

**Coherent neutron scattering amplitudes.** By G. E. BACON (for THE NEUTRON DIFFRACTION COMMISSION), *The University, Sheffield S10 2TN, England*

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An up-to-date table of coherent neutron scattering amplitudes is presented

A full list of scattering amplitudes was published by the Neutron Diffraction Commission in 1969 (*Acta Cryst. A25*, 391). Since then new values of several elements have been determined by Koester & Knopf (1971) using Christiansen-filter and gravity-mirror methods and there have been some measurements by Shull (1968) using Pendelosung fringes. The standard deviations of these new measurements are considered to be much smaller than those of the earlier data but it is doubtful whether it is worthwhile at the present moment to seek to give estimated accuracies to all the values

Table 1. *Coherent scattering amplitudes, b, in units of  $10^{-12}$  cm*

Z	Element or Isotope	b	Z	Element or Isotope	b
1	$^1\text{H}$	-0.374	25	Mn	-0.39
	$^2\text{H}$	0.667 <sup>1</sup>	26	Fe	0.95
	$^3\text{H}$	0.47		$^{54}\text{Fe}$	0.42
2	$^4\text{He}$	0.30		$^{56}\text{Fe}$	1.01
3	Li	-0.214 <sup>7</sup>		$^{57}\text{Fe}$	0.23
	$^6\text{Li}$	0.18 + 0.025 <i>i</i>	27	Co	0.25
	$^7\text{Li}$	-0.233 <sup>7</sup>	28	Ni	1.03
4	Be	0.774		$^{58}\text{Ni}$	1.44
5	B	0.54 + 0.021 <i>i</i>		$^{60}\text{Ni}$	0.28
	$^{11}\text{B}$	0.60		$^{61}\text{Ni}$	0.76
6	$^{12}\text{C}$	0.665		$^{62}\text{Ni}$	-0.87
	$^{13}\text{C}$	0.60		$^{64}\text{Ni}$	-0.037
7	$^{14}\text{N}$	0.94	29	Cu	0.76
8	O	0.580		$^{63}\text{Cu}$	0.67
	$^{17}\text{O}$	0.578		$^{65}\text{Cu}$	1.11
	$^{18}\text{O}$	0.600	30	Zn	0.57
9	F	0.56		$^{64}\text{Zn}$	0.55
10	Ne	0.46		$^{66}\text{Zn}$	0.63
11	Na	0.36		$^{68}\text{Zn}$	0.67
12	Mg	0.52	31	Ga	0.72
13	Al	0.35	32	Ge	0.819 <sup>3</sup>
14	Si	0.42	33	As	0.64
15	P	0.51	34	Se	0.80 <sup>4</sup>
16	S	0.28	35	Br	0.68
17	Cl	0.96	36	Kr	0.74
	$^{35}\text{Cl}$	1.18	37	Rb	0.71 <sup>5</sup>
	$^{37}\text{Cl}$	0.26		$^{85}\text{Rb}$	0.83
18	A	0.20	38	Sr	0.69 <sup>6</sup>
	$^{36}\text{A}$	2.43 <sup>2</sup>	39	Y	0.79
19	K	0.37	40	Zr	0.71
	$^{39}\text{K}$	0.37	41	Nb	0.71
20	Ca	0.47	42	Mo	0.69 <sup>7</sup>
	$^{40}\text{Ca}$	0.49	43	$^{99}\text{Tc}$	0.68
	$^{44}\text{Ca}$	0.18	44	Ru	0.73
21	Sc	1.18	45	Rh	0.58
22	Ti	-0.34	46	Pd	0.60
	$^{46}\text{Ti}$	0.48	47	Ag	0.60
	$^{47}\text{Ti}$	0.33		$^{107}\text{Ag}$	0.83
	$^{48}\text{Ti}$	-0.58		$^{109}\text{Ag}$	0.43
	$^{49}\text{Ti}$	0.08	48	Cd	$0.37 + 0.16i$
	$^{50}\text{Ti}$	0.55		$^{113}\text{Cd}$	$-1.5 + 1.2i$
23	V	-0.05	49	In	0.39
24	Cr	0.352			
	$^{52}\text{Cr}$	0.49			

Table 1. (cont.)

50	Sn	0.61	73	Ta	0.70
	$^{116}\text{Sn}$	0.58	74	W	0.48
	$^{117}\text{Sn}$	0.64		$^{182}\text{W}$	0.839
	$^{118}\text{Sn}$	0.58		$^{183}\text{W}$	0.439
	$^{119}\text{Sn}$	0.60		$^{184}\text{W}$	0.769
	$^{120}\text{Sn}$	0.64		$^{186}\text{W}$	-0.12
	$^{122}\text{Sn}$	0.55	75	Re	0.92
	$^{124}\text{Sn}$	0.59	76	Os	1.07
51	Sb	0.56		$^{188}\text{Os}$	0.78
52	Te	0.54		$^{189}\text{Os}$	1.10
	$^{120}\text{Te}$	0.52		$^{190}\text{Os}$	1.14
	$^{123}\text{Te}$	0.57	77	$^{192}\text{Os}$	1.19
	$^{124}\text{Te}$	0.55		Ir	1.06
	$^{125}\text{Te}$	0.56	78	Pt	0.95
	I	0.53	79	Au	0.76
53	Xe	0.48	80	Hg	1.27
	Cs	0.55 <sup>8</sup>	81	Tl	0.89
54	Ba	0.52	82	Pb	0.94
	La	0.83	83	Bi	0.86
55	Ce	0.48	90	Th	1.03
	$^{140}\text{Ce}$	0.47	92	U	0.85
	$^{142}\text{Ce}$	0.45		$^{235}\text{U}$	0.98
56	Pr	0.44		$^{238}\text{U}$	0.85
57	Nd	0.72	93	Np	1.055
	$^{142}\text{Nd}$	0.77	94	$^{239}\text{Pu}$	0.75
	$^{144}\text{Nd}$	0.28		$^{240}\text{Pu}$	0.35
	$^{146}\text{Nd}$	0.87		$^{242}\text{Pu}$	0.81
	$^{152}\text{Sm}$	-0.5			
	$^{154}\text{Sm}$	0.8			
	Eu	0.55			
	Gd	1.5			
	Dy	1.69			
66	$^{160}\text{Dy}$	0.67			
	$^{161}\text{Dy}$	1.03			
	$^{162}\text{Dy}$	-0.14			
	$^{163}\text{Dy}$	0.50			
	$^{164}\text{Dy}$	4.94			
	Ho	0.85			
	Er	0.79			
	Tm	0.72			
	Yb	1.26			
	Lu	0.73			
	Hf	0.78			

