isolated atoms. Thus empirically the HFS f values may be at least as good as the HF in the majority of the experimentally important cases. There are other inherent limitations and defects in these calculations. For example: (1) they do not make allowances for the dispersion effects which occur when λ is in the vicinity of an X-ray absorption edge, (2) they assume spherical symmetry, (3) the wave functions from which the f values are computed are not corrected for spin-orbit effects, and (4) the wave functions are not corrected for relativistic effects.

Conclusions and comments

Despite the intrinsic approximations in these calculations, it is felt that the scattering factors presented here represent a substantial improvement over most values available. They possess the inherent advantages of being relatively complete and of having been obtained in a coherent fashion, the same type of approximation being involved in the calculations for each of the atoms. There are numerous obvious extensions of these calculations. In preparation at present are the following: (1) the scattering amplitudes for electron scattering both within the first Born approximation and in the case where consideration is taken of the phase change, (2) the inelastic scattering factors, (3) X-ray and electron scattering factors for ions, and (4) analytic approximations to the X-ray and electron scattering factors.

We are indebted to Mr Loyd Dreher and to Mr Robert Pohler, whose assistance has made these computations possible. The computations were carried out on The University of Texas CDC 1604 computer.

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Hartree Scattering Factors for Elements 37 through 98*

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Hartree scattering factors are given for atoms of atomic number 37 through 98 and for several of their ions. The values are listed in tabular form and as analytic functions. Values are also given for two low-lying excited states of cerium. Differences between the Hartree and Thomas–Fermi–Dirac scattering factors are discussed.

Introduction

Atomic scattering factors obtained from Hartree self-consistent-field (SCF) calculations have been available in the past for only a very few atoms and ions above atomic number 36. Boyd, Larson & Waber (1963) have recently completed Hartree SCF calculations for all atoms of the periodic table, many ions, and many excited states. In this paper we present scattering factors for the ground states of elements of atomic number 37 and higher, for several of their ions, and for two excited states of cerium. (For elements of lower atomic number, scattering factors which have been obtained from more accurate wave functions are already available in standard references.)

We have published in a Los Alamos Scientific Laboratory report (Cromer, Larson & Waber, 1963) a set of Hartree SCF scattering factors for all atoms in the periodic table, in a more detailed form than in the present paper. Although this publication duplicates light element work by others, it has the advantage of presenting in a single unit complete information on Hartree SCF scattering factors.

Calculations

Details of the Hartree SCF calculations will be given elsewhere by Boyd, Larson & Waber (1964). The scattering factors were computed from the total radial density functions by straightforward means (James, 1948). Calculations were performed for the most part with an IBM 7090 computer and, in the

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Table 1. *Hartree scattering factors for elements 37 through 98*

s_x	RB	RB+1	SR	SR+2	Y	Y+3	ZR	ZR+4	NB	MO	TC	RU	RH	PD	PD+2	AG
0.	37.00	36.00	38.00	36.00	39.00	36.00	40.00	36.00	41.00	42.00	43.00	44.00	45.00	46.00	44.00	47.00
0.05	35.77	35.35	36.62	35.46	37.58	35.54	38.63	35.60	39.71	40.76	41.75	42.85	43.88	45.02	43.36	45.95
0.10	33.57	33.60	34.11	33.98	34.88	34.25	35.85	34.47	36.98	38.05	38.97	40.20	41.28	42.55	41.60	43.43
0.15	31.23	31.27	31.77	31.89	32.39	32.39	33.17	32.79	34.17	35.14	35.99	37.18	38.24	39.46	39.10	40.39
0.20	28.83	28.83	29.53	29.58	30.14	30.23	30.80	30.80	31.61	32.44	33.24	34.27	35.24	36.31	36.27	37.28
0.25	26.60	26.59	27.35	27.35	28.00	28.06	28.63	28.71	29.28	30.00	30.75	31.59	32.46	33.37	33.45	34.31
0.30	24.67	24.66	25.37	25.34	26.02	26.03	26.62	26.70	27.19	27.82	28.51	29.20	29.96	30.73	30.83	31.60
0.35	23.01	23.01	23.63	23.61	24.24	24.23	24.81	24.87	25.33	25.89	26.52	27.10	27.76	28.42	28.50	29.19
0.40	21.57	21.57	22.11	22.10	22.67	22.67	23.21	23.25	23.70	24.22	24.78	25.28	25.85	26.43	26.48	27.09
0.50	19.06	19.06	19.57	19.57	20.07	20.06	20.56	20.56	21.03	21.48	21.94	22.36	22.81	23.26	23.27	23.75
0.60	16.81	16.81	17.36	17.36	17.88	17.88	18.38	18.37	18.86	19.30	19.72	20.13	20.52	20.90	20.90	21.29
0.70	14.73	14.73	15.34	15.34	15.90	15.90	16.44	16.42	16.95	17.42	17.85	18.27	18.66	19.04	19.03	19.39
0.80	12.87	12.87	13.49	13.49	14.07	14.07	14.64	14.63	15.18	15.69	16.16	16.62	17.03	17.43	17.42	17.79
0.90	11.27	11.27	11.85	11.85	12.42	12.42	12.99	12.98	13.54	14.07	14.58	15.06	15.52	15.95	15.94	16.34
1.00	9.94	9.94	10.45	10.45	10.98	10.98	11.52	11.51	12.05	12.58	13.10	13.60	14.08	14.54	14.54	14.97
1.10	8.88	8.88	9.31	9.31	9.77	9.77	10.25	10.24	10.74	11.24	11.74	12.24	12.73	13.20	13.20	13.65
1.20	8.03	8.03	8.39	8.39	8.77	8.77	9.18	9.18	9.62	10.07	10.54	11.01	11.48	11.95	11.95	12.41
1.30	7.38	7.38	7.66	7.66	7.97	7.97	8.32	8.32	8.69	9.08	9.50	9.93	10.37	10.81	10.81	11.26
1.40	6.87	6.87	7.09	7.09	7.34	7.34	7.62	7.62	7.93	8.26	8.62	9.00	9.39	9.80	9.81	10.23
1.50	6.46	6.46	6.64	6.64	6.84	6.84	7.07	7.07	7.32	7.59	7.89	8.22	8.56	8.93	8.93	9.31
1.60	6.12	6.12	6.27	6.27	6.44	6.44	6.62	6.62	6.82	7.05	7.30	7.57	7.87	8.19	8.19	8.52
1.70	5.83	5.83	5.97	5.97	6.11	6.11	6.26	6.26	6.43	6.61	6.82	7.04	7.29	7.56	7.56	7.85
1.80	5.58	5.58	5.70	5.70	5.83	5.83	5.96	5.96	6.10	6.25	6.42	6.61	6.82	7.05	7.05	7.29
1.90	5.34	5.34	5.46	5.46	5.58	5.58	5.70	5.70	5.82	5.96	6.10	6.26	6.43	6.62	6.62	6.83
1.99	5.13	5.13	5.26	5.26	5.38	5.38	5.49	5.49	5.61	5.72	5.85	5.99	6.13	6.30	6.30	6.47

