystal, 485
- Potential-energy minima, 437
- PowderCell*, 444
- Power spectrum, 376
- Poynting vector, 644
- Prediction of crystal structures, 458
- Pressure tensor  
 mechanical, 470  
 thermodynamic, 470
- Pretransitional lengthening of correlation lengths, 551
- Prime factor algorithm, 52, 54  
 multidimensional, 59
- Primitive basis, 177
- Primitive coefficients, 180
- Primitive lattice, 71
- Primitive root mod  $p$ , 55
- Principal axes, 128
- Principal central projections and sections, 66
- Principal projections, 76
- Principal sections and projections, 67
- PRJMS*, 444–445
- Probability  
*a posteriori*, 512  
*a priori*, 504
- Probability densities, convolution of, 102
- Probability density distributions, 197  
 ideal, 200
- Probability density functions, 203  
 non-ideal, 212  
 of  $|E|$ , non-ideal, 205
- Probability density of samples for images, 366
- Probability theory, 102  
 analytical methods of, 102
- Probability trees, 513
- Processing X-ray fibre diffraction data, 574
- Product function, 250
- Programmers' Hierarchical Interactive Graphics System (PHIGS), 419
- Projected charge-density approximation, 305
- Projection approximation, 648
- Projection diffraction groups, 311
- Projection matching, three-dimensional, 383
- Projection operator, 649
- Projection(s), 25  
 and sections, duality between, 41  
 and sections, principal central, 66  
 bounded, 67, 92  
 centrosymmetric, 251–252  
 orthographic, 427–428  
 principal, 76  
 tilt, 389  
 use in three-dimensional reconstruction, 366
- Projector, 70
- Prolate spheroidal wavefunctions, 39
- Propagation direction, 630
- Propagation equation, 626
- Proper least-squares plane, 413
- Proper noncrystallographic symmetry, 258
- Proper rotation, 123, 128
- Protein crystallography, 286
- Protein crystals, 287
- Protein Data Bank, 438
- Proteins, electron crystallography of, 389
- PRXBLD*, 442
- Pseudo-distances, 28
- Pseudorotation, 437
- Pseudotranslational symmetry, 225
- Punched-card machines, 76
- Pure imaginary transforms, 87
- Quartet phase relationships, 225
- Quasicrystal structures, display of, 445
- Quasicrystals  
 decagonal, 354  
 diffuse scattering from, 527  
 icosahedral, 352  
 symmetry determination of, 352
- Quasilattice, 595
- Quasi-long-range order (QLRO), 548
- Quasimoments, 21
- Quasi-normalized structure factors, 218
- Quasiperiodic order, 603
- Quintet phase relationships, 227
- R* factors  
 fibre diffraction, 582  
 kinematical, 584
- Rader algorithm, 52
- Rader/Winograd algorithms, generalized, 90
- Rader/Winograd factorization, crystallographic extension of, 82
- Radial dependence of atomic electron distribution, 12
- Radial functions, 13
- Radiation damage, 299
- Radius of integration, 261
- Radon measure, 30
- Radon transform, 366
- Random conical tilt, 377, 381
- Random copolymers, 571
- Random-start method, 233
- Random-walk problem, 104  
 exact solution, 207
- Rank of tensor, 5
- Rapidly decreasing functions, 37, 39
- Raster-graphics devices, 432–433
- Rational approximant, 595
- Ray transform, 366
- Real antisymmetric transforms, 88
- Real crystal, 176
- Real-space averaging, 273–274  
 of electron density, 259, 273
- Real-space molecular replacement, 273
- Real-space translation functions, 271
- Real spherical harmonic functions, 12
- Real symmetric transforms, 88
- Real-valued transforms, 85
- Real waves, 640
- Reciprocal axes, 405
- Reciprocal Bravais lattice, 121
- Reciprocal cell, multiple, 121
- Reciprocal lattice, 2, 5, 43, 48, 62, 121, 177  
 point-group symmetry of, 114  
 weighted, 114–115  
 weighted, statistical properties of, 195