- Both diffraction data and gravity-mirror measurements support this higher value.
- Krohn & Ringo (1966).
- Shull (1968).
- This new value is supported by a gravity-mirror measurement and by Krebs-Larsen *et al.* (1971).
- Copley (1970), Wang (1970), Meriel (1970).
- Cooper (1970), Loopstra & Rietveld (1969).
- Koester & Knopf (1971).
- Cox & Minkiewicz (1971), Chadwick *et al.* (1971).
- Alexandrov *et al.* (1968).

listed. The compiler hopes that publication of the following, somewhat conservative list, will serve to maintain the interest of all neutron crystallographers in continual refin-

ement of these values. He invites any reader who disputes the accuracy of any of the values to provide him with improved information.

References are given for most of the values which have been significantly changed since the previous list.

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**Sixth-order elastic coefficients in cubic crystals.** By DAVID Y. CHUNG, Department of Physics and Astronomy, Howard University, Washington, D.C. 20001, U.S.A.

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The sixth-order elastic coefficients have been enumerated by the method of symmetry operations. For  $n > 5$  the conjecture of Krishnamurty [*Acta Cryst.* (1963), 16, 839] that there should be  $(n^2 - 2n + 3)$   $n$ th-order elastic coefficients of a cubic crystal (with point group  $O_h$ ) was shown to be incorrect.

The numbers of independent elastic coefficients of order two and three for all crystal classes have been derived by Bhagavantam & Suryanarayana (1949) from the character method. By the method of reduction of a representation, Jahn (1949) obtained identical results. Recently Jahn's (1949) method has been extended to fourth- and fifth-order

elastic coefficients by Krishnamurty & Gopala-Krishnamurty (1968), and to sixth- and seventh-order coefficients by Chung (1972). Krishnamurty (1963), in enumerating the forth-order elastic coefficients by the character method, has conjectured that the number of  $n$ th-order elastic coefficients, symmetric in all the  $n$  suffixes, of a cubic crystal ( $O_h$  point group) would be  $n^2 - 2n + 3$  ( $n \geq 2$ ); whereas for an isotropic solid ( $R_\infty^i$ ) would be  $n$ .

Krishnamurty & Appalanarasimham (1969) recently pointed out that there should not be  $n$   $n$ th-order elastic coefficients of an isotropic solid for  $n > 5$ . In this note, it is shown that the other conjecture, namely  $n^2 - 2n + 3$  constants for cubic crystals, does not hold true either for  $n > 5$ .

It is known that the elastic energy should be invariant with respect to the crystal symmetry operations. Using this principle Hearmon (1953) obtained the independent coefficients for all crystal classes. We applied the same method to sixth-order coefficients for a cubic crystal. The resulting 32 independent coefficients and their equivalence are given in Table 1.

One notices that the number of independent coefficients 32 is quite different from  $n^2 - 2n + 3 = 27$  for  $n = 6$  predicted by Krishnamurty (1963). However, it agrees very well with the group theoretical prediction of Chung (1972).

111111 = 222222 = 333333
111112 = 111113 = 122222 = 133333 = 222223 = 233333
111122 = 111133 = 112222 = 113333 = 222233 = 223333
111123 = 122223 = 123333
111144 = 222255 = 333366
111155 = 111166 = 222266 = 333344 = 333355 = 222244
112222 = 111333 = 222333
112223 = 111233 = 112223 = 112333 = 122233 = 122333
112244 = 111344 = 122255 = 133366 = 222355 = 233366
112555 = 113366 = 133344 = 222366 = 233355 = 122244
112666 = 111355 = 122266 = 133355 = 222344 = 233344
114456 = 222456 = 333456
112233
112244 = 112255 = 113344 = 113366 = 223355 = 223366
112266 = 113355 = 223344
112344 = 122355 = 123366
112355 = 112366 = 122344 = 122366 = 123344 = 123355
112456 = 113456 = 122456 = 133456 = 223456 = 233456
114444 = 225555 = 336666
114455 = 114466 = 224455 = 225566 = 334466 = 335566
115555 = 116666 = 224444 = 226666 = 334444 = 335555
115566 = 224466 = 334455
123456
124444 = 125555 = 134444 = 136666 = 235555 = 236666
124455 = 235566 = 134466
124466 = 125566 = 134455 = 135566 = 234455 = 234466
126666 = 135555 = 234444
144456 = 245556 = 345666
145556 = 145666 = 244456 = 245666 = 344456 = 345556
444444 = 555555 = 666666
444455 = 444466 = 445555 = 446666 = 555566 = 556666
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