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# ACCUMULATED TABLE OF BOND VALENCE PARAMETERS
Data_BOND_VALENCE_PARAMETERS_2006-05-02
# BVPARM.CIF
_audit_conform_dict_name      cif_core.dic
_audit_conform_dict_version    2.2

#*****
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# Materials Research, McMaster University, Hamilton, Ontario Canada.
# idbrown@mcmaster.ca
#
#*****DISCLAIMER*****
#
# The values reported here are taken from the literature and
# other sources and the author does not warrant their correctness
# nor accept any responsibility for errors. Users are advised to
# consult the primary sources.
#
#*****
#
# The parameters given in the main table are the values of Ro and
# B used in the equation:
#
#      bond valence = exp((Ro-R)/B)
#
# where R is the bond length. All values are in Angstrom units.
# Where significantly different values have been reported in the
# literature, they are listed in decreasing order of reliability.
#
#      Bond valence parameters for atoms whose oxidation state is
# given as 9 do not have an oxidation state
# specified in the original citation. They may apply to a
# particular, but unspecified, oxidation state or they may be
# intended to apply to all oxidation states.
#
# The ammonium ion is listed under the symbol NH.
#
#      The list below is formatted and is designed to be read
# either as a crystallographic information file (CIF) or as a
# fixed format file once the text has been stripped off.
#*****#3
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;2001-03-13 Ref m deleted.
2001-06-01
2001-06-21 new ref c and d added.
2002-03-22 new ref q added
2003-02-17 refs m, z and aa added
2003-02-19 corrected CIF errors
2004-08-12 correction of errors
2006-05-02 refs ag to ai added
;
_audit_author_name        'I. David Brown'
_audit_author_address
;          Brockhouse Institute for Materials Research
          McMaster University

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Tuesday January 20, 2009

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Hamilton, Ontario, Canada L8S 4M1
;
_audit_contact_author_name   'I. David Brown'
_audit_contact_author_email  idbrown@mcmaster.ca

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_valence_ref_id
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a 'Brown and Altermatt, (1985), Acta Cryst. B41, 244-247 (empirical)'
b 'Brese and O'Keeffe, (1991), Acta Cryst. B47, 192-197 (extrapolated)'
c 'Adams, 2001, Acta Cryst. B57, 278-287 (includes second neighbours)'
d 'Hu et al. (1995) Inorg. Chim. Acta, 232, 161-165.'
e 'I.D.Brown Private communication'
f 'Brown et al. (1984) Inorg. Chem. 23, 4506-4508'
g 'Palenik (1997) Inorg. Chem. 36 4888-4890'
h 'Kanowitz and Palenik (1998) Inorg. Chem. 37 2086-2088'
i 'Wood and Palenik (1998) Inorg. Chem. 37 4149-4151'
j 'Liu and Thorp (1993) Inorg. Chem. 32 4102-4105'
k 'Palenik (1997) Inorg. Chem. 36 3394-3397'
l 'Shields, Raithby, Allen and Motherwell (1999) Acta Cryst. B56, 455-465'
m 'Chen, Zhou and Hu (2002) Chinese Sci. Bul. 47, 978-980.'
n 'Kihlbourg (1963) Ark. Kemi 21 471; Schroeder 1975 Acta Cryst. B31, 2294'
o 'Allmann (1975) Monatshefte Chem. 106, 779'
p 'Zachariesen (1978) J.Less Common Metals 62, 1'
q 'Krivovichev and Brown (2001) Z. Krist. 216, 245'
r 'Burns, Ewing and Hawthorne (1997) Can. Miner. 35,1551-1570'
s 'Garcia-Rodriguez, et al. (2000) Acta Cryst. B56, 565-569'
t 'Mahapatra et al. (1996) J. Amer.Chem. Soc. 118, 11555'
u 'Wood and Palenik (1999) Inorg. Chem. 38, 1031-1034'
v 'Wood and Palenik (1999) Inorg. Chem. 38, 3926-3930'
w 'Wood, Abboud, Palenik and Palenik (2000) Inorg. Chem. 39, 2065-2068'
x 'Tytko, Mehnike and Kurad (1999) Structure and Bonding 93, 1-66'
y 'Gundemann, et al.(1999) J. Phys. Chem. A 103, 4752-4754'
z 'Zocchi (2000) Solid State Sci. 2 383-387'
aa 'Jensen, Palenik and Tiekiak (2001) Polyhedron 20, 2137'
ab 'Roulhac and Palenik (2002) Inorg. Chem. 42, 118-121'
ac 'Holsa et al.(2002) J.Solid State Chem 165, 48-55'
ae 'Trzesowska, Kruszynski & Bartezak (2004) Acta Cryst. B60, 174-178'
af 'Locock & Burns (2004) Z.Krist. 219, 267-271'
ag 'Hu & Zhou (2004) Z. Krist. 219 614-620'
ah 'Trzesowska, Kruszynski & Bartczak (2005) Acta Cryst. B61 429-434'
ai 'Palenik (2003) Inorg. Chem. 42, 2725-2728'

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Ac 3  Cl -1  2.63  0.37  b ?
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Ag 1  S -2  2.119  0.37  a ?
Ag 1  F -1  1.80  0.37  b ?
Ag 1  Cl -1  2.09  0.37  b ?
Ag 2  F -1  1.79  0.37  e unchecked
Ag 3  F -1  1.83  0.37  e unchecked

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Ag 9	Br	-1	2.22	0.37	b	?	
Ag 9	I	-1	2.38	0.37	b	?	
Ag 9	Se	-2	2.26	0.37	b	?	
Ag 9	Te	-2	2.51	0.37	b	?	
Ag 9	N	-3	1.85	0.37	b	?	
Ag 9	P	-3	2.22	0.37	b	?	
Ag 9	As	-3	2.30	0.37	b	?	
Ag 9	H	-1	1.50	0.37	b	?	
Al 3	O	-2	1.620	0.37	e	?	
Al 3	O	-2	1.644	0.38	o	?	
Al 3	S	-2	2.21	0.37	e	unchecked	
Al 3	S	-2	2.13	0.37	b	?	
Al 3	Se	-2	2.27	0.37	b	?	
Al 3	Te	-2	2.48	0.37	b	?	
Al 3	F	-1	1.545	0.37	a	?	
Al 3	Cl	-1	2.032	0.37	a	?	
Al 3	Br	-1	2.20	0.37	b	?	
Al 3	I	-1	2.41	0.37	b	?	
Al 3	N	-3	1.79	0.37	b	?	
Al 3	P	-3	2.24	0.37	b	?	
Al 3	As	-3	2.30	0.37	b	?	
Al 3	H	-1	1.45	0.37	b	?	
Am 3	O	-2	2.11	0.37	b	?	
Am 3	O	-2	2.13	0.35	p	?	
Am 3	F	-1	2.00	0.37	b	?	
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Am 3	Cl	-1	2.48	0.37	b	?	
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Am 4	O	-2	2.12	0.37	e	unchecked	
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Am 5	O	-2	2.07	0.35	p	?	
Am 5	F	-1	1.95	0.40	p	?	
Am 6	O	-2	2.05	0.35	p	?	
Am 6	F	-1	1.95	0.40	p	?	
Am 5	O	-2	2.12	0.37	e	unchecked	
As 2	S	-2	2.24	0.37	e	unchecked	
As 2	Se	-2	2.38	0.37	e	unchecked	
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As 3	S	-2	2.272	0.37	a	?	
As 3	Se	-2	2.40	0.37	e	unchecked	
As 3	Te	-2	2.65	0.37	e	unchecked	
As 3	F	-1	1.70	0.37	b	?	
As 3	Cl	-1	2.16	0.37	b	?	
As 3	Br	-1	2.35	0.37	e	unchecked	
As 3	I	-1	2.58	0.37	e	unchecked	
As 3	C	-4	1.93	0.37	b	?	
As 5	O	-2	1.767	0.37	a	?	
As 5	S	-2	2.28	0.37	e	unchecked	
As 5	F	-1	1.620	0.37	a	?	
As 5	Cl	-2	2.14	0.37	b	?	
Au 1	Cl	-1	2.02	0.37	e	unchecked	
Au 1	I	-1	2.35	0.37	e	unchecked	
Au 3	O	-2	1.89	0.37	e	?	
Au 3	O	-2	1.833	0.37	b	?	
Au 3	S	-2	2.39	0.35	e	unchecked	
Au 3	F	-1	1.89	0.37	e	unchecked	
Au 3	F	-1	1.81	0.37	b	?	
Au 3	Cl	-1	2.17	0.37	b	?	
Au 3	Br	-1	2.32	0.37	e	unchecked	
Au 3	I	-1	2.54	0.37	e	unchecked	
Au 3	N	-3	1.94	0.35	e	unchecked	
Au 5	F	-1	1.80	0.37	e	unchecked	
Au 9	S	-2	2.03	0.37	b	?	
Au 9	Se	-2	2.18	0.37	b	?	
Au 9	Te	-2	2.41	0.37	b	?	
Au 9	Br	-1	2.12	0.37	b	?	
Au 9	I	-1	2.34	0.37	b	?	