- Reciprocal-lattice sum, 453
- Reciprocal-lattice vectors, 450
- Reciprocal metric, 4
- Reciprocal space, 2, 450  
 symmetry in, 119
- Reciprocal-space group, 175, 179, 192
- Reciprocal-space procedures, 251
- Reciprocal-space representation of space groups, 114
- Reciprocal sum potential, 462
- Reciprocal unit-cell parameters, 4
- Reciprocity, 37
- Reciprocity property, 36
- Reciprocity relationship, 304
- Reciprocity theorem, 37, 41, 43, 63, 106  
 of scattering theory, 308–309
- Reconstruction  
 image, 361  
 single-particle, 366, 375  
 three-dimensional, 366
- Recursion for B-splines, 477
- REDUCE, 122
- Reduced orbit, 74
- Reducibility of the representation, 71
- Reducible matrix group, 176
- Reference bases, choice of, 7
- Refinement  
 aspherical multipole, 459  
 in single-particle reconstruction, 383  
 least-squares, 289  
 molecular-dynamics, 581  
 of phases, 233  
 restrained least-squares, 581
- Reflected intensity, 640
- Reflecting power, 635–636
- Reflection case, 631
- Reflection conditions, 73
- Reflection domain, middle of, 631
- Reflection geometry, 631–632
- Reflection high-energy electron diffraction (RHEED), 356
- Reflections  
 acentric, 74  
 equivalent, 285  
 main, 592  
 satellite, 592  
 substructure, 218  
 superstructure, 218
- Refraction, neutron, 654
- Refractive index, 300
- Regularization, 34  
 by convolution, 42
- Reindexing  
 additive, 61  
 multiplicative, 61
- Relationship between structure factors of symmetry-related reflections, 115
- Relationships between direct and reciprocal bases, 3
- Relatively prime integers, 406
- Relativistic effects, 301
- Representation domain, 179
- Representation method, 223
- Representation of space groups in reciprocal space, 114
- Representation of surfaces by dots, 433
- Representation of surfaces by lines, 433
- Representation of surfaces by shading, 433
- Representation operators, 72, 78
- Representation property, 68
- Representations, irreducible, 175
- Representative operators of a space group, 123
- Repulsion energy, 449
- Residual lattice, 48
- Resolution  
 extended, 274  
 image, 306  
 instrumental, 307
- Restacking, 558
- Restrained least-squares refinement, 581
- RHEED (reflection high-energy electron diffraction), 356
- Rhombohedral lattice, 90
- Riemann integral, 26
- Riemann–Lebesgue lemma, 36
- Right action, 68, 70
- Right cosets, 69
- Right representation, 68
- Rigid-body motion, 18
- Rigid-body superposition, 422
- Rigid rotation, 8
- Ring systems  
 condensed, 437  
 flexible, 436  
 fused, 442
- Rings*, 442
- RMBD (rocking microbeam diffraction), 356
- Robertson's sorting board, 76
- Rocking curve, 633, 638, 660  
 width at half-height, 636  
 width of, 633
- Rocking microbeam diffraction (RMBD), 356
- Rodrigues' formula, 468–469
- Root-mean-square differences between crystal structures, 445
- Root-mean-square error, 291
- Rotation, 426, 429  
 improper, 123, 128  
 molecular, 558  
 optical, 286  
 proper, 123, 128  
 rigid, 8  
 screw, 18
- Rotation axes, improper, 258
- Rotation-function Eulerian space groups, 265

## SUBJECT INDEX

- Rotation functions, 260
  - fast, 268
  - locked, 267–268
- Rotation matrix, 267, 419
  - trace of, 263
- Rotation of multipoles, 475
- Rotation operator, 6
  - inverse, 114
- Rotation part of space-group operation, 115
- Rotation vector, 421
- Rotational filtering, 365
- Rotational structure (form) factor, 526
- Rotational symmetry, noncrystallographic, 260
- Row–column method, 58
  
- SAD–MAD (single anomalous dispersion–multiple anomalous dispersion), 238
- Saddlepoint approximation, 102–103
- Saddlepoint equation, 105