s_x	AG+1	CD	CD+2	IN	SN	SB	TE	I	XE	CS	BA	LA	LA+3	CE	CE+3	CE+4
0.	46.00	48.00	46.00	49.00	50.00	51.00	52.00	53.00	54.00	55.00	56.00	57.00	54.00	58.00	55.00	54.00
0.05	45.25	46.91	45.38	47.73	48.69	49.68	50.68	51.69	52.71	53.27	54.07	55.05	53.20	56.13	54.21	53.29
0.10	43.22	44.31	43.66	45.00	45.80	46.67	47.60	48.56	49.55	50.12	50.63	51.40	51.02	52.67	52.04	51.32
0.15	40.43	41.22	41.17	41.97	42.65	43.37	44.14	44.95	45.82	46.63	47.26	47.89	47.97	49.21	48.99	48.49
0.20	37.36	38.14	38.29	38.94	39.64	40.30	40.95	41.62	42.33	43.14	43.90	44.54	44.63	45.77	45.62	45.29
0.25	34.37	35.19	35.34	36.04	36.79	37.46	38.09	38.70	39.31	40.00	40.73	41.39	41.42	42.47	42.35	42.12
0.30	31.62	32.46	32.55	33.31	34.10	34.82	35.48	36.09	36.67	37.27	37.91	38.54	38.55	39.50	39.40	39.21
0.35	29.19	29.99	30.02	30.80	31.60	32.36	33.05	33.70	34.29	34.86	35.44	36.03	36.03	36.89	36.80	36.63
0.40	27.08	27.81	27.80	28.56	29.33	30.08	30.80	31.47	32.10	32.68	33.24	33.81	33.80	34.58	34.51	34.36
0.50	23.74	24.29	24.27	24.88	25.50	26.16	26.84	27.51	28.17	28.80	29.38	29.96	29.95	30.59	30.56	30.49
0.60	21.28	21.70	21.68	22.14	22.62	23.13	23.68	24.26	24.86	25.47	26.06	26.64	26.63	27.17	27.18	27.19
0.70	19.39	19.74	19.73	20.09	20.46	20.85	21.27	21.73	22.22	22.73	23.27	23.80	23.80	24.25	24.29	24.34
0.80	17.79	18.13	18.13	18.45	18.77	19.10	19.43	19.79	20.17	20.58	21.02	21.47	21.47	21.86	21.89	21.95
0.90	16.34	16.70	16.71	17.04	17.36	17.67	17.96	18.26	18.57	18.90	19.25	19.62	19.62	19.95	19.97	20.01
1.00	14.97	15.37	15.37	15.74	16.08	16.40	16.70	16.99	17.27	17.55	17.84	18.14	18.14	18.43	18.44	18.46
1.10	13.65	14.08	14.09	14.49	14.86	15.21	15.54	15.84	16.12	16.40	16.66	16.93	16.93	17.19	17.20	17.21
1.20	12.41	12.86	12.86	13.28	13.69	14.07	14.42	14.75	15.06	15.35	15.62	15.88	15.88	16.13	16.13	16.14
1.30	11.26	11.71	11.71	12.14	12.56	12.96	13.34	13.70	14.03	14.35	14.64	14.91	14.91	15.17	15.17	15.17
1.40	10.23	10.65	10.65	11.08	11.49	11.90	12.30	12.68	13.03	13.37	13.69	13.99	13.99	14.26	14.26	14.26
1.50	9.31	9.71	9.71	10.11	10.51	10.91	11.31	11.69	12.07	12.42	12.76	13.08	13.08	13.37	13.37	13.38
1.60	8.52	8.88	8.88	9.25	9.62	10.01	10.39	10.77	11.15	11.51	11.86	12.20	12.20	12.50	12.51	12.52
1.70	7.85	8.17	8.17	8.49	8.84	9.19	9.55	9.92	10.28	10.65	11.00	11.35	11.35	11.65	11.66	11.68
1.80	7.29	7.56	7.56	7.85	8.15	8.47	8.81	9.15	9.49	9.84	10.19	10.53	10.53	10.85	10.85	10.87
1.90	6.83	7.05	7.05	7.30	7.57	7.85	8.15	8.46	8.78	9.11	9.44	9.77	9.77	10.08	10.09	10.11
1.99	6.47	6.67	6.67	6.88	7.12	7.37	7.63	7.91	8.21	8.51	8.82	9.14	9.14	9.44	9.45	9.46

s_x	PR	PR+3	PR+4	ND	ND+3	PM	PM+3	SM	SM+3	EU	EU+2	EU+3	GD	GD+3	TB	TB+3
0.	59.00	56.00	55.00	60.00	57.00	61.00	58.00	62.00	59.00	63.00	61.00	60.00	64.00	61.00	65.00	62.00
0.05	57.17	55.22	54.30	58.20	56.23	59.23	57.24	60.26	58.25	61.29	60.17	59.26	62.26	60.27	63.34	61.28
0.10	53.74	53.07	52.34	54.80	54.10	55.86	55.14	56.92	56.17	57.97	57.88	57.21	58.78	58.24	60.09	59.28
0.15	50.27	50.03	49.52	51.33	51.08	52.39	52.13	53.46	53.18	54.52	54.65	54.23	55.25	55.29	56.66	56.34
0.20	46.79	46.64	46.31	47.82	47.67	48.87	48.71	49.92	49.76	50.98	51.04	50.81	51.76	51.87	53.11	52.93
0.25	43.43	43.31	43.09	44.42	44.30	45.42	45.30	46.44	46.32	47.47	47.46	47.34	48.32	48.38	49.55	49.42
0.30	40.39	40.29	40.11	41.31	41.20	42.25	42.15	43.21	43.11	44.18	44.16	44.09	45.05	45.08	46.17	46.08
0.35	37.70	37.61	37.46	38.54	38.45	39.41	39.33	40.30	40.22	41.22	41.20	41.13	42.06	42.07	43.09	43.01
0.40	35.32	35.25	35.11	36.09	36.02	36.89	36.82	37.72	37.65	38.57	38.57	38.50	39.36	39.37	40.32	40.25
0.50	31.23	31.20	31.12	31.89	31.86	32.58	32.54	33.29	33.25	34.02	34.03	33.98	34.73	34.73	35.54	35.50
0.60	27.74	27.75	27.74	28.32	28.33	28.92	28.93	29.54	29.54	30.18	30.19	30.18	30.83	30.83	31.51	31.51
0.70	24.75	24.79	24.83	25.27	25.30	25.79	25.82	26.33	26.36	26.89	26.89	26.91	27.49	27.49	28.05	28.07
0.80	22.28	22.32	22.37	22.72	22.76	23.17	23.20	23.64	23.67	24.11	24.11	24.15	24.64	24.64	25.11	25.15
0.90	20.30	20.33	20.37	20.67	20.69	21.04	21.07	21.43	21.46	21.83	21.83	21.86	22.28	22.28	22.68	22.71
1.00	18.73	18.74	18.77	19.03	19.05	19.35	19.36	19.67	19.69	20.00	20.00	20.02	20.37	20.37	20.70	20.72
1.10	17.45	17.46	17.47	17.72	17.72	17.98	17.99	18.26	18.26	18.54	18.53	18.54	18.84	18.83	19.12	19.13
1.20	16.38	16.38	16.38	16.62	16.62	16.86	16.86	17.10	17.10	17.34	17.34	17.34	17.59	17.59	17.84	17.84
1.30	15.41	15.42	15.42	15.65	15.65	15.88	15.88	16.11	16.11	16.33	16.33	16.33	16.56	16.56	16.78	16.78
1.40	14.51	14.52	14.52	14.76	14.76	14.99	14.99	15.22	15.22	15.44	15.44	15.44	15.65	15.65	15.86	15.86
1.50	13.64	13.65	13.65	13.90	13.91	14.15	14.15	14.39	14.39	14.61	14.61	14.61	14.83	14.83	15.04	15.03
1.60	12.79	12.80	12.81	13.07	13.07	13.33	13.33	13.58	13.58	13.82	13.81	13.82	14.04	14.04	14.26	14.26
1.70	11.96	11.97	11.98	12.25	12.26	12.53	12.53	12.79	12.79	13.04	13.04	13.04	13.28	13.28	13.51	13.51
1.80	11.15	11.16	11.18	11.45	11.46	11.74	11.75	12.02	12.02	12.28	12.28	12.28	12.54	12.53	12.77	12.77
1.90	10.39	10.40	10.41	10.69	10.70	10.98	10.99	11.26	11.27	11.54	11.54	11.54	11.81	11.80	12.05	12.05
1.99	9.74	9.75	9.76	10.04	10.05	10.33	10.34	10.61	10.62	10.89	10.89	10.90	11.16	11.16	11.41	11.42