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Au 9	N	-3	1.72	0.37	b	?	
Au 9	P	-3	2.14	0.37	b	?	
Au 9	As	-3	2.22	0.37	b	?	
Au 9	H	-1	1.37	0.37	b	?	
B 3	O	-2	1.371	0.37	a	?	
B 3	S	-2	1.77	0.37	e	unchecked	
B 3	S	-2	1.82	0.37	b	?	
B 3	Se	-2	1.95	0.37	b	?	
B 3	Te	-2	2.20	0.37	b	?	
B 3	F	-1	1.281	0.37	a	?	
B 3	F	-1	1.31	0.37	b	?	
B 3	Cl	-1	1.74	0.37	b	?	
B 3	Br	-1	1.88	0.37	b	?	
B 3	I	-1	2.10	0.37	b	?	
B 3	N	-3	1.47	0.37	b	?	
B 3	P	-3	1.88	0.37	b	?	
B 3	As	-3	1.97	0.37	b	?	
B 3	H	-1	1.14	0.37	b	?	
B 3	B	3	1.402	0.37	e	unchecked	
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Ba 2	S	-2	2.769	0.37	a	?	
Ba 2	Se	-2	2.88	0.37	b	?	
Ba 2	Te	-2	3.08	0.37	b	?	
Ba 2	F	-1	2.188	0.37	a	?	
Ba 2	Cl	-1	2.69	0.37	b	?	
Ba 2	Br	-1	2.88	0.37	b	?	
Ba 2	I	-1	3.13	0.37	b	?	
Ba 2	N	-3	2.47	0.37	b	?	
Ba 2	P	-3	2.88	0.37	b	?	
Ba 2	As	-3	2.96	0.37	b	?	
Ba 2	H	-1	2.22	0.37	b	?	
Be 2	O	-2	1.381	0.37	a	?	
Be 2	S	-2	1.83	0.37	b	?	
Be 2	Se	-2	1.97	0.37	b	?	
Be 2	Te	-2	2.21	0.37	b	?	
Be 2	F	-1	1.281	0.37	a	?	
Be 2	Cl	-1	1.76	0.37	b	?	
Be 2	Br	-1	1.90	0.37	b	?	
Be 2	I	-1	2.10	0.37	b	?	
Be 2	N	-3	1.50	0.37	b	?	
Be 2	P	-3	1.95	0.37	b	?	
Be 2	As	-3	2.00	0.37	b	?	
Be 2	H	-1	1.11	0.37	b	?	
Bi 3	O	-2	2.094	0.37	a	?	
Bi 3	S	-2	2.570	0.37	a	?	
Bi 2	Se	-2	2.70	0.35	e	unchecked	
Bi 3	F	-1	1.99	0.37	b	?	
Bi 3	Cl	-1	2.48	0.37	b	?	
Bi 3	Cl	-1	2.40	0.37	e	unchecked	
Bi 3	Br	-1	2.59	0.37	e	unchecked	
Bi 3	I	-1	2.82	0.37	e	unchecked	
Bi 3	N	-3	2.02	0.35	e	unchecked	
Bi 5	O	-2	2.06	0.37	b	?	
Bi 5	F	-1	1.97	0.37	b	?	
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Bi 9	Br	-1	2.62	0.37	b	?	
Bi 9	I	-1	2.84	0.37	b	?	
Bi 9	S	-2	2.55	0.37	b	?	
Bi 9	Se	-2	2.72	0.37	b	?	
Bi 9	Te	-2	2.87	0.37	b	?	
Bi 9	N	-3	2.24	0.37	b	?	
Bi 9	P	-3	2.63	0.37	b	?	
Bi 9	As	-3	2.72	0.37	b	?	
Bi 9	H	-1	1.97	0.37	b	?	
Bk 3	O	-2	2.08	0.37	b	?	
Bk 3	O	-2	2.10	0.35	p	?	
Bk 3	F	-1	1.96	0.37	b	?	
Bk 3	F	-1	1.95	0.40	p	?	
Bk 3	Cl	-1	2.35	0.37	e	unchecked	