- Saddlepoint expansion, 104
- Saddlepoint method, 36, 105
- SAED (selected-area electron diffraction), 307, 584
- Sampling, 25, 44
  - and periodization, duality between, 44
  - considerations, 99
  - of Gaussian density, 479
  - theorems, 65
- Satellite reflections, 503, 592
- Satellite tobacco necrosis virus, 259
- Sayre's equation, 91, 230
- Sayre's squaring method, 94
- Scalar pressure, 470
- Scalar products, 5, 404
  - mixed, matrices of, 8
- Scale, 426
- Scale factors, 287
- Scaling of heavy-atom-derivative data sets, 255
- Scaling symmetry, 603
- Scanning microbeam diffraction (SMBD), 356
- Scanning transmission electron microscope (STEM), 304
- Scattering
  - classical Thomson, 10
  - coherent, 488
  - Compton, 489
  - critical, 551
  - diffuse, 540
  - forward, 647
  - from mesomorphic structures, 547
  - incoherent, 488
  - incoherent inelastic, 488
  - inelastic, 300, 540
  - inelastic neutron, 488
  - inelastic X-ray, 490
  - kinematical, 300
  - Laue, 520
  - low-angle, 508
  - magnetic, 11, 656
  - multiple, 540
  - of neutrons by thermal vibrations, 488
  - of X-rays by thermal vibrations, 487
  - phonon, 543
  - plasmon, 541
  - thermal diffuse, 300
  - X-ray, 10, 62
- Scattering cross sections, 550, 654
- Scattering diagrams, 651
- Scattering factors
  - atomic, 10, 284
  - complex, 255
  - dynamical, 543
  - spherical atomic, 10
- Scattering lengths, 654
  - atomic, 11
  - neutron, 293
  - non-spin-flip, 657
  - spin-flip, 657
- Scattering matrix method, 363
- Scattering operator, 14
- Scattering power, 285
- Scattering theory, reciprocity theorem of, 308–309
- SCHAKAL*, 444
- Scherzer defocus, 305
  - conditions, 362
- Scherzer phase function, 362
- Schrödinger equation, 300
- Schur–Auerbach, theorem of, 176
- Schur's lemma, 71, 78
- Scrambling, 53
- Screen coordinates, 426, 428
- Screen space, 430
- Screw correlations, 20
- Screw rotation, 18
- Screw shifts, 518
- Script*, 442
- Search directions, 94
- Second Bethe approximation, 302
- Second-order Born approximation, 11
- SECS*, 442
- Section, 25
- Sections and projections, 25, 66
  - duality between, 41
  - principal, 67
- Selected-area electron diffraction (SAED), 307, 584
- Selection of origin, 247
- Selection rules, 101
- Self-energy terms, 449
- Self-Patterson, 100
  - vectors, 260
- Self-rotation function, 100
- Self-seeding, 583
- Self-vectors, 251
- Semi-direct product, 69
- Semi-norm on a vector space, 28
- Semi-reciprocal space, 648
- Separating exponent, 479
- Series-termination errors, 64, 91, 99
- Seven-beam approximation, 652
- Shadows, 434
- Shannon interpolation, 25, 50
- Shannon interpolation formula, 47, 92
- Shannon interpolation theorem, 65
- Shannon sampling criterion, 47, 68, 93
- Shannon sampling theorem, 47, 65, 275
- Shape-dependent term of Ewald sum, 469
- Sharpened Patterson functions, 245–246
- SHELX*, 443
- Shift of space-group origin, 120
- Shift property, 51, 65
- Short cyclic convolutions, 57
- Short-range order (SRO), 505, 548
  - correlation functions, 518
  - in multicomponent systems, 520
  - parameters, 541, 545
  - Warren parameters, 520
- Shubnikov groups, 308
- Sign conventions for electron diffraction, 301–302
- Signal-to-noise ratio in electron microscopy, 376, 385
- Simulated annealing, 576
- Simultaneous iterative reconstruction technique (SIRT), 370
- Sine strips, 76
- Single anomalous dispersion–multiple anomalous dispersion (SAD–MAD), 238
- Single-crystal electron-diffraction patterns, 356
- Single isomorphous replacement (SIR), 252, 283
  - difference electron density, 253
  - phasing, 253
- Single isomorphous replacement–multiple isomorphous replacement (SIR–MIR), 236