Table 1 (*cont.*)

s_x	TB+4	DY	DY+3	HO	HO+3	ER	ER+3	TM	TM+3	YB	YB+2	YB+3	LU	LU+3	HF	TA
0.	61.00	66.00	63.00	67.00	64.00	68.00	65.00	69.00	66.00	70.00	68.00	67.00	71.00	68.00	72.00	73.00
0.05	60.35	64.37	62.29	65.39	63.30	66.42	64.31	67.44	65.32	68.46	67.25	66.33	69.39	67.34	70.42	71.45
0.10	58.52	61.14	60.31	62.19	61.34	63.24	62.38	64.29	63.41	65.34	65.16	64.44	66.11	65.47	67.05	68.03
0.15	55.80	57.72	57.40	58.79	58.46	59.86	59.51	60.92	60.57	61.99	62.11	61.62	62.67	62.68	63.47	64.33
0.20	52.57	54.18	53.99	55.25	55.06	56.32	56.13	57.39	57.19	58.46	58.54	58.26	59.22	59.33	59.96	60.73
0.25	49.20	50.60	50.47	51.66	51.52	52.72	52.58	53.78	53.64	54.84	54.86	54.71	55.70	55.77	56.46	57.21
0.30	45.93	47.19	47.09	48.21	48.11	49.23	49.14	50.27	50.17	51.31	51.30	51.21	52.24	52.26	53.04	53.79
0.35	42.89	44.05	43.97	45.02	44.95	46.01	45.93	47.00	46.92	48.00	47.99	47.93	48.93	48.94	49.76	50.53
0.40	40.15	41.22	41.15	42.13	42.07	43.07	43.00	44.01	43.95	44.96	44.95	44.90	45.87	45.87	46.70	47.48
0.50	35.43	36.33	36.29	37.13	37.10	37.96	37.92	38.79	38.76	39.65	39.65	39.61	40.47	40.47	41.27	42.04
0.60	31.48	32.20	32.20	32.91	32.90	33.64	33.63	34.38	34.37	35.14	35.14	35.12	35.89	35.89	36.64	37.38
0.70	28.09	28.66	28.68	29.28	29.30	29.92	29.93	30.57	30.59	31.24	31.25	31.25	31.94	31.94	32.64	33.34
0.80	25.18	25.64	25.67	26.18	26.21	26.73	26.76	27.30	27.33	27.89	27.89	27.92	28.52	28.52	29.16	29.81
0.90	22.75	23.12	23.15	23.58	23.61	24.06	24.09	24.55	24.57	25.05	25.05	25.08	25.60	25.60	26.17	26.76
1.00	20.76	21.07	21.10	21.46	21.48	21.86	21.88	22.27	22.29	22.69	22.69	22.72	23.16	23.16	23.66	24.17
1.10	19.15	19.43	19.44	19.74	19.76	20.08	20.09	20.42	20.43	20.77	20.77	20.79	21.16	21.16	21.58	22.01
1.20	17.86	18.10	18.10	18.36	18.37	18.64	18.65	18.93	18.93	19.22	19.22	19.23	19.54	19.54	19.88	20.24
1.30	16.78	17.01	17.01	17.24	17.24	17.47	17.47	17.71	17.71	17.96	17.96	17.96	18.22	18.22	18.50	18.80
1.40	15.86	16.07	16.07	16.28	16.28	16.49	16.49	16.70	16.70	16.92	16.92	16.92	17.14	17.14	17.37	17.61
1.50	15.04	15.24	15.24	15.44	15.44	15.64	15.63	15.83	15.83	16.03	16.03	16.03	16.22	16.22	16.43	16.63
1.60	14.26	14.46	14.46	14.67	14.66	14.86	14.86	15.05	15.05	15.24	15.24	15.24	15.42	15.42	15.61	15.79
1.70	13.51	13.72	13.72	13.93	13.93	14.13	14.13	14.32	14.32	14.51	14.51	14.51	14.69	14.69	14.87	15.05
1.80	12.78	13.00	13.00	13.22	13.22	13.43	13.43	13.63	13.63	13.82	13.82	13.82	14.01	14.01	14.19	14.37
1.90	12.06	12.29	12.29	12.52	12.52	12.74	12.74	12.95	12.95	13.15	13.15	13.15	13.35	13.35	13.54	13.72
1.99	11.43	11.66	11.67	11.90	11.91	12.13	12.13	12.35	12.35	12.56	12.56	12.56	12.76	12.77	12.97	13.15

s_x	W	RE	OS	IR	PT	AU	AU+1	HG	HG+2	TL	TL+1	PB	BI	BI+3	PO	AT
0.	74.00	75.00	76.00	77.00	78.00	79.00	78.00	80.00	78.00	81.00	80.00	82.00	83.00	80.00	84.00	85.00
0.05	72.47	73.50	74.52	75.55	76.64	77.66	76.98	78.62	77.12	79.42	78.86	80.37	81.34	79.12	82.34	83.34
0.10	69.04	70.06	71.09	72.13	73.36	74.41	74.22	75.27	74.69	75.96	75.90	76.72	77.56	76.71	78.45	79.37
0.15	65.24	66.18	67.15	68.13	69.33	70.37	70.42	71.19	71.19	71.93	72.00	72.61	73.30	73.28	74.02	74.78
0.20	61.53	62.37	63.25	64.15	65.19	66.16	66.25	66.99	67.16	67.79	67.83	68.50	69.15	69.36	69.79	70.43
0.25	57.96	58.72	59.51	60.32	61.19	62.07	62.12	62.91	63.05	63.73	63.75	64.50	65.19	65.34	65.83	66.44
0.30	54.52	55.24	55.97	56.71	57.45	58.23	58.25	59.05	59.12	59.87	59.86	60.66	61.40	61.46	62.09	62.73
0.35	51.26	51.97	52.66	53.35	54.01	54.72	54.71	55.48	55.49	56.27	56.26	57.05	57.81	57.81	58.54	59.22
0.40	48.21	48.91	49.59	50.25	50.87	51.52	51.51	52.23	52.21	52.96	52.96	53.71	54.46	54.43	55.20	55.91
0.50	42.77	43.47	44.14	44.79	45.39	45.99	45.97	46.61	46.57	47.23	47.23	47.88	48.55	48.52	49.24	49.93
0.60	38.10	38.80	39.48	40.13	40.75	41.34	41.34	41.93	41.91	42.50	42.50	43.07	43.65	43.65	44.25	44.86
0.70	34.04	34.73	35.40	36.06	36.70	37.31	37.31	37.90	37.90	38.46	38.46	39.01	39.55	39.55	40.09	40.63
0.80	30.48	31.14	31.80	32.45	33.09	33.72	33.72	34.31	34.32	34.89	34.89	35.44	35.98	35.99	36.50	37.01
0.90	27.37	27.98	28.61	29.23	29.86	30.47	30.48	31.08	31.08	31.66	31.66	32.23	32.78	32.78	33.31	33.82
1.00	24.71	25.26	25.82	26.40	26.99	27.57	27.58	28.16	28.16	28.74	28.74	29.31	29.87	29.87	30.41	30.93
1.10	22.47	22.94	23.44	23.95	24.48	25.02	25.02	25.57	25.57	26.12	26.12	26.67	27.22	27.22	27.76	28.28
1.20	20.62	21.02	21.44	21.88	22.34	22.81	22.81	23.31	23.31	23.81	23.81	24.32	24.84	24.84	25.36	25.87
1.30	19.11	19.44	19.79	20.16	20.54	20.95	20.95	21.38	21.38	21.82	21.82	22.28	22.75	22.75	23.23	23.71
1.40	17.87	18.14	18.43	18.73	19.06	19.39	19.39	19.76	19.75	20.14	20.14	20.53	20.95	20.94	21.38	21.81
1.50	16.85	17.07	17.31	17.56	17.83	18.11	18.11	18.41	18.41	18.73	18.73	19.06	19.42	19.41	19.79	20.17
1.60	15.98	16.18	16.38	16.59	16.81	17.05	17.04	17.29	17.29	17.56	17.56	17.84	18.13	18.13	18.45	18.77
1.70	15.23	15.40	15.58	15.77	15.96	16.15	16.15	16.36	16.36	16.58	16.58	16.82	17.06	17.06	17.32	17.60
1.80	14.54	14.71	14.88	15.05	15.22	15.39	15.39	15.57	15.57	15.76	15.76	15.96	16.16	16.16	16.38	16.61
1.90	13.90	14.07	14.23	14.40	14.56	14.72	14.72	14.89	14.88	15.05	15.05	15.22	15.40	15.40	15.59	15.78
1.99	13.34	13.51	13.69	13.85	14.01	14.17	14.17	14.33	14.33	14.48	14.48	14.64	14.80	14.80	14.97	15.13