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Bk 3	Cl	-1	2.46	0.37	b	?	
Bk 3	Cl	-1	2.42	0.40	p	?	
Bk 3	Br	-1	2.56	0.40	p	?	
Bk 4	O	-2	2.07	0.35	p	?	
Bk 4	F	-1	1.93	0.40	p	?	
Br 3	O	-2	1.90	0.37	e	unchecked	
Br 3	F	-1	1.75	0.37	e	unchecked	
Br 5	O	-2	1.84	0.37	e	unchecked	
Br 5	F	-1	1.76	0.37	e	unchecked	
Br 7	O	-2	1.81	0.37	b	?	
Br 7	F	-1	1.72	0.37	b	?	
Br 7	Cl	-1	2.19	0.37	b	?	
C 2	O	-2	1.366	0.37	e	unchecked	
C 2	Cl	-1	1.410	0.37	e	unchecked	
C 4	O	-2	1.390	0.37	a	?	
C 4	O	-2	1.40	0.26	o	?	
C 4	C	4	1.54	0.37	e	?	
C 4	S	-2	1.80	0.37	e	unchecked	
C 4	F	-1	1.32	0.37	b	?	
C 4	F	-1	1.41	0.37	e	unchecked	
C 4	Cl	-1	1.76	0.37	b	?	
C 4	Br	-1	1.91	0.37	e	unchecked	
C 4	N	-3	1.442	0.37	a	?	
C 9	Se	-2	1.97	0.37	b	?	
C 9	I	-1	2.12	0.37	b	?	
C 9	Br	-1	1.90	0.37	b	?	
C 9	S	-2	1.82	0.37	b	?	
C 9	Te	-2	2.21	0.37	b	?	
C 9	N	-3	1.47	0.37	b	?	
C 9	P	-3	1.89	0.37	b	?	
C 9	As	-3	1.99	0.37	b	?	
C 9	H	-1	1.10	0.37	b	?	
Ca 2	O	-2	1.967	0.37	a	?	
Ca 2	O	-2	1.896	0.41	o	?	
Ca 2	S	-2	2.45	0.37	b	?	
Ca 2	Se	-2	2.56	0.37	b	?	
Ca 2	Te	-2	2.76	0.37	b	?	
Ca 2	F	-1	1.842	0.37	a	?	
Ca 2	Cl	-1	2.37	0.37	b	?	
Ca 2	Br	-1	2.507	0.37	e	unchecked	
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Ca 2	I	-1	2.72	0.37	b	?	
Ca 2	N	-3	2.14	0.37	b	?	
Ca 2	P	-3	2.55	0.37	b	?	
Ca 2	As	-3	2.62	0.37	b	?	
Ca 2	H	-1	1.83	0.37	b	?	
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Cd 2	Te	-2	2.59	0.37	b	?	
Cd 2	F	-1	1.811	0.37	b	?	
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Cd 2	Br	-1	2.35	0.37	b	?	
Cd 2	I	-1	2.57	0.37	b	?	
Cd 2	I	-1	2.60	0.37	e	unchecked	
Cd 2	N	-3	1.96	0.37	b	?	
Cd 2	P	-3	2.34	0.37	b	?	
Cd 2	As	-3	2.43	0.37	b	?	
Cd 2	H	-1	1.66	0.37	b	?	
Ce 3	O	-2	2.151	0.37	b	?	
Ce 3	O	-2	2.121	0.37	ab	'in trans-metal complexes'	
Ce 3	O	-2	2.116	0.37	ae	'in trans-metal complexes'	
Ce 3	S	-2	2.65	0.37	e	unchecked	
Ce 3	F	-1	2.036	0.37	b	?	
Ce 3	F	-1	2.00	0.40	p	?	
Ce 3	Cl	-1	2.52	0.37	b	?	
Ce 3	Cl	-1	2.49	0.40	p	?	
Ce 3	Br	-1	2.65	0.35	e	?	

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Ce 3	Br	-1	2.65	0.40	p	?	
Ce 3	I	-1	2.87	0.40	p	?	
Ce 4	O	-2	2.028	0.37	b	?	
Ce 4	O	-2	2.068	0.37	ab	'in organic compounds'	
Ce 4	S	-2	2.65	0.35	e	unchecked	
Ce 4	F	-1	1.995	0.37	b	?	
Ce 4	F	-1	1.97	0.40	p	?	
Ce 9	Cl	-1	2.41	0.37	b	?	
Ce 9	Br	-1	2.69	0.37	b	?	
Ce 9	I	-1	2.92	0.37	b	?	
Ce 9	S	-2	2.62	0.37	b	?	
Ce 9	Se	-2	2.74	0.37	b	?	
Ce 9	Te	-2	2.92	0.37	b	?	
Ce 9	N	-3	2.254	0.37	ah	?	
Ce 9	N	-3	2.34	0.37	b	?	
Ce 9	P	-3	2.70	0.37	b	?	
Ce 9	As	-3	2.78	0.37	b	?	
Ce 9	H	-1	2.04	0.37	b	?	
Cf 3	O	-2	2.07	0.37	b	?	
Cf 3	F	-1	1.95	0.37	b	?	
Cf 3	F	-1	1.94	0.40	p	?	
Cf 3	Cl	-1	2.45	0.37	b	?	
Cf 3	Cl	-1	2.41	0.40	p	?	
Cf 3	Br	-1	2.55	0.40	p	?	
Cf 4	O	-2	2.06	0.35	p	?	
Cf 4	F	-1	1.92	0.40	p	?	
Cl 3	O	-2	1.71	0.37	e	unchecked	
Cl 3	F	-1	1.69	0.37	e	unchecked	
Cl 5	O	-2	1.67	0.37	e	unchecked	
Cl 7	O	-2	1.632	0.37	a	?	
Cl 7	F	-1	1.55	0.37	b	?	
Cl 7	Cl	-1	2.00	0.37	b	?	
Cf 3	Cl	-1	2.45	0.37	b	?	
Cm 3	O	-2	2.23	0.37	b	?	
Cm 3	O	-2	2.12	0.35	p	?	
Cm 3	F	-1	2.12	0.37	b	?	
Cm 3	F	-1	1.96	0.40	p	?	
Cm 3	Cl	-1	2.62	0.37	b	?	
Cm 3	Cl	-1	2.44	0.40	p	?	
Cm 4	O	-2	2.08	0.35	p	?	
Cm 4	F	-1	1.94	0.40	p	?	
Co 1	H	-1	1.000	0.35	e	unchecked	
Co 2	O	-2	1.692	0.37	a	?	
Co 2	O	-2	1.685	0.37	i	'from transition metal complexes'	
Co 2	S	-2	1.94	0.37	e	unchecked	
Co 2	F	-1	1.64	0.37	b	?	
Co 2	Cl	-1	2.033	0.37	a	?	
Co 2	Cl	-1	2.01	0.37	b	?	
Co 2	N	-3	1.65	0.37	e	unchecked	
Co 3	O	-2	1.637	0.37	i	'from transition metal complexes'	
Co 3	O	-2	1.70	0.37	b	?	
Co 3	S	-2	2.02	0.37	e	unchecked	
Co 3	F	-1	1.62	0.37	b	?	
Co 3	Cl	-1	2.05	0.37	b	?	
Co 3	N	-3	1.75	0.37	e	unchecked	
Co 3	C	2	1.634	0.37	b	?	
Co 4	O	-2	1.72	0.37	e	unchecked	
Co 4	F	-1	1.55	0.37	e	unchecked	
Co 9	O	-2	1.655	0.42	o	?	
Co 9	Br	-1	2.18	0.37	b	?	
Co 9	I	-1	2.37	0.35	b	?	
Co 9	S	-2	2.06	0.37	b	?	
Co 9	Se	-2	2.24	0.37	b	?	
Co 9	Te	-2	2.46	0.37	b	?	
Co 9	N	-3	1.84	0.37	b	?	
Co 9	P	-3	2.21	0.37	b	?	
Co 9	As	-3	2.28	0.37	b	?	
Co 9	H	-1	1.44	0.37	b	?	
Cr 2	O	-2	1.73	0.37	b	?	