- Single-particle reconstruction, 366, 375
- Singular value decomposition, 370
- SIR (single isomorphous replacement), 252, 283
  - difference electron density, 253
  - phasing, 253
- SIR–MIR (single isomorphous replacement–multiple isomorphous replacement), 236
- SIRT (simultaneous iterative reconstruction technique), 370
- Site-symmetry group, 180
- Site-symmetry restrictions, 12
- Size distribution, 504
- Size effect, 521
- Skew-circulant matrix, 56
- Sliding filter, 436
- Small-angle-scattering approximation, 300
- Small values of  $\mu_e$ , 641
- SMB (symmetrical many-beam) method, 312
  
- SMBD (scanning microbeam diffraction), 356
- Smectic films, 554
- Smectic-A phase, 547, 550–551
  - modulated, 553
- Smectic-B phase, 547
- Smectic-C phase, 551
  - modulated, 553
- Smectic-D phase, 561
- Smectic-F phase, 556
- Smectic-I phase, 556
- Smooth particle mesh Ewald method, 475
- Sobolev space, 41
- Software, Hall symbols in, 123
- Solids
  - electron band theory, 629
  - theory of, 9
- Solution of dynamical theory, 633
- Solvable space groups, 71
- Solvent flattening, 92
- Solvent regions, 66
- Sound velocities, 490–491
- Southern bean mosaic virus, 259, 274
- Space-group algorithm, 119
- Space-group determination by convergent-beam electron diffraction, 307
- Space-group notation, explicit-origin, 127
- Space-group operation, 115
  - intrinsic and location-dependent components of translation part, 116
  - rotation part, 115
  - translation part, 115
- Space-group origin, shift of, 120
- Space-group-specific Fourier summations, 116
- Space-group-specific structure-factor formulae, 116
- Space-group-specific symmetry factors, 114
- Space-group symbols
  - computer-adapted, 117, 122, 127
  - explicit, 123–124
  - Hall, 123, 127, 130
  - Hermann–Mauguin, 119
- Space-group symmetry, 576
- Space-group tables, 119
- Space-group types, 71
  - affine, 177
  - crystallographic, 177
- Space groups, 71, 176, 282
  - cubic, 118
  - Eulerian, 263
  - finite, 177
  - hexagonal, 119
  - holosymmetric, 180
  - in reciprocal space, 162
  - monoclinic, 118
  - orthorhombic, 118
  - reciprocal-space representation of, 114
  - representative operators of, 123
  - rotation-function, 264
  - solvable, 71
  - symmorphic, 71, 177
  - tetragonal, 119
  - triclinic, 118
  - trigonal, 119
- Spaces
  - data, 426–427, 429–430
  - display, 426–427, 429–431, 434
  - picture, 426–428, 434
  - screen, 430
- Special Harker planes, 249
- Special  $\mathbf{k}$  vector, 178
- Special position, 72
  - condition, 72
- Special reflection, 73
- Spectrometer, triple-axis, 490
- Specular reflection, 554
- Spherical angles, 262
- Spherical atomic scattering factor, 10
- Spherical atoms, 116
- Spherical coordinates, 467
- Spherical Dirichlet kernel, 64, 91
- Spherical Fejér kernel, 64
- Spherical harmonic addition theorem, 468
- Spherical harmonic expansion, atom-centred, 12
- Spherical harmonic functions, real, 12
- Spherical harmonics, 268

## SUBJECT INDEX

- Spherical interference function, 261  
 Spherical polar coordinates, 263  
 Spherical-wave *Pendellösung*, 641  
 Spin-flip scattering lengths, 657  
 Spin orbitals, occupied natural, 15  
 Spiro links, 442  
 Spot boundaries, 575  
 Squarability criterion, 293  
 Square-integrable functions, 41  
 Square-summable sequences, 47  
 Squaring method equation, 91  
 SRO (short-range order), 505, 548  
     correlation functions, 518  
     in multicomponent systems, 520  
     parameters, 541, 545  
     Warren parameters, 520  
 Stacked transformations, 431  
 Standard basis of  $\mathbb{R}^n$ , 42  