s_x	RN	FR	RA	AC	TH	TH+4	PA	U	U+4	NP	PU	PU+4	AM	CM	BK	CF
0.	86.00	87.00	88.00	89.00	90.00	86.00	91.00	92.00	88.00	93.00	94.00	90.00	95.00	96.00	97.00	98.00
0.05	84.35	84.89	85.66	86.61	87.57	85.00	88.68	89.71	87.00	90.74	91.83	89.01	92.86	93.83	94.85	95.88
0.10	80.32	80.92	81.42	82.14	82.86	82.24	84.18	85.23	84.24	86.27	87.56	86.27	88.62	89.43	90.48	91.53
0.15	75.58	76.39	77.05	77.65	78.24	78.34	79.57	80.57	80.29	81.59	82.93	82.31	83.98	84.72	85.77	86.82
0.20	71.09	71.85	72.61	73.24	73.84	74.00	74.99	75.93	75.84	76.90	78.10	77.78	79.12	79.91	80.94	81.98
0.25	67.03	67.68	68.39	69.03	69.66	69.74	70.60	71.46	71.41	72.35	73.38	73.21	74.32	75.16	76.14	77.13
0.30	63.33	63.92	64.55	65.17	65.80	65.81	66.57	67.34	67.30	68.13	69.02	68.93	69.88	70.70	71.60	72.53
0.35	59.87	60.47	61.06	61.66	62.27	62.25	62.93	63.62	63.58	64.33	65.10	65.04	65.87	66.64	67.46	68.30
0.40	56.59	57.23	57.83	58.44	59.03	59.00	59.63	60.25	60.22	60.89	61.57	61.54	62.27	62.97	63.71	64.47
0.50	50.62	51.29	51.94	52.58	53.20	53.18	53.72	54.28	54.30	54.85	55.40	55.43	55.99	56.61	57.22	57.85
0.60	45.49	46.13	46.76	47.39	48.02	48.01	48.53	49.07	49.11	49.60	50.10	50.16	50.63	51.19	51.73	52.27
0.70	41.18	41.74	42.32	42.90	43.49	43.49	43.99	44.52	44.55	45.03	45.51	45.57	46.00	46.53	47.02	47.51
0.80	37.52	38.03	38.55	39.07	39.60	39.60	40.11	40.61	40.63	41.10	41.57	41.61	42.04	42.53	42.99	43.44
0.90	34.33	34.81	35.30	35.79	36.27	36.27	36.77	37.26	37.25	37.73	38.20	38.20	38.65	39.10	39.54	39.97
1.00	31.44	31.93	32.42	32.89	33.35	33.35	33.85	34.33	34.31	34.79	35.26	35.24	35.71	36.14	36.57	36.99
1.10	28.80	29.30	29.79	30.27	30.73	30.73	31.23	31.70	31.68	32.17	32.64	32.61	33.09	33.51	33.94	34.36
1.20	26.39	26.89	27.38	27.86	28.33	28.33	28.82	29.30	29.28	29.77	30.24	30.21	30.69	31.13	31.56	31.99
1.30	24.20	24.69	25.17	25.65	26.12	26.11	26.60	27.07	27.06	27.54	28.01	27.99	28.47	28.91	29.35	29.79
1.40	22.26	22.72	23.17	23.63	24.09	24.09	24.55	25.01	25.01	25.47	25.94	25.92	26.39	26.84	27.28	27.72
1.50	20.57	20.98	21.40	21.83	22.26	22.26	22.69	23.13	23.13	23.57	24.02	24.01	24.46	24.90	25.34	25.78
1.60	19.12	19.48	19.85	20.24	20.63	20.63	21.03	21.43	21.43	21.85	22.26	22.26	22.69	23.11	23.54	23.97
1.70	17.89	18.20	18.52	18.86	19.21	19.21	19.56	19.93	19.93	20.31	20.69	20.69	21.08	21.48	21.89	22.29
1.80	16.86	17.12	17.39	17.68	17.99	17.98	18.30	18.62	18.62	18.95	19.30	19.30	19.65	20.02	20.39	20.77
1.90	15.99	16.21	16.44	16.68	16.94	16.94	17.21	17.49	17.49	17.78	18.08	18.09	18.40	18.73	19.06	19.41
1.99	15.32	15.50	15.70	15.91	16.14	16.14	16.37	16.61	16.61	16.87	17.13	17.13	17.41	17.71	18.01	18.32

Table 2. *Coefficients for the five-parameter analytic fit of Hartree scattering factors in the range* $0 \le s_x \le 0{\cdot}64$ Å^{-1}