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Cr 2	F -1	1.67	0.37	b	?
Cr 2	F -1	1.74	0.37	e	unchecked
Cr 2	Cl -1	2.09	0.37	b	?
Cr 2	Br -1	2.26	0.37	e	unchecked
Cr 2	I -1	2.48	0.37	e	unchecked
Cr 2	N -3	1.83	0.35	e	unchecked
Cr 3	O -2	1.724	0.37	a	?
Cr 3	O -2	1.708	0.37	w	'from transition metal complexes'
Cr 3	S -2	2.162	0.37	e	unchecked
Cr 3	F -1	1.657	0.37	a	?
Cr 3	F -1	1.64	0.37	b	?
Cr 3	Cl -1	2.08	0.37	b	?
Cr 3	Br -1	2.28	0.37	e	unchecked
Cr 3	N -3	1.81	0.37	e	unchecked
Cr 4	O -2	1.81	0.37	e	unchecked
Cr 4	F -1	1.56	0.37	e	unchecked
Cr 5	O -2	1.76	0.37	w	'from transition metal complexes'
Cr 5	O -2	1.78	0.37	e	unchecked
Cr 6	O -2	1.794	0.37	a	?
Cr 6	F -1	1.74	0.37	b	?
Cr 6	Cl -1	2.12	0.37	b	?
Cr 9	O -2	1.79	0.34	o	?
Cr 9	O -2	1.724	0.37	w	'from transition metal complexes'
Cr 9	Br -1	2.26	0.37	b	?
Cr 9	I -1	2.45	0.37	b	?
Cr 9	S -2	2.18	0.37	b	?
Cr 9	Se -2	2.29	0.37	b	?
Cr 9	Te -2	2.52	0.37	b	?
Cr 9	N -3	1.85	0.37	b	?
Cr 9	P -3	2.27	0.37	b	?
Cr 9	As -3	2.34	0.37	b	?
Cr 9	H -1	1.52	0.37	b	?
Cs 1	O -2	2.417	0.37	a	?
Cs 1	O -2	2.2862	0.408	c	'7 A cut-off'
Cs 1	S -2	2.89	0.37	b	?
Cs 1	S -2	2.5253	0.517	c	'7 A cut-off'
Cs 1	S -2	2.93	0.37	e	unchecked
Cs 1	Se -2	2.98	0.37	b	?
Cs 1	Se -2	2.6424	0.553	c	'7 A cut-off'
Cs 1	Te -2	3.16	0.37	b	?
Cs 1	Te -2	2.7647	0.603	c	'8 A cut-off'
Cs 1	F -1	2.33	0.37	b	?
Cs 1	F -1	2.1980	0.410	c	'7 A cut-off'
Cs 1	F -1	2.38	0.37	e	unchecked
Cs 1	Cl -1	2.791	0.37	a	?
Cs 1	Cl -1	2.4715	0.495	c	'7 A cut-off'
Cs 1	Br -1	2.95	0.37	b	?
Cs 1	Br -1	2.5035	0.543	c	'7 A cut-off'
Cs 1	I -1	3.18	0.37	b	?
Cs 1	I -1	2.6926	0.609	c	'8 A cut-off'
Cs 1	I -1	3.29	0.37	e	unchecked
Cs 1	N -3	2.83	0.37	e	unchecked
Cs 1	N -3	2.53	0.37	b	?
Cs 1	P -3	2.93	0.37	b	?
Cs 1	As -3	3.04	0.37	b	?
Cs 1	H -1	2.44	0.37	b	?
Cu 1	O -2	1.610	0.37	e	unchecked
Cu 1	O -2	1.504	0.37	l	'from transition metal complexes'
Cu 1	S -2	1.898	0.37	a	?
Cu 1	S -2	1.811	0.37	l	'from transition metal complexes'
Cu 1	Se -2	1.900	0.37	l	'from transition metal complexes'
Cu 1	F -1	1.6	0.37	b	?
Cu 1	Cl -1	1.858	0.37	l	'from transition metal complexes'
Cu 1	Cl -1	1.89	0.37	e	unchecked
Cu 1	Br -1	2.03	0.37	e	unchecked
Cu 1	I -1	2.108	0.37	a	?
Cu 1	I -1	2.155	0.37	l	'from transition metal complexes'
Cu 1	N -3	1.520	0.37	l	'3-coordinate N'
Cu 1	N -3	1.480	0.37	l	'2-coordinate N'

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Cu 1	N -3	1.630	0.37	l	'4-coordinate N'
Cu 1	P -3	1.774	0.37	l	'from transition metal complexes'
Cu 1	As -3	1.856	0.37	l	'from transition metal complexes'
Cu 1	C -4	1.446	0.37	l	'from transition metal complexes'
Cu 2	O -2	1.679	0.37	a	?
Cu 2	O -2	1.649	0.37	j	'from transition metal complexes'
Cu 2	O -2	1.655	0.37	l	'from transition metal complexes'
Cu 2	S -2	2.054	0.37	a	?
Cu 2	S -2	2.060	0.37	j	'from transition metal complexes'
Cu 2	S -2	2.024	0.37	l	'from transition metal complexes'
Cu 2	S -2	1.86	0.37	b	?
Cu 2	Se -2	2.02	0.37	b	?
Cu 2	Se -2	2.124	0.37	l	?
Cu 2	Te -2	2.27	0.37	b	?
Cu 2	F -1	1.594	0.37	a	?
Cu 2	Cl -1	2.00	0.37	b	?
Cu 2	Br -1	1.99	0.37	b	?
Cu 2	Br -1	2.134	0.37	l	'from transition metal complexes'
Cu 2	I -1	2.16	0.37	b	?
Cu 2	I -1	2.36	0.37	l	'from transition metal complexes'
Cu 2	N -3	1.751	0.37	j	'from transition metal complexes'
Cu 2	N -3	1.713	0.37	l	'from transition metal complexes'
Cu 2	N -3	1.61	0.37	b	?
Cu 2	N -3	1.709	0.37	l	'2-coordinate N'
Cu 2	N -3	1.704	0.37	l	'3-coordinate N'
Cu 2	N -3	1.763	0.37	l	'4-coordinate N'
Cu 2	P -3	1.97	0.37	b	?
Cu 2	P -3	2.05	0.37	l	'from transition metal complexes'
Cu 2	As -3	2.08	0.37	b	?
Cu 2	C -4	1.72	0.37	l	'from transition metal complexes'
Cu 2	H -1	1.21	0.37	b	?
Cu 3	O -2	1.735	0.37	t	?
Cu 3	O -2	1.739	0.37	e	unchecked
Cu 3	F -1	1.58	0.37	e	unchecked
Cu 3	Cl -1	2.078	0.37	l	'from transition metal complexes'
Cu 3	N -3	1.768	0.37	l	'from transition metal complexes'
Cu 3	N -3	1.753	0.37	t	?
Cu 3	C -4	1.84	0.37	l	'from transition metal complexes'
Dy 2	O -2	1.90	0.37	e	unchecked
Dy 3	O -2	2.001	0.37	a	?
Dy 3	O -2	2.005	0.37	ae	'from transition metal complexes'
Dy 3	F -1	1.922	0.37	b	?
Dy 3	F -1	1.89	0.40	p	?
Dy 3	Cl -1	2.41	0.37	b	?
Dy 3	Cl -1	2.38	0.40	p	?
Dy 3	Br -1	2.53	0.40	p	?
Dy 3	I -1	2.76	0.40	p	?
Dy 9	Br -1	2.56	0.37	b	?
Dy 9	I -1	2.77	0.37	b	?
Dy 9	S -2	2.47	0.37	b	?
Dy 9	Se -2	2.61	0.37	b	?
Dy 9	Te -2	2.80	0.37	b	?
Dy 9	N -3	2.124	0.37	ah	?
Dy 9	N -3	2.18	0.37	b	?
Dy 9	P -3	2.57	0.37	b	?
Dy 9	As -3	2.64	0.37	b	?
Dy 9	H -1	1.89	0.37	b	?
Er 2	O -2	1.88	0.37	e	unchecked
Er 2	S -2	2.52	0.37	e	unchecked
Er 3	O -2	1.988	0.37	a	?
Er 3	O -2	2.010	0.37	b	?
Er 3	O -2	1.979	0.37	ae	'from transition metal complexes'
Er 3	S -2	2.52	0.37	e	unchecked
Er 3	Se -2	2.58	0.37	e	unchecked
Er 3	F -1	1.904	0.37	a	?
Er 3	F -1	1.87	0.40	p	?
Er 3	Cl -1	2.39	0.37	b	?
Er 3	Cl -1	2.36	0.40	p	?
Er 3	Br -1	2.51	0.40	p	?