 Standard coordinates, 42, 63, 71–72  
 Standard Gaussian function, 38, 41  
 Standard lattice, 42  
 Standard  $n$ -torus, 42  
 Standard uncertainty of distance from an atom to a plane, 412  
 Standards for graphics, 419  
 Standing waves, 633  
     anti-nodes of, 633  
     nodes of, 633  
 Star, arms of, 178  
 Star of  $\mathbf{k}$ , 178  
 Starting models, 578  
 Statistical properties of the weighted reciprocal lattice, 195  
 Statistical theory of communication, 104  
 Statistical theory of phase determination, 104  
 Statistics  
     crystallographic, 204  
     structure-factor, 117  
 Status of centrosymmetry, 123  
 Steepest descents, Booth's method, 96  
 STEM (scanning transmission electron microscope), 304  
 Stereochemical information, 576  
 Stereoviews, 428  
 Stirling's formula, 106  
 Structural connectivity, 435  
 Structural similarity, 425, 445  
 Structure amplitude, 10  
 Structure determination  
     by X-ray fibre diffraction analysis, 576  
     using electron-diffraction data, 583  
 Structure-factor algebra, 75, 105–106  
 Structure-factor formalism, generalized, 22  
 Structure-factor formulae, space-group-specific, 116  
 Structure-factor statistics, 117  
 Structure factors, 6, 8, 10, 62, 282, 466  
     calculation of, 73  
     for one-phonon scattering, 487  
     Fourier–Bessel, 569  
     from model atomic parameters, 93  
     geometric, 116–117, 135  
     in terms of form factors, 63  
     inequalities among, 221  
     joint probability distribution of, 105  
     normalized, 216, 231, 246  
     quasi-normalized, 218  
     rotational, 526  
     tables of, 117, 135  
     trigonometric, 116–117, 135  
     trigonometric, even absolute moments of, 206  
     trigonometric, moment of, 205  
     unitary, 218  
     *via* model electron-density maps, 93  
 Structure invariants, 216  
 Structure seminvariants, 216  
     algebraic relationships, 228  
     one-phase, 229, 231  
     two-phase, 229  
 Structure theorem, 35  
     for distributions with compact support, 43, 47  
*STRUPLO*, 444  
*STRUPLO for Windows*, 443–444  
*STRUVIR*, 443–444
- Sturkey's solution, 648  
 Subcentric arrangement, 212  
 Subdivision and decimation of period lattices, duality between, 48  
 Sublattice, 48  
 Subspace sectioning, 436, 441  
 Substitutional disorder, 545, 572  
 Substitutional order, 543  
 Substructure reflections, 218  
 Sum function, 250  
 Sum of images, 249  
 Summable functions, 27  
 Summation convention, 5  
 Summation problem in crystallography, 46  
 Superposition methods, 249  
 Superposition of Patterson functions, 250  
 Superpositions  
     general, 422  
     multiple simultaneous, 425  
     rigid-body, 422  
 Superstructure reflections, 218  
 Support, 25  
     compact, 25, 36, 44  
     of a distribution, 30  
     of a tensor product, 34  
 Support condition, 34, 44  
     generalized, 34  
 Surface effects, 553  
 Surface phase, 557  
 Surface plasmons, 300  
 Surface representation in cryo-EM, 386  
 Surfaces  
     atomic, 590, 596  
     dispersion, 629, 650, 657  
     fractal atomic, 597  
     representation of, 433  
     van der Waals, 433, 439  
*Sybyl*, 442  
 Symbolic programming techniques, 114  
 Symbolically oriented languages, 117  
 Symmetric rectangular density modulation, 601  
 Symmetrical many-beam (SMB) method, 312  
 Symmetry, 176, 263, 431  
     conjugate, 35, 40  
     conjugate and parity-related, 85  
     crystal, 68  
     crystallographic, 258  
     cyclic, 83  
     dihedral, 84  
     effects on Fourier image, 114  
     helical, 101, 375, 569, 576  