ATOM	A(1)	B(1)	A(2)	B(2)	C	E
RB	16.5333	3.9759	7.2534	36.0201	12.8639	0.321
RB+1	17.0149	2.7482	8.4814	25.1250	10.4753	0.051
SR	17.0896	5.3456	5.6899	56.3175	14.9150	0.406
SR+2	16.8228	2.4559	8.7587	20.0379	10.4040	0.027
Y	17.4464	5.6240	5.7065	66.6780	15.6319	0.347
Y+3	16.6524	2.2060	9.0139	16.4670	10.3255	0.015
ZR	17.5948	5.5840	6.1580	62.3425	16.0655	0.293
ZR+4	16.4874	1.9965	9.2427	13.8517	10.2655	0.009
NB	17.6565	5.5257	6.6853	52.1563	16.4722	0.262
MO	17.9633	5.5544	6.9719	47.8551	16.8927	0.233
TC	18.6250	5.6956	6.8701	49.9512	17.3497	0.217
RU	18.9913	5.6681	7.1817	41.8513	17.6727	0.192
RH	19.7051	5.7197	7.1316	39.8075	18.0159	0.176
PD	20.0027	5.4734	7.7869	33.1066	18.1133	0.122
PD+2	18.2359	4.3969	8.6012	20.1813	17.1380	0.040
AG	21.4452	5.7610	6.8141	36.9677	18.6050	0.151
AG+1	19.8766	4.9129	8.1985	24.0012	17.8845	0.058
CD	22.6820	5.8314	6.2562	42.5278	18.9385	0.151
CD+2	19.7388	4.4323	8.5801	18.4994	17.6624	0.029
IN	23.7881	5.8427	5.7728	51.7357	19.2639	0.179
SN	24.3943	5.5672	6.1130	55.9134	19.3529	0.158
SB	24.7214	5.1748	6.8531	54.0641	19.3118	0.131
TE	24.9089	4.7758	7.7619	49.8839	19.2316	0.110
I	24.9994	4.4114	8.7482	45.3012	19.1647	0.097
XE	25.0082	4.0941	9.7690	41.0062	19.1415	0.088
CS	24.9633	4.1869	9.6892	40.4741	19.9520	0.231
BA	25.1350	4.7150	8.8835	47.6319	21.4966	0.342
LA	25.2977	4.9555	8.8401	52.7840	22.4435	0.341
LA+3	24.7310	2.9399	11.2094	22.2741	18.0449	0.018
CE	26.0655	4.8170	8.8664	46.2950	22.6077	0.330
CE+3	25.1585	2.9115	11.4725	21.3889	18.3546	0.018
CE+4	24.6439	2.6640	11.6186	19.0921	17.7282	0.011
PR	26.7024	4.8264	8.7660	45.3141	23.0767	0.321
PR+3	25.6538	2.8919	11.6529	20.6155	18.6784	0.018
PR+4	25.1529	2.6492	11.8038	18.3999	18.0341	0.011
ND	27.3846	4.8353	8.6138	44.7743	23.5558	0.313
ND+3	26.2086	2.8704	11.7876	19.9157	18.9891	0.017
PM	28.0905	4.8354	8.4393	44.4364	24.0330	0.305
PM+3	26.8016	2.8519	11.8733	19.2942	19.3106	0.017
SM	28.8108	4.8289	8.2478	44.2862	24.5139	0.297
SM+3	27.4297	2.8322	11.9260	18.7335	19.6302	0.016
EU	29.5335	4.8144	8.0515	44.2451	24.9972	0.288
EU+2	28.4660	3.0727	11.7534	20.8289	20.7554	0.027
EU+3	28.0815	2.8126	11.9488	18.2262	19.9561	0.015
GD	30.1636	4.9709	7.6514	52.4089	25.8435	0.277
GD+3	28.7569	2.7882	11.9605	17.7494	20.2693	0.015
TB	30.9679	4.7659	7.6590	44.3971	25.9752	0.273
TB+3	29.4474	2.7635	11.9513	17.3147	20.5885	0.014
TB+4	28.9643	2.5569	12.1364	15.4637	19.8912	0.008
DY	31.6701	4.7330	7.4692	44.5656	26.4728	0.265
DY+3	30.1455	2.7399	11.9205	16.9169	20.9216	0.013
HO	32.3624	4.6967	7.2851	44.7812	26.9751	0.257
HO+3	30.8564	2.7121	11.8875	16.5394	21.2440	0.012
ER	33.0370	4.6567	7.1066	45.0403	27.4890	0.250
ER+3	31.5735	2.6827	11.8479	16.1841	21.5668	0.012
TM	33.6996	4.6143	6.9349	45.3208	28.0079	0.242
TM+3	32.2908	2.6547	11.7932	15.8574	21.9047	0.011
YB	34.3459	4.5688	6.7729	45.6107	28.5333	0.235
YB+2	33.3530	2.8655	11.3993	17.8694	23.2277	0.019
YB+3	33.0087	2.6263	11.7312	15.5500	22.2492	0.011
LU	34.8547	4.6251	6.5320	56.1354	29.3382	0.220
LU+3	33.7321	2.5946	11.6741	15.2513	22.5830	0.010
HF	35.0288	4.4811	7.0486	54.8053	29.6916	0.194
TA	35.1026	4.3540	7.5990	51.4121	30.0821	0.176
W	35.1202	4.2657	8.1109	47.8895	30.5602	0.165
RE	35.1186	4.2156	8.5579	44.7416	31.1167	0.157
OS	35.1293	4.1977	8.9299	42.0246	31.7365	0.150
IR	35.1819	4.2081	9.2170	39.7756	32.3979	0.145
PT	35.0496	4.1106	9.9935	33.7924	32.7642	0.127
AU	35.2109	4.1429	10.1868	32.1853	33.4126	0.121
AU+1	34.6042	3.5668	11.5912	23.6873	31.7383	0.054
HG	35.8174	4.3428	9.5646	35.1501	34.4244	0.131
HG+2	34.3561	3.2398	12.4275	19.0264	31.1814	0.029
TL	36.5754	4.5741	8.6870	40.6731	35.4608	0.160
TL+1	36.0217	4.0914	9.6435	29.4016	34.2289	0.083
PB	37.2236	4.6412	8.4498	46.4014	36.0897	0.156
BI	37.6775	4.5367	8.8179	48.6453	36.3122	0.137
BI+3	36.5195	3.6605	9.5868	22.1225	33.8522	0.036
PO	38.0076	4.3479	9.5162	47.9631	36.3187	0.115
AT	38.2553	4.1290	10.3919	45.7646	36.2174	0.098
RN	38.4392	3.9054	11.3707	42.9587	36.0719	0.084
FR	38.4322	3.8667	11.5458	41.7445	36.5842	0.162
RA	38.2966	4.0698	11.1797	45.2636	37.9482	0.241
AC	38.2488	4.1918	11.2328	48.8186	38.9807	0.253
TH	38.2017	4.3113	11.3396	52.7127	39.9792	0.255
TH+4	39.0571	2.7317	13.5315	22.0728	33.3944	0.013
PA	38.5521	4.2686	11.6431	45.3758	40.2732	0.247
U	38.8814	4.3315	11.6605	44.2456	40.9304	0.244
U+4	39.1181	2.6930	14.6122	20.3739	34.2522	0.012
NP	39.3215	4.3992	11.5864	43.4582	41.5702	0.241
PU	39.8734	4.2972	11.9458	37.9977	41.6298	0.226
PU+4	39.3876	2.7025	15.3433	18.9922	35.2521	0.012
AM	40.4823	4.3498	11.7823	37.4681	42.1900	0.223
CM	41.1934	4.5778	11.0092	42.5817	43.3005	0.229
BK	41.9515	4.6209	10.7471	42.6494	43.8149	0.224
CF	42.7543	4.6529	10.4717	42.8391	44.2982	0.220

later stages of the work, with an IBM 7094. Scattering factors were computed at 200 points in the range $s_x = \sin\theta/\lambda$ from 0 to 1·99 Å^{-1} at intervals of 0·01 Å^{-1}. This large number of points was used to facilitate fitting the curves to analytic functions. The calculations for the 200 points required about 20 seconds per atom when using the 7094 computer.