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Er 3	I	-1	2.75	0.40	p	?	
Er 9	Br	-1	2.54	0.37	b	?	
Er 9	I	-1	2.75	0.37	b	?	
Er 9	S	-2	2.46	0.37	b	?	
Er 9	Se	-2	2.59	0.37	b	?	
Er 9	Te	-2	2.78	0.37	b	?	
Er 9	N	-3	2.086	0.37	ah	?	
Er 9	N	-3	2.16	0.37	b	?	
Er 9	P	-3	2.55	0.37	b	?	
Er 9	As	-3	2.63	0.37	b	?	
Er 9	H	-1	1.86	0.37	b	?	
Es 3	O	-2	2.08	0.35	p	?	
Eu 2	O	-2	2.147	0.37	b	?	
Eu 2	S	-2	2.584	0.37	a	?	
Eu 2	F	-1	2.04	0.37	b	?	
Eu 2	Cl	-1	2.53	0.37	b	?	
Eu 2	Br	-1	2.67	0.37	e	unchecked	
Eu 2	I	-1	2.90	0.37	e	unchecked	
Eu 2	N	-3	2.34	0.37	e	unchecked	
Eu 3	O	-2	2.074	0.37	a	?	
Eu 3	O	-2	2.038	0.37	ae	'from transition metal complexes'	
Eu 3	S	-2	2.58	0.35	e	unchecked	
Eu 3	F	-1	1.961	0.37	b	?	
Eu 3	F	-1	1.93	0.40	p	?	
Eu 3	Cl	-1	2.48	0.37	e	unchecked	
Eu 3	Cl	-1	2.42	0.40	p	?	
Eu 3	Br	-1	2.57	0.40	p	?	
Eu 3	I	-1	2.79	0.40	p	?	
Eu 9	Br	-1	2.61	0.37	b	?	
Eu 9	I	-1	2.83	0.37	b	?	
Eu 9	S	-2	2.53	0.37	b	?	
Eu 9	Se	-2	2.66	0.37	b	?	
Eu 9	Te	-2	2.85	0.37	b	?	
Eu 9	N	-3	2.161	0.37	ah	?	
Eu 9	N	-3	2.24	0.37	b	?	
Eu 9	P	-3	2.62	0.37	b	?	
Eu 9	As	-3	2.70	0.37	b	?	
Eu 9	H	-1	1.95	0.37	b	?	
Fe 2	O	-2	1.734	0.37	a	?	
Fe 2	O	-2	1.713	0.37	h	?	
Fe 2	O	-2	1.700	0.37	j	?	
Fe 2	S	-2	2.12	0.37	e	unchecked	
Fe 2	S	-2	2.125	0.37	j	'from transition metal complexes'	
Fe 2	F	-1	1.65	0.37	b	?	
Fe 2	Cl	-1	2.06	0.37	b	?	
Fe 2	Cl	-1	2.15	0.37	e	unchecked	
Fe 2	Br	-1	2.21	0.35	e	unchecked	
Fe 2	I	-1	2.47	0.35	e	?	
Fe 2	N	-3	1.769	0.37	j	'from transition metal complexes'	
Fe 3	O	-2	1.759	0.37	a	?	
Fe 3	O	-2	1.751	0.37	h	'from transition metal complexes'	
Fe 3	O	-2	1.765	0.37	j	'from transition metal complexes'	
Fe 3	S	-2	2.149	0.37	a	?	
Fe 3	S	-2	2.134	0.37	j	?	
Fe 3	F	-1	1.679	0.37	a	?	
Fe 3	Cl	-1	2.09	0.37	b	?	
Fe 3	Cl	-1	2.15	0.37	e	unchecked	
Fe 3	N	-3	1.815	0.37	j	'from transition metal complexes'	
Fe 3	C	2	1.689	0.37	a	?	
Fe 4	S	-2	2.23	0.35	e	unchecked	
Fe 6	O	-2	1.76	0.35	e	unchecked	
Fe 9	O	-2	1.795	0.30	ag	'for all oxidation states'	
Fe 9	O	-2	1.74	0.38	o	?	
Fe 9	Br	-1	2.26	0.37	b	?	
Fe 9	I	-1	2.47	0.37	b	?	
Fe 9	S	-2	2.16	0.37	b	?	
Fe 9	Se	-2	2.28	0.37	b	?	
Fe 9	Te	-2	2.53	0.37	b	?	
Fe 9	N	-3	1.86	0.37	b	?	

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Fe 9	P	-3	2.27	0.37	b	?	
Fe 9	As	-3	2.35	0.37	b	?	
Fe 9	H	-1	1.53	0.37	b	?	
Ga 1	Se	-1	2.55	0.37	e	unchecked	
Ga 3	O	-2	1.730	0.37	a	?	
Ga 3	S	-2	2.163	0.37	a	?	
Ga 3	F	-1	1.62	0.37	b	?	
Ga 3	F	-1	1.69	0.37	e	unchecked	
Ga 3	Cl	-1	2.07	0.37	b	?	
Ga 3	Br	-1	2.20	0.35	e	?	
Ga 3	I	-1	2.46	0.37	e	unchecked	
Ga 9	Br	-1	2.24	0.37	b	?	
Ga 9	I	-1	2.45	0.37	b	?	
Ga 9	S	-2	2.17	0.37	b	?	
Ga 9	Se	-2	2.30	0.37	b	?	
Ga 9	Te	-2	2.54	0.37	b	?	
Ga 9	N	-3	1.84	0.37	b	?	
Ga 9	P	-3	2.26	0.37	b	?	
Ga 9	As	-3	2.34	0.37	b	?	
Ga 9	H	-1	1.51	0.37	b	?	
Gd 2	O	-2	2.01	0.37	e	unchecked	
Gd 2	F	-1	2.40	0.37	e	unchecked	
Gd 3	O	-2	2.065	0.37	b	?	
Gd 3	O	-2	2.031	0.37	ae	'from transition metal complexes'	
Gd 3	S	-2	2.53	0.37	e	unchecked	
Gd 3	F	-1	1.95	0.37	b	?	
Gd 3	F	-1	1.92	0.40	p	?	
Gd 3	Cl	-1	2.445	0.37	b	?	
Gd 3	Cl	-1	2.41	0.40	p	?	
Gd 3	Cl	-1	2.47	0.37	e	unchecked	
Gd 3	Br	-1	2.56	0.40	p	?	
Gd 3	I	-1	2.78	0.40	p	?	
Gd 9	Br	-1	2.60	0.37	b	?	
Gd 9	I	-1	2.82	0.37	b	?	
Gd 9	S	-2	2.53	0.37	b	?	
Gd 9	Se	-2	2.65	0.37	b	?	
Gd 9	Te	-2	2.84	0.37	b	?	
Gd 9	N	-3	2.146	0.37	ah	?	
Gd 9	N	-3	2.22	0.37	b	?	
Gd 9	N	-3	2.10	0.37	e	?	
Gd 9	P	-3	2.61	0.37	b	?	
Gd 9	As	-3	2.68	0.37	b	?	
Gd 9	H	-1	1.93	0.37	b	?	
Ge 4	O	-2	1.748	0.37	a	?	
Ge 4	S	-2	2.217	0.37	a	?	
Ge 4	Se	-2	2.35	0.37	e	unchecked	
Ge 4	F	-1	1.66	0.37	b	?	
Ge 4	Cl	-1	2.14	0.37	b	?	
Ge 9	Br	-1	2.30	0.37	b	?	
Ge 9	I	-1	2.50	0.37	b	?	
Ge 9	S	-2	2.23	0.37	b	?	
Ge 9	Se	-2	2.35	0.37	b	?	
Ge 9	Te	-2	2.56	0.37	b	?	
Ge 9	N	-3	1.88	0.37	b	?	
Ge 9	P	-3	2.32	0.37	b	?	
Ge 9	As	-3	2.43	0.37	b	?	
Ge 9	H	-1	1.55	0.37	b	?	
H 1	O	-2	0.569	0.94	e	'1.05<O-H<1.70 A, best general value'	
H 1	O	-2	0.907	0.28	e	'O-H < 1.05 A'	
H 1	O	-2	0.990	0.59	e	'1.70 A < O-H'	
Hf 3	F	-1	2.62	0.37	e	unchecked	
Hf 4	O	-2	1.923	0.37	b	?	
Hf 4	F	-1	1.85	0.37	b	?	
Hf 4	F	-1	1.82	0.40	p	?	
Hf 4	Cl	-1	2.24	0.37	e	unchecked	
Hf 4	Cl	-1	2.30	0.37	b	?	
Hf 9	Br	-1	2.47	0.37	b	?	
Hf 9	S	-2	2.39	0.37	b	?	
Hf 9	Se	-2	2.52	0.37	b	?	

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Hf 9	Te -2	2.72	0.37	b ?			
Hf 9	I -1	2.68	0.37	b ?			
Hf 9	N -3	2.09	0.37	b ?			
Hf 9	P -3	2.48	0.37	b ?			
Hf 9	As -3	2.56	0.37	b ?			
Hf 9	H -1	1.78	0.37	b ?			
Hg 1	O -2	1.90	0.37	b ?			
Hg 1	F -1	1.81	0.37	b ?			
Hg 1	Cl -1	2.28	0.37	b ?			
Hg 2	O -2	1.972	0.37	a ?			
Hg 2	O -2	1.93	0.37	b ?			
Hg 2	S -2	2.308	0.37	a ?			
Hg 2	F -1	2.17	0.37	e unchecked			
Hg 2	F -1	1.90	0.37	b ?			
Hg 2	Cl -1	2.28	0.37	e ?			
Hg 2	Cl -1	2.25	0.37	b ?			
Hg 2	Br -1	2.38	0.37	e unchecked			
Hg 2	I -1	2.62	0.37	e unchecked			
Hg 9	Br -1	2.40	0.37	b ?			
Hg 9	I -1	2.59	0.37	b ?			
Hg 9	S -2	2.32	0.37	b ?			
Hg 9	Se -2	2.47	0.37	b ?			
Hg 9	Te -2	2.61	0.37	b ?			
Hg 9	N -3	2.02	0.37	b ?			
Hg 9	P -3	2.42	0.37	b ?			
Hg 9	As -3	2.50	0.37	b ?			
Hg 9	H -1	1.71	0.37	b ?			
Hg 2	Hg 2	2.51	0.35	f ?			
Ho 3	O -2	2.025	0.37	a ?			
Ho 3	O -2	1.992	0.37	ae 'from transition metal complexes'			
Ho 3	S -2	2.49	0.37	e unchecked			
Ho 3	F -1	1.908	0.37	b ?			
Ho 3	F -1	1.88	0.40	p ?			
Ho 3	Cl -1	2.401	0.37	b ?			
Ho 3	Cl -1	2.37	0.40	p ?			
Ho 3	Br -1	2.52	0.40	p ?			
Ho 3	I -1	2.76	0.40	p ?			
Ho 9	Br -1	2.55	0.37	b ?			
Ho 9	I -1	2.77	0.37	b ?			
Ho 9	S -2	2.48	0.37	b ?			
Ho 9	Se -2	2.61	0.37	b ?			
Ho 9	Te -2	2.80	0.37	b ?			
Ho 9	N -3	2.118	0.37	ah ?			
Ho 9	N -3	2.18	0.37	b ?			
Ho 9	P -3	2.56	0.37	b ?			
Ho 9	As -3	2.64	0.37	b ?			
Ho 9	H -1	1.88	0.37	b ?			
I 0	I 0	2.195	0.35	e unchecked			
I 1	F -1	2.32	0.37	e unchecked			
I 1	Cl -1	2.47	0.37	e unchecked			
I 3	O -2	2.02	0.37	e unchecked			
I 3	F -1	1.90	0.37	b ?			
I 3	Cl -1	2.39	0.37	e unchecked			
I 5	O -2	2.003	0.37	a ?			
I 5	F -1	1.84	0.37	e unchecked			
I 5	F -1	1.90	0.37	b ?			
I 5	Cl -1	2.38	0.37	b ?			
I 7	O -2	1.93	0.37	b ?			
I 7	F -1	1.83	0.37	b ?			
I 7	Cl -1	2.31	0.37	b ?			
In 1	Cl -1	2.56	0.37	e unchecked			
In 3	O -2	1.902	0.37	a ?			
In 3	S -2	2.370	0.37	a ?			
In 3	F -1	1.792	0.37	a ?			
In 3	Cl -1	2.28	0.37	b ?			
In 3	Br -1	2.51	0.35	e unchecked			
In 3	I -1	2.63	0.37	e unchecked			
In 3	Co -1	2.593	0.35	e unchecked			
In 3	Mn -2	2.604	0.35	e unchecked			