     helical, approximate, 570  
     Hermitian, 64, 74, 85  
     in Fourier space, 120  
     in reciprocal space, 119  
     noncrystallographic, 66, 258  
     noncrystallographic, molecular averaging by, 92  
     noncrystallographic, proper, 258  
     noncrystallographic, rotational, 260  
     of Patterson function, 244  
     permissible, 114  
     pseudotranslational, 225  
     scaling, 603  
 Symmetry elements  
     Eulerian, 264  
     three-dimensional, 308–309  
     two-dimensional, 308–310  
 Symmetry factors, 116  
     space-group-specific, 114  
     tables of, 114  
 Symmetry-generating algorithm, 123  
 Symmetry group, 176  
 Symmetry lines, 180  
 Symmetry operation, 176  
 Symmetry planes, 180  
 Symmetry points, 180  
 Symmetry property, 39  
 Symmetry-related reflections, relationship between structure factors of, 115  
 Symmorphic space groups, 71, 177  
 Synchrotron radiation, 282, 293  
 Systematic absences, 73, 121  
 Systematic errors, 408  
 Szegő's theorem, 44, 67, 106
- Table lookup schemes, 474  
 Tangent formula, 223, 292  
     application of, 231  
     modified, 233  
     weighted, 224  
 TDS (thermal diffuse scattering), 300, 484, 540  
 TEM (transmission electron microscope), 303  
 Temperature factors, 73, 287  
     anisotropic, 73  
     artificial, 94, 100  
     atomic, 17  
     isotropic, 73  
 Tempered distributions, 36, 39, 41, 47, 72  
     definition and examples of, 40  
     Fourier transforms of, 39–40  
 Tensor-algebraic formulation, 2, 5  
 Tensor formulation of vector product, 6  
 Tensor product, 27, 34, 52  
     of distributions, 33  
     of matrices, 51, 58, 60  
     structure of, 77  
     support of, 34  
 Tensor product B-spline, 480  
 Tensor product property, 35, 67, 101  
     of a Fourier transform, 76  
 Tensors, 5  
     anisotropic displacement, 6  
     antisymmetric, 6  
     libration, 18  
     metric, 4–5  
     permutation, 405  
     rank of, 5  
     translation, 18  
     translation, libration and screw-motion, 6  
 Test-function spaces, 29  
 Test functions, 39  
 Tetragonal family, 118  
 Tetragonal space groups, 90, 119  
 Text processing, 122  
 Texture electron-diffraction patterns, 357, 394  
 THEED (transmission high-energy electron diffraction), 356  
 Theory of distributions, 25, 28  
 Theory of solids, 9  
 Thermal diffuse scattering (TDS), 300, 484, 540  
 Thermal fluctuations, 550  
 Thermal neutrons, 293  
 Thermal streaks, 545  
 Thermodynamic pressure tensor, 470  
 Thermotropic phase, 548  
 Thick crystals, 363, 638  
 Thin crystals, 639  
     comparison of geometrical and dynamical theory, 637  
 Thin films, 554  
     crystal defects in, 542  
 Thomson scattering, classical, 10  
 Thon rings, 378  
 Three-axis joystick, 430  
 Three-beam approximation, 652  
 Three-beam inversion, 652  
 Three-dimensional Dirac delta function, 464  
 Three-dimensional electron-diffraction data, 391  
     from a single crystal orientation, 585  
     from two crystal orientations, 585  
 Three-dimensional fast Fourier transform (3DFFT), 475–476  
 Three-dimensional Hermite polynomials, 21  
 Three-dimensional isotropic harmonic oscillator, 17  
 Three-dimensional Patterson function, 577  
 Three-dimensional projection matching, 383  
 Three-dimensional reconstruction, 366  
 Three-dimensional structure determination by electron crystallography, 391  
 Three-dimensional symmetry elements, 308–309  
 Three-generator symbol, 123  
 Through-focus series method, 363  
 Tie point, 628  
 Tilt projections, 389  
 Tilted hexatic phase, 556  
 Toeplitz–Carathéodory–Herglotz theorem, 45  