Explanation of the tables

The results are given in three different forms. Table 1 lists the values of f as a function of s_x at the intervals used in *International Tables for X-ray Crystallography* (1962). Tables 2 and 3 give the coefficients a_i, b_i and c which fit the function

$$f(s_x) = \sum_{i=1}^{n} a_i \exp(-b_i s_x^2) + c\,. \qquad (1)$$

In Table 2, $n=2$ in equation (1) and the coefficients fit the curves in the range $s_x=0$ to $s_x=0{\cdot}64$, the practical limit when using Cu $K\alpha$ radiation. In Table 3, $n=4$ and the entire curve from $s_x=0$ to $s_x=1{\cdot}99$ is fitted. The scheme used was that of Forsyth & Wells (1959), in which the points are weighted by the factor $w=\exp\{-(s_x-0{\cdot}5)^2\}$ so that the curve is fitted best near $s_x=0{\cdot}5$ and $\left(\sum_{i=1}^{n} a_i + c\right)$ is not required to equal $f(0)$. In Tables 2 and 3, following Forsyth & Wells, the quantity

$$E = \frac{100}{f(0)}\left(\frac{\Sigma w_j \delta_j^2}{\Sigma w_j}\right)^{\frac{1}{2}},$$

the error of the fit as a percentage of the scattering factor at $s_x=0$, is also given.

In general, the nine-parameter fit of the entire curve is very good. Except for values of $s_x > 1{\cdot}90$ for elements 77 through 86 the magnitude of the difference between the true curve and the analytic expression is $<0{\cdot}1$ electron at all points. The five-parameter fit is not as good but is certainly adequate for most work. It happens that for each element the magnitude of E is equal, within a factor of about 2,

Table 3. *Coefficients for the nine-parameter analytic fit of Hartree scattering factors in the range* $0 \leq s_x \leq 1{\cdot}99$ Å^{-1}

ATOM	A(1)	B(1)	A(2)	B(2)	A(3)	B(3)	A(4)	B(4)	C	E
RB	16.5142	2.0124	9.3058	20.1847	5.5015	0.4031	1.5961	197.5854	4.0558	0.040
RB+1	17.3342	1.8798	7.1219	16.4621	5.6220	0.2208	3.1319	37.3740	2.7876	0.004
SR	17.2535	1.7136	9.5762	16.2184	5.1740	0.2455	2.6828	160.5856	3.2961	0.021
SR+2	17.7192	1.6546	8.0681	14.6977	6.9256	0.1201	2.3613	30.5154	0.9256	0.002
Y	17.6338	1.5156	9.9155	14.0658	5.4951	0.1599	3.5069	127.3560	2.4227	0.024
Y+3	18.1839	1.4552	8.9869	13.0441	1.6377	26.3317	-13.4044	-0.0332	20.5960	0.004
ZR	17.6473	1.3819	10.4321	12.9203	4.8685	0.1747	4.0279	103.6089	2.9910	0.032
ZR+4	18.1821	1.3214	10.0832	11.8785	0.6535	27.7977	-84.9411	-0.0050	92.0237	0.008
NB	15.7473	1.3608	11.2084	12.6192	5.1880	0.4507	4.1132	86.8618	4.6961	0.045
MO	16.0315	0.8728	11.8176	12.2235	4.5749	2.0642	4.2377	77.4332	5.2900	0.049
TC	19.2788	0.9275	11.1498	9.0096	4.2116	27.9883	2.8748	104.0926	5.4762	0.029
RU	19.3706	0.8635	12.1463	8.8756	4.9840	28.6028	2.0624	107.2206	5.4296	0.018
RH	19.3996	0.8009	13.2539	8.5500	5.1668	28.3901	1.8113	108.4500	5.3625	0.011
PD	19.4218	0.7426	14.0808	8.1549	5.6880	26.5853	1.5231	84.7432	5.2835	0.010
PD+2	19.3998	0.7410	14.2563	8.1389	4.9092	24.2898	0.1589	76.7400	5.2767	0.011
AG	19.4063	0.6865	15.3199	7.7399	5.5348	26.0246	1.5496	107.4603	5.1842	0.014
AG+1	19.4119	0.6865	15.1795	7.7414	5.6057	24.3718	0.6205	66.5566	5.1830	0.014
CD	19.3721	0.6331	16.4245	7.2446	5.0163	24.8556	2.1200	96.8479	5.0620	0.016
CD+2	19.3883	0.6337	16.2846	7.2913	5.1777	21.9446	0.0864	86.9545	5.0637	0.017
IN	19.3439	0.5848	17.7412	6.8188	4.8449	27.6025	2.1182	129.8031	4.9352	0.021
SN	19.3014	0.5374	18.5993	6.2897	4.5484	27.7752	2.7704	110.3681	4.7678	0.020
SB	19.2753	5.7629	19.2639	0.4924	4.7174	29.0928	3.1664	96.0526	4.5675	0.019
TE	19.7565	5.2466	19.2411	0.4491	5.4572	30.3364	3.2205	87.0985	4.3187	0.018
I	20.0896	4.7556	19.2485	0.4072	6.6026	30.4497	3.0490	80.9784	4.0067	0.017
XE	20.3365	4.3012	19.3104	0.3663	7.9384	29.4767	2.8053	76.2643	3.6078	0.017
CS	20.5568	3.9191	19.4002	0.3312	10.2541	29.0119	1.5535	268.7687	3.2197	0.022
BA	20.5732	3.5068	19.7214	0.2879	10.5693	23.7801	2.6838	212.6900	2.4436	0.018
LA	20.7784	3.1939	20.1376	0.2521	10.9920	21.3700	3.4251	167.2029	1.6519	0.020
LA+3	20.7479	3.1843	20.1808	0.2505	11.2606	21.3634	0.2274	73.1375	1.5852	0.019
CE	21.5670	3.1245	20.0793	0.2446	11.6905	20.7801	2.8792	184.4509	1.7689	0.015
CE+3	21.3257	3.0267	20.4455	0.2305	11.6024	19.8448	0.4493	54.9910	1.1795	0.015
CE+4	20.9812	0.2126	20.8721	2.8873	11.7235	18.7112	0.0755	94.0054	0.3488	0.019
PR	22.1949	2.9915	20.1377	0.2310	12.1342	19.6858	2.8784	178.0122	1.6365	0.015
PR+3	21.9393	2.8868	20.7102	0.2130	11.7571	18.4000	0.8067	43.9672	0.7883	0.012
PR+4	21.5331	2.7679	21.3081	0.1965	12.0743	17.6263	0.1692	62.9981	-0.0833	0.015
ND	22.8448	2.8737	20.1050	0.2206	12.5154	18.7051	2.8901	171.8270	1.6248	0.016
ND+3	22.5774	2.7609	20.9568	0.1978	11.7455	17.0565	1.2900	37.0673	0.4312	0.009
PM	23.5072	2.7687	19.9531	0.2138	12.8518	17.8342	2.9026	166.1495	1.7627	0.018
PM+3	23.2299	2.6451	21.1856	0.1845	11.5999	15.7978	1.8830	32.4657	0.1021	0.007
SM	24.1752	2.6741	19.6771	0.2101	13.1515	17.0537	2.9160	160.9784	2.0557	0.020
SM+3	23.8893	2.5381	21.3819	0.1730	11.3730	14.6350	2.5391	29.2025	-0.1834	0.005
EU	24.8393	2.5887	19.2688	0.2100	13.4207	16.3526	2.9286	156.1363	2.5161	0.022
EU+2	24.7469	2.4972	20.8995	0.1749	10.8265	13.7528	4.1079	30.2277	0.4163	0.003
EU+3	24.5558	2.4381	21.5415	0.1629	11.1384	13.5842	3.1882	26.8253	-0.4244	0.003
GD	25.3127	2.4346	19.4286	0.1930	13.4300	14.9463	3.6693	131.5278	2.1290	0.021
GD+3	25.2239	2.3460	21.6119	0.1548	10.9406	12.6563	3.7821	25.0111	-0.5597	0.002
TB	26.1346	2.4409	18.1660	0.2196	13.8860	15.1471	2.9472	147.8025	3.8363	0.026
TB+3	25.8913	2.2598	21.6016	0.1482	10.7728	11.8211	4.3358	23.5336	-0.6031	0.002

or less, to the magnitude of the maximum deviation of the analytic curve from the true curve.