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In 9	Br -1	2.41	0.37	b ?			
In 9	I -1	2.63	0.37	b ?			
In 9	S -2	2.36	0.37	b ?			
In 9	Se -2	2.47	0.37	b ?			
In 9	Te -2	2.69	0.37	b ?			
In 9	N -3	2.03	0.37	b ?			
In 9	P -3	2.43	0.37	b ?			
In 9	As -3	2.51	0.37	b ?			
In 9	H -1	1.72	0.37	b ?			
Ir 4	O -2	1.87	0.37	e unchecked			
Ir 4	F -1	1.80	0.37	e unchecked			
Ir 5	O -2	1.916	0.37	b ?			
Ir 5	O -2	2.01	0.37	e unchecked			
Ir 5	F -1	1.82	0.37	b ?			
Ir 5	Cl -1	2.30	0.37	b ?			
Ir 9	S -2	2.38	0.37	b ?			
Ir 9	Se -2	2.51	0.37	b ?			
Ir 9	Te -2	2.71	0.37	b ?			
Ir 9	Br -1	2.45	0.37	b ?			
Ir 9	I -1	2.66	0.37	b ?			
Ir 9	N -3	2.06	0.37	b ?			
Ir 9	P -3	2.46	0.37	b ?			
Ir 9	As -3	2.54	0.37	b ?			
Ir 9	H -1	1.76	0.37	b ?			
K 1	O -2	2.132	0.37	a ?			
K 1	O -2	2.113	0.37	u ?			
K 1	O -2	1.9548	0.430	c '6 A cut-off'			
K 1	O -2	1.84	0.48	o ?			
K 1	S -2	2.59	0.37	b ?			
K 1	S -2	2.1516	0.580	c '7 A cut-off'			
K 1	S -2	2.63	0.37	e unchecked			
K 1	Se -2	2.72	0.37	b ?			
K 1	Se -2	2.2811	0.612	c '7 A cut-off'			
K 1	Te -2	2.93	0.37	b ?			
K 1	Te -2	2.4102	0.653	c '7 A cut-off'			
K 1	F -1	1.992	0.37	a ?			
K 1	F -1	1.8307	0.429	c '6 A cut-off'			
K 1	Cl -1	2.519	0.37	a ?			
K 1	Cl -1	2.0707	0.559	c '6 A cut-off'			
K 1	Br -1	2.66	0.37	b ?			
K 1	Br -1	2.1529	0.603	c '7 A cut-off'			
K 1	I -1	2.88	0.37	b ?			
K 1	I -1	2.2821	0.658	c '7 A cut-off'			
K 1	I -1	2.92	0.37	e unchecked			
K 1	N -3	2.26	0.37	b ?			
K 1	N -3	2.30	0.37	e unchecked			
K 1	P -3	2.64	0.37	b ?			
K 1	As -3	2.83	0.37	b ?			
K 1	H -1	2.10	0.37	b ?			
Kr 2	F -1	1.88	0.37	e ?			
La 3	O -2	2.172	0.37	a ?			
La 3	O -2	2.172	0.33	ac ?			
La 3	O -2	2.148	0.37	ae 'from transition metal complexes'			
La 3	S -2	2.643	0.37	a ?			
La 3	Se -2	2.74	0.37	b ?			
La 3	Te -2	2.94	0.37	b ?			
La 3	F -1	2.02	0.40	p ?			
La 3	F -1	2.08	0.37	e unchecked			
La 3	Cl -1	2.545	0.37	b ?			
La 3	Cl -1	2.57	0.37	e unchecked			
La 3	Cl -1	2.58	0.40	p ?			
La 3	Br -1	2.72	0.37	b ?			
La 3	Br -1	2.66	0.40	p ?			
La 3	I -1	2.93	0.37	b ?			
La 3	I -1	2.88	0.40	p ?			
La 3	N -3	2.261	0.37	ah ?			
La 3	N -3	2.34	0.37	b ?			
La 3	P -3	2.73	0.37	b ?			
La 3	As -3	2.80	0.37	b ?			

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La 3	H -1	2.06	0.37	b ?	
Li 1	O -2	1.466	0.37	a ?	
Li 1	O -2	1.1745	0.514	c '6 A cut-off'	
Li 1	O -2	1.29	0.48	o ?	
Li 1	S -2	1.94	0.37	b ?	
Li 1	S -2	1.4607	0.656	c '6 A cut-off'	
Li 1	Se -2	2.09	0.37	b ?	
Li 1	Se -2	1.6272	0.681	c '7 A cut-off'	
Li 1	Te -2	2.30	0.37	b ?	
Li 1	Te -2	1.7340	0.717	c '7 A cut-off'	
Li 1	F -1	1.360	0.37	a ?	
Li 1	F -1	1.0968	0.503	c '6 A cut-off'	
Li 1	Cl -1	1.91	0.37	b ?	
Li 1	Cl -1	1.3873	0.640	c '6 A cut-off'	
Li 1	Cl -1	1.94	0.37	e unchecked	
Li 1	Br -1	2.02	0.37	b ?	
Li 1	Br -1	1.5150	0.674	c '7 A cut-off'	
Li 1	I -1	2.22	0.37	b ?	
Li 1	I -1	1.6754	0.722	c '7 A cut-off'	
Li 1	N -3	1.61	0.37	b ?	
Lu 3	O -2	1.971	0.37	b ?	
Lu 3	O -2	1.947	0.37	ae 'from transition metal complex'	
Lu 3	S -2	2.43	0.37	b ?	
Lu 3	Se -2	2.56	0.37	b ?	
Lu 3	Te -2	2.75	0.37	b ?	
Lu 3	F -1	1.876	0.37	b ?	
Lu 3	F -1	1.84	0.40	p ?	
Lu 3	Cl -1	2.361	0.37	b ?	
Lu 3	Cl -1	2.33	0.40	p ?	
Lu 3	Br -1	2.50	0.37	b ?	
Lu 3	Br -1	2.48	0.40	p ?	
Lu 3	I -1	2.73	0.37	b ?	
Lu 3	I -1	2.73	0.40	p ?	
Lu 3	N -3	2.046	0.37	ah ?	
Lu 3	N -3	2.11	0.37	b ?	
Lu 3	P -3	2.51	0.37	b ?	
Lu 3	As -3	2.59	0.37	b ?	
Lu 3	H -1	1.82	0.37	b ?	
Mg 2	O -2	1.693	0.37	a ?	
Mg 2	O -2	1.636	0.42	o ?	
Mg 2	S -2	2.18	0.37	b ?	
Mg 2	Se -2	2.32	0.37	b ?	
Mg 2	Te -2	2.53	0.37	b ?	
Mg 2	F -1	1.578	0.37	a ?	
Mg 2	Cl -1	2.08	0.37	b ?	
Mg 2	Br -1	2.28	0.37	b ?	
Mg 2	I -1	2.46	0.37	b ?	
Mg 2	N -3	1.85	0.37	b ?	
Mg 2	P -3	2.29	0.37	b ?	
Mg 2	As -3	2.38	0.37	b ?	
Mg 2	H -1	1.53	0.37	b ?	
Mn 2	O -2	1.790	0.37	a ?	
Mn 2	O -2	1.765	0.37	j ?	
Mn 2	S -2	2.22	0.37	e unchecked	
Mn 2	F -1	1.698	0.37	a ?	
Mn 2	Cl -1	2.133	0.37	a ?	
Mn 2	Br -1	2.34	0.37	e unchecked	
Mn 2	I -2	2.52	0.37	e unchecked	
Mn 2	N -3	1.849	0.37	j 'from transition metal complexes'	
Mn 2	N -3	1.65	0.35	e unchecked	
Mn 3	O -2	1.760	0.37	a ?	
Mn 3	O -2	1.732	0.37	j 'from transition metal complexes'	
Mn 3	F -1	1.66	0.37	b ?	
Mn 3	Cl -1	2.14	0.37	b ?	
Mn 3	N -3	1.837	0.37	j 'from transition metal complexes'	
Mn 4	O -2	1.753	0.37	a ?	
Mn 4	O -2	1.750	0.37	j 'from transition metal complexes'	
Mn 4	F -1	1.71	0.37	b ?	
Mn 4	F -1	1.63	0.37	e unchecked	