 Toeplitz determinants, 45, 67  
 Toeplitz forms, 44, 67  
     asymptotic distribution of eigenvalues of, 45, 68

## SUBJECT INDEX

- Toeplitz matrices, 45  
 Tomography, electron, 377, 382  
 Topography, neutron, 661  
 Topological dual, 30, 39–40  
 Topological vector spaces, 28  
 Topology, 27, 39  
   general, 27  
   in function spaces, 27  
   metrizable, 28  
   not metrizable, 30  
   on  $\mathcal{D}(\Omega)$ , 29  
   on  $\mathcal{D}_k(\Omega)$ , 29  
   on  $\mathcal{E}(\Omega)$ , 29  
 Topology analysis, 445  
 Torsion angles, 406  
 Total cross section, 11  
 Total-reflection domain, 638  
   width of, 633, 638  
 Trace of rotation matrix, 263  
 Transfer function, 52  
   of lens, 304  
 Transformation properties of direct and reciprocal base vectors and lattice-point coordinates, 116  
 Transformations  
   affine, 120  
   compound, 429  
   direct-space, 120  
   general, 423  
   linear, 7  
   modelling, 431  
   nonlinear, 264  
   of coordinates, 5, 7, 33  
   stacked, 431  
   to a Cartesian system, 3  
   unitary, 37  
   viewing, 426–427, 429–430, 432  
   viewport, 426, 428  
   windowing, 426  
 Transformed variance–covariance matrix, 407  
 Transforms  
   complex antisymmetric, 87  
   complex symmetric, 87  
   Hankel, 101  
   Hermitian-antisymmetric, 87  
   of an axially periodic fibre, 101  
   of delta functions, 40  
   polynomial, 61  
   pure imaginary, 87  
   Radon, 366  
   ray, 366  
   real antisymmetric, 88  
   real symmetric, 88  
   real-valued, 85  
 Translate, 26  
 Translation, 18, 25, 426, 429  
   part of space-group operation, 115  
   part of space-group operation, intrinsic and location-dependent components of, 116  
 Translation, libration and screw-motion tensors, 6  
 Translation functions, 100, 269  
   general, 269  
   locked, 271  
   real-space, 271  
 Translation subgroup, 177  
 Translation tensor, 18  
 Translation vector, 258  
 Translational components of noncrystallographic rotation elements, 258  
 Translational displacement, 18  
 Translational invariance, 650  
 Translations, conversion to phase shifts, 35  
 Transmission case, 631  
 Transmission electron microscope (TEM), 303  
 Transmission geometry, 631–633  
   intensities of plane waves in, 634  
 Transmission high-energy electron diffraction (THEED), 356  
 Transposition formula, 80–81  
   for intermediate results, 77  
 Triads, mutually reciprocal, 2  
 Triangular inequality, 27  
 Triclinic space groups, 89, 118  
 Trigonal space groups, 90, 119  
 Trigonometric functions  
   B-spline approximation of, 477  
   interpolation of, 478  
   least-squares approximation of, 478  
 Trigonometric moment problem, 44  
 Trigonometric structure-factor expressions, vectors of, 104  
 Trigonometric structure factors, 116–117, 135  
   even absolute moments of, 206  
   moment of, 205  
 Triple-axis spectrometer, 490  
 Triple point, 552  
 Triplet relationships using structural information, 224  
 Triplets, search of, 231  
 Triply periodic, 627  
 Tunability, 294  
 Twiddle factors, 53, 58, 60, 62, 80  
 Two-beam approximation, 302, 649  
 Two-beam case, 629  
 Two-beam dynamical approximation, 394  
 Two-beam dynamical diffraction formulae, 303  
 Two-centre orbital products, 17  
 Two-centre terms, 15  
 Two-dimensional disorder, 514  
 Two-dimensional hexatic phase, 555  
 Two-dimensional symmetry elements, 308–310  
 Two-phase structure seminvariants, first rank, 229  
 Two-wavelength method, 293  
 Type of irreps, 181  
 Type of rotation (proper or improper), 123  
  
 Uni-arm  $\mathbf{k}$  vector, 181  
 Uniaxial nematic order, 549  