Effect of configuration

Scattering factors were also computed from the wave functions of atoms in several excited states. Changes in the configurations of outer electrons can produce differences as great as 0·7 electron. An example of this effect for cerium is shown in Table 4. Below $s_x = 0{\cdot}5$, the more stable states have larger scattering factors. For $s_x > 0{\cdot}5$ the scattering factors are essentially the same.

Comparison of Thomas-Fermi-Dirac and Hartree scattering factors

The differences, at $s_x = 0{\cdot}05$ Å^{-1}, between the Thomas–Fermi–Dirac (TFD) and Hartree (H) scattering factors are plotted against Z, the atomic number, in Fig. 1. Note that at this small value of s_x, the difference is always positive. At small s_x values the difference between two scattering curves reflects the difference between the respective radial density functions at

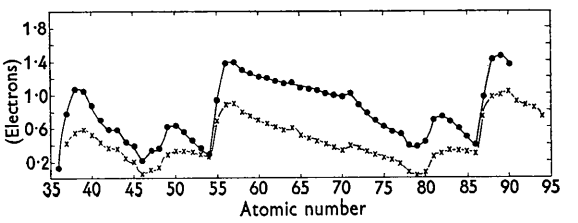

Fig. 1. Plot of $f_{TFD} - f_H$ *versus* Z at $s_x = 0{\cdot}05$, and plot of δ, the number of electrons in the Hartree density function outside 4·675 Bohr radii, *versus* Z.

● Electrons outside TFD discontinuity.
× $f_{TFD} - f_H$ at $s_x = 0{\cdot}05$.

Table 3 (*cont.*)

ATOM	A(1)	B(1)	A(2)	B(2)	A(3)	B(3)	A(4)	B(4)	C	E
TB+4	25.6590	2.1986	22.6978	0.1340	11.5775	11.8625	3.0041	22.2210	-1.9390	0.002
DY	26.7543	2.3774	17.5330	0.2296	14.0805	14.6300	2.9545	144.0925	4.6461	0.027
DY+3	26.5627	2.1801	21.4745	0.1434	10.7287	11.1224	4.7442	22.4382	-0.5121	0.002
HO	27.3401	2.3198	16.9187	0.2427	14.2608	14.1502	2.9622	140.5160	5.4854	0.029
HO+3	27.2309	2.1055	21.2387	0.1401	10.7124	10.4939	5.1149	21.4753	-0.2994	0.002
ER	27.8965	2.2682	16.3492	0.2594	14.4143	13.7220	2.9656	137.4589	6.3405	0.030
ER+3	27.8971	2.0363	20.8519	0.1387	10.7618	9.9551	5.4012	20.6752	0.0850	0.002
TM	28.4033	2.2223	15.8754	0.2792	14.5534	13.3267	2.9670	134.5847	7.1657	0.031
TM+3	28.5595	1.9721	20.3541	0.1389	10.8491	9.4812	5.6337	19.9825	0.6003	0.002
YB	28.8530	2.1819	15.5181	0.3023	14.6735	12.9635	2.9681	131.8887	7.9514	0.031
YB+2	29.3481	1.9637	18.4873	0.1629	11.5681	9.5586	5.7304	22.9149	2.8596	0.005
YB+3	29.2165	1.9126	19.7203	0.1411	10.9900	9.0767	5.7924	19.4015	1.2772	0.003
LU	29.2842	2.0645	15.2765	0.2925	14.6089	11.8505	3.7588	115.5326	8.0298	0.028
LU+3	29.8657	1.8563	19.0669	0.1443	11.1270	8.6996	5.9490	18.8440	1.9874	0.003
HF	29.5377	1.9836	14.9772	0.3032	14.5507	11.2965	4.3739	96.7527	8.5161	0.029
TA	29.5857	1.9213	14.7541	0.3285	14.5902	11.0144	4.8215	84.7554	9.1965	0.031
W	29.3788	1.8703	14.7860	10.8776	14.7475	0.3632	5.1297	76.5858	9.9018	0.034
RE	28.8739	1.8259	15.1645	10.7930	15.0335	0.4038	5.3231	70.7407	10.5438	0.035
OS	27.9724	1.7910	15.7149	0.4508	15.7093	10.7153	5.4197	66.4032	11.1205	0.036
IR	26.4763	1.7741	16.9913	0.5066	16.3881	10.6267	5.4363	63.2119	11.6428	0.037
PT	24.9683	1.7438	18.3297	0.5481	17.2974	10.5880	5.3354	54.5868	11.9990	0.037
AU	22.0195	1.7765	21.0803	0.6128	18.1701	10.4154	5.2590	52.3563	12.3991	0.037
AU+1	31.0910	1.3638	17.5193	8.9561	12.7498	0.2981	6.4650	31.9786	10.1503	0.015
HG	26.6359	0.7118	18.7561	10.2800	16.5302	2.0187	5.1493	57.8082	12.8658	0.037
HG+2	33.4136	1.2069	17.8625	8.1639	13.0979	0.1532	6.6894	24.6522	6.9228	0.008
TL	34.4672	0.8371	16.7874	11.6599	11.8240	3.5233	4.3857	78.2228	13.4505	0.046
TL+1	21.7465	0.6022	20.4389	1.5600	19.7267	8.8670	5.5358	42.2926	12.5162	0.023
PB	36.1149	0.8403	13.7530	4.5402	13.7165	12.4123	4.7855	82.0069	13.5724	0.040
BI	36.8680	0.8232	17.4494	5.2824	9.6440	13.9966	5.4009	77.6668	13.5950	0.033
BI+3	29.9892	1.0836	21.0752	7.1837	11.6322	0.3476	5.8041	26.3466	11.4825	0.011
PO	37.2499	0.7978	20.9040	5.6479	6.5211	18.1007	5.7292	73.6946	13.5683	0.026
AT	37.3710	0.7662	22.5060	5.5777	6.1489	23.6453	5.4736	71.8624	13.4832	0.018
RN	37.3405	0.7313	23.1931	5.3025	7.3853	27.7083	4.7153	71.5307	13.3570	0.011
FR	37.3175	0.6992	23.6784	5.0339	11.0892	32.8751	1.6591	280.9454	13.2361	0.013
RA	37.0921	0.6610	23.6303	4.6101	11.4606	27.5458	2.7811	233.0863	13.0270	0.006
AC	36.9437	0.6275	23.8438	4.2987	11.8162	25.2345	3.5449	186.2107	12.8371	0.009
TH	36.7851	0.5953	24.0510	4.0096	12.0856	23.0425	4.4267	154.3940	12.6339	0.011
TH+4	36.7349	0.5936	23.8855	3.9689	12.7150	22.6239	0.0560	128.5321	12.6086	0.010
PA	37.0896	0.5765	24.3770	3.9828	13.3409	22.5782	3.6094	170.6033	12.5645	0.010
U	37.2011	0.5537	24.7273	3.8671	13.9892	21.4042	3.6294	164.9693	12.4327	0.011
U+4	36.9548	0.5465	24.4545	3.7223	14.0530	20.1567	0.2083	68.7280	12.3296	0.009
NP	37.3223	0.5322	25.1400	3.7690	14.5642	20.3493	3.6491	159.9586	12.3023	0.011
PU	37.6021	0.5162	25.7684	3.7753	15.3933	20.1111	2.9721	179.9459	12.2428	0.012
PU+4	37.2009	0.5038	25.2397	3.5332	14.9558	17.9797	0.5718	45.7443	12.0321	0.008
AM	37.7195	0.4966	26.3530	3.6992	15.8209	19.2760	2.9702	175.8520	12.1137	0.013
CM	37.6825	0.4733	26.7809	3.5366	15.9106	17.8125	3.7019	147.8731	11.8971	0.013
BK	37.7918	0.4552	27.4536	3.4709	16.2534	17.1326	3.7167	144.5725	11.7560	0.013
CF	37.8937	0.4378	28.1851	3.4084	16.5505	16.5194	3.7301	141.5922	11.6109	0.014