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Mn 4	Cl -1	2.13	0.37	b ?	
Mn 4	N -3	1.822	0.37	j 'from transition metal complexes'	
Mn 6	O -2	1.79	0.37	e ?	
Mn 7	O -2	1.827	0.37	e unchecked	
Mn 7	O -2	1.79	0.37	b ?	
Mn 7	F -1	1.72	0.37	b ?	
Mn 7	Cl -1	2.17	0.37	b ?	
Mn 9	O -2	1.754	0.37	g 'from transition metal complexes'	
Mn 9	Br -1	2.26	0.37	b ?	
Mn 9	I -1	2.49	0.37	b ?	
Mn 9	S -2	2.20	0.37	b ?	
Mn 9	Se -1	2.32	0.37	b ?	
Mn 9	Te -2	2.55	0.37	b ?	
Mn 9	N -3	1.87	0.37	b ?	
Mn 9	P -3	2.24	0.37	b ?	
Mn 9	As -3	2.36	0.37	b ?	
Mn 9	H -1	1.55	0.37	b ?	
Mo 3	O -2	1.834	0.37	m ?	
Mo 3	F -1	1.76	0.35	e unchecked	
Mo 3	Cl -1	2.22	0.37	e unchecked	
Mo 3	Br -1	2.34	0.37	e unchecked	
Mo 3	N -3	1.96	0.37	e unchecked	
Mo 4	O -2	1.886	0.37	j 'from transition metal complexes'	
Mo 4	O -2	1.856	0.37	m ?	
Mo 4	S -2	2.235	0.37	j 'from transition metal complexes'	
Mo 4	F -1	1.80	0.37	e unchecked	
Mo 4	Cl -1	2.17	0.37	e unchecked	
Mo 4	N -3	2.043	0.37	j 'from transition metal complexes'	
Mo 5	O -2	1.907	0.37	j 'from transition metal complexes'	
Mo 5	O -2	1.878	0.37	m ?	
Mo 5	S -2	2.288	0.37	j 'from transition metal complexes'	
Mo 5	Cl -1	2.26	0.37	e unchecked	
Mo 5	N -3	2.009	0.37	j 'from transition metal complexes'	
Mo 6	O -2	1.907	0.37	a ?	
Mo 6	O -2	1.915	0.41	x ?	
Mo 6	O -2	1.87	0.26	n ?	
Mo 6	O -2	1.900	0.37	m ?	
Mo 6	S -2	2.331	0.37	j 'from transition metal complexes'	
Mo 6	F -1	1.81	0.37	b ?	
Mo 6	Cl -1	2.28	0.37	b ?	
Mo 6	N -3	2.009	0.37	j 'from transition metal complexes'	
Mo 9	O -2	1.879	0.30	z 'applies to all oxidation states'	
Mo 9	Br -1	2.43	0.37	b ?	
Mo 9	I -1	2.64	0.37	b ?	
Mo 9	S -2	2.35	0.37	b ?	
Mo 9	Se -2	2.49	0.37	b ?	
Mo 9	Te -2	2.69	0.37	b ?	
Mo 9	N -3	2.04	0.37	b ?	
Mo 9	P -3	2.44	0.37	b ?	
Mo 9	As -3	2.52	0.37	b ?	
Mo 9	H -1	1.73	0.37	b ?	
N 3	O -2	1.361	0.37	a ?	
N 3	S -2	1.73	0.37	e unchecked	
N 3	F -1	1.37	0.37	b ?	
N 3	Cl -1	1.75	0.37	b ?	
N -3	N -3	1.44	0.35	e unchecked	
N 5	O -2	1.432	0.37	a ?	
N 5	O -2	1.41	0.43	o ?	
N 5	F -1	1.36	0.37	b ?	
N 5	Cl -1	1.80	0.37	b ?	
Na 1	O -2	1.803	0.37	a ?	
Na 1	O -2	1.756	0.37	v ?	
Na 1	O -2	1.5766	0.475	c '6 A cut-off'	
Na 1	O -2	1.661	0.44	o ?	
Na 1	S -2	2.300	0.37	a ?	
Na 1	S -2	2.28	0.37	b ?	
Na 1	S -2	1.8213	0.626	c '6 A cut-off'	
Na 1	Se -2	2.41	0.37	b ?	
Na 1	Se -2	1.8908	0.654	c '7 A cut-off'	

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Na 1	Te -2	2.64	0.37	b	?		
Na 1	Te -2	2.0400	0.690	c	'7 A cut-off'		
Na 1	F -1	1.677	0.37	a	?		
Na 1	F -1	1.4485	0.465	c	'6 A cut-off'		
Na 1	Cl -1	2.15	0.37	b	?		
Na 1	Cl -1	1.6833	0.608	c	'6 A cut-off'		
Na 1	Cl -1	2.22	0.37	e	unchecked		
Na 1	Br -1	2.33	0.37	b	?		
Na 1	Br -1	1.7719	0.646	c	'7 A cut-off'		
Na 1	I -1	2.56	0.37	b	?		
Na 1	I -1	1.9555	0.695	c	'7 A cut-off'		
Na 1	N -3	1.93	0.37	b	?		
Na 1	N -3	2.01	0.37	e	unchecked		
Na 1	P -3	2.36	0.37	b	?		
Na 1	As -3	2.53	0.37	b	?		
Na 1	H -1	1.68	0.37	b	?		
Nb 3	O -2	1.91	0.35	e	unchecked		
Nb 3	F -1	1.71	0.37	e	unchecked		
Nb 3	Cl -1	2.20	0.37	e	unchecked		
Nb 3	Br -1	2.35	0.37	e	unchecked		
Nb 4	O -2	1.88	0.37	e	unchecked		
Nb 4	F -1	1.90	0.37	e	unchecked		
Nb 4	Cl -1	2.26	0.35	e	unchecked		
Nb 4	Br -1	2.62	0.37	e	unchecked		
Nb 5	O -2	1.911	0.37	a	?		
Nb 5	O -2	1.916	0.37	x	?		
Nb 5	F -1	1.87	0.37	b	?		
Nb 5	Cl -1	2.27	0.37	b	?		
Nb 5	I -1	2.77	0.37	e	unchecked		
Nb 5	N -3	2.01	0.35	e	unchecked		
Nb 9	Br -1	2.45	0.37	b	?		
Nb 9	I -1	2.68	0.37	b	?		
Nb 9	S -2	2.37	0.37	b	?		
Nb 9	Se -2	2.51	0.37	b	?		
Nb 9	Te -2	2.70	0.37	b	?		
Nb 9	N -3	2.06	0.37	b	?		
Nb 9	P -3	2.46	0.37	b	?		
Nb 9	As -3	2.54	0.37	b	?		
Nb 9	H -1	1.75	0.37	b	?		
Nd 2	O -2	1.95	0.37	e	unchecked		
Nd 2	S -2	2.60	0.35	e	unchecked		
Nd 3	O -2	2.105	0.37	a	?		
Nd 3	O -2	2.117	0.37	b	?		
Nd 3	O -2	2.086	0.37	ae	'from transition metal complexes'		
Nd 3	S -2	2.59	0.37	b	?		
Nd 3	Se -2	2.71	0.37	b	?		
Nd 3	Te -2	2.89	0.37	b	?		
Nd 3	F -1	2.008	0.37	b	?		
Nd 3	F -1	1.98	0.40	p	?		
Nd 3	Cl -1	2.492	0.37	b	?		
Nd 3	Cl -1	2.46	0.40	p	?		
Nd 3	Br -1	2.66	0.37	b	?		
Nd 3	Br -1	2.61	0.40	p	?		
Nd 3	I -1	2.87	0.37	b	?		
Nd 3	I -1	2.84	0.40	p	?		
Nd 3	N -3	2.201	0.37	ah	?		
Nd 3	N -3	2.30	0.37	b	?		
NH 1	O -2	2.226	0.37	s	?		
NH 1	F -1	2.129	0.37	s	?		
NH 1	Cl -1	2.619	0.37	s	?		
Ni 2	O -2	1.654	0.37	a	?		
Ni 2	O -2	1.670	0.37	j	'from transition metal complexes'		
Ni 2	S -2	1.98	0.37	e	unchecked		
Ni 2	S -2	1.937	0.37	j	'from transition metal complexes'		