 Uniformity, assumption of, 203, 209  
 Uniformizable space, 28  
 Unit cell, 178–179, 460  
   dipole moment of, 461  
   neutral, 461  
 Unit-cell parameters  
   direct, 4  
   reciprocal, 4  
 Unit cube, 42  
 Unitary matrix group, 176  
 Unitary structure factors, 218  
 Unitary transformations, 37  
 Unscrambling, 81  
 Uranium, 287  
  
 Valence density, 12  
 van der Waals surfaces, 433, 439  
 Van Hove correlation functions, 489  
 Variance, 407  
 Variance–covariance matrix, 406  
   transformed, 407  
 Variances, 411–412  
 Vector interactions in a Patterson map, 248  
 Vector lattice, 177  
 Vector machines, 432  
 Vector map, 244  
 Vector overlap, 251  
 Vector processing, 61  
 Vector product, 405  
   components of, 405  
   tensor formulation of, 6  
 Vector radix Cooley–Tukey algorithm, 58  
 Vector radix FFT algorithms, 59  
 Vector relationships, 405  
 Vector-search procedures, 251  
 Vector space  
   complete, 26  
   norm on, 28  
   semi-norm on, 28  
   topological, 28  
 Vectors  
   angle between two, 404  
   components of, 5  
   cross-Patterson, 260  
   four-dimensional, 424  
   interatomic, 65  
   length of, 404  
   of trigonometric structure-factor expressions, 104  
   origin-shift, 123  
   polarization, 11, 655  
   Poynting, 644  
   rotation, 421  
   self-Patterson, 260  
   translation, 258  
 VENUS, 443–445  
 Very small angle neutron scattering, 660  
 Vibrating crystals, 660  
 Vibrational–librational correlations, 525  
 Viewing transformation, 426–427, 429–430, 432  
 Viewport, 426, 428  
 Viewport transformation, 426, 428  
 Vitamin B<sub>12</sub>, 286  
 Voronoi diagram, 373  
  
 Waller–Hartree formula, 541, 543  
 Warren short-range-order parameters, 520  
 Wavefield, 628, 630  
 Wavefunctions, prolate spheroidal, 39  
 Wavelengths, 299  
 Wavevectors, 635  
 Weak enantiomorphic images, 247  
 Weak-phase-object approximation, 304  
 Weak phase objects, 361, 583  
   periodic, 364  
 Weighted difference map, 97, 99  
 Weighted lattice distribution, 44  
 Weighted reciprocal lattice, 114–115  
   statistical properties of, 195  
 Weighted reciprocal-lattice distribution, 62  
 Weighted tangent formula, 224  
 Weighting factor, 289  
 Weights  
   anisotropic, 413  
   Gaussian, 413  
 Whole pattern (WP), 310  
 Width of rocking curve, 633  
   at half-height, 636  
 Width of total-reflection domain, 633, 638  
 Wigner potential, 466  
 Wigner–Seitz cell, 178  
 Wilson plot, 287  
 Window, 426, 429, 434  
 Windowing, 426, 428  
 Windowing transformation, 426  
 Wing, 184  
 Winograd algorithms, 52, 56  
 Winograd small FFT algorithms, 57  
 Winograd small FFTs, nesting of, 60  
 Wintgen letter, 180  
 Wintgen position, 180  
 Wintgen symbol, 180  
 World coordinates, 426  
 WP (whole pattern), 310  
 Wyckoff letter, 180  
 Wyckoff position, 115, 180  
 Wyckoff symbols, 72  
  
*XmLmctep*, 443–444  
 X-ray analysis, 287  
 X-ray fibre diffraction analysis, 567  
   data processing, 574  
   structure determination by, 576  
 X-ray scattering, 62, 293  
   cross section, 550  
   elastic component, 10  
   inelastic component, 10  
 X-ray topographs, 626  
 X-rays, 293  
   diffuse scattering of, 492  
   interaction with matter, 626  
*X-Seed*, 443–444  
*Xtal-3D*, 444–445  
*XtalDraw*, 443–444  
  
 z buffer, 433  
 ZAP (zone-axis pattern), 310  
 Zero-absorption case, 633  
 Zeroth-order Laue zone (ZOLZ) reflections, 308, 324  
 Zonal data sets  
   view down the chain axis, 584  
   view onto the chain axes, 585  
 Zone-axis pattern (ZAP), 310  
 Zones and rows, average intensity of, 196