Table 4. *Effect of configuration on scattering factor of* Ce

s_x	$f_{Ce}(4f^26s^2)$*	$f_{Ce}(4f^15d^16s^2)$	$f_{Ce}(5d^26s^2)$
0·00	58·00	58·00	58·00
0·05	56·13	56·08	56·07
0·10	52·67	52·45	52·29
0·15	49·21	48·91	48·60
0·20	45·77	45·53	45·18
0·25	42·47	42·31	42·00
0·30	39·50	39·38	39·13
0·35	36·89	36·80	36·60
0·40	34·58	34·51	34·37
0·45	32·50	32·45	32·36
0·50	30·59	30·57	30·52
0·55	28·81	28·82	28·81
0·60	27·17	27·19	27·21
0·65	25·65	25·68	25·72
0·70	24·25	24·29	24·34
0·75	22·99	23·03	23·09
0·80	21·86	21·89	21·95
0·85	20·85	20·88	20·92
0·90	19·95	19·97	20·01
0·95	19·15	19·16	19·19
1·00	18·43	18·44	18·46

* Presumed ground state.

large radii. The TFD radial density is required to drop abruptly to zero at a certain radius, r_D, in order to provide the proper number of electrons, Z, in the radial domain. This radius, r_D, varies in a nearly linear manner from about 4·54 Bohr units at $Z=37$ to about 4·82 Bohr units at $Z=94$.

In Fig. 1 the number of electrons, δ, outside 4·765 Bohr units (which is the nearest value to r_D at which the quantities were computed) is also plotted against Z. The two curves in Fig. 1 are seen to be very similar in shape.

For $s_x=0{\cdot}05$ Å^{-1}, the ratio $R=(\sin 4\pi rs)/(4\pi rs)$ decreases from unity as r increases and becomes zero the first time at $r\approx 9{\cdot}45$ Bohr units, well outside r_D. *All* of the electrons in a TFD atom thus scatter with phases of the same sign; this is not true for the Hartree atoms because there is a non-vanishing probability of finding electrons at large radial distances. In the range 0 to r_D, R is a slowly decreasing function of r and is always larger than

$$R_0=(\sin 4\pi r_D 0{\cdot}05)/(4\pi r_D 0{\cdot}05)=0{\cdot}63\ .$$

Beyond r_D the ratio R is always smaller than R_0 and eventually its sign alternates.

The integral of U, the charge density, can be broken into two parts, one for the range zero to r_D and the second for r_D to infinity. In the Hartree model, there are a small number of electrons δ which lie outside r_D. Because both the TFD and H densities are normalized to Z, the number of electrons in the atom or ion, one can write

$$\int_0^\infty \Delta U dr=\int_0^{r_D}(U_{\mathrm{TFD}}-U_{\mathrm{H}})dr+\int_{r_D}^\infty (U_{\mathrm{TFD}}-U_{\mathrm{H}})dr$$
$$=[Z-(Z-\delta)]+[0-\delta]=0\ . \qquad (2)$$

The difference between scattering factors can be written in a similar fashion, *i.e.*

$$\Delta f=\int_0^{r_D} R\Delta U dr+\int_{r_D}^\infty R\Delta U dr\ . \qquad (3)$$

Canfield & Waber (1963) show that U_{TFD} and U_{H} are quite similar in magnitude for radii in the range $0<\varepsilon\leq r\leq r_D$. Thus the first integral of (3) is always larger than δR_0. Because of the alternating sign of R, the second integral of (3) will be less than δR_0 by some factor γ which is small. Thus

$$\Delta f\geq \delta R_0-\gamma\delta R_0\ , \qquad (4)$$

and for small s_x, Δf should have a strong dependence on the variation of δ with Z. An inference from this argument is that when relativistic-exchange charge densities become available for calculating scattering factors, the quantity $(f_{\mathrm{TFD}}-f_{\mathrm{RE}})$ will be positive for small s_x and behave similarly with Z.

At $s_x=0{\cdot}1$ Å^{-1}, the ratio R first becomes negative at $r\approx 4{\cdot}72$ Bohr units, and this radius is approximately r_D. Thus f_{TFD} must be greater than f_{H} for s_x less than about 0·1 Å^{-1}, but for s greater than about 0·1 Å^{-1} this need not be true. The differences become complicated owing to the presence of several maxima in the Hartree density (which arise from the shell structure) while the TFD density has a single maximum. The differences for $s_x=0{\cdot}25$, 0·5 and 1·0 Å^{-1} are plotted in Fig. 2.

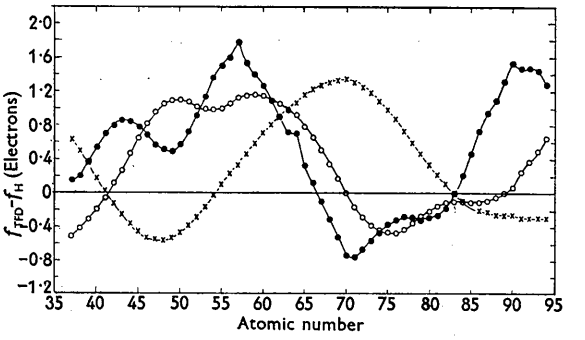

Fig. 2. Plot of $f_{\mathrm{TFD}}-f_{\mathrm{H}}$ *versus* Z at $s_x=0{\cdot}25$, 0·50 and 1·00 Å^{-1}.

● $s_x=0{\cdot}25$.
○ $s_x=0{\cdot}50$.
× $s_x=1{\cdot}00$.

The minima in the curves of Fig. 1 occur at atoms with filled outer shells, for these atoms have very low electron densities outside r_D. It is of interest to note some of the discontinuities in the curves of Fig. 1. These are caused by changes in configuration. For example in La, $Z=57$, there is one $5d$ electron whereas there are none at $Z=56$ or 58. A similar situation occurs at Gd, $Z=64$. At Yb, $Z=70$, the $4f$ shell has just been filled and at $Z=71$ the $5d$ shell starts to fill. Another case is at $Z=43$ where there are two $5s$ electrons in Tc and only one in Mo and Ru. Also, one notes the effect of the contraction of the atoms as the $4d$ or $4f$ shells are filled. Some of the configurational discontinuities are still apparent in the $s_x=0{\cdot}25$ Å^{-1} curve of Fig. 2 but at higher s_x these discontinuities are smoothed out.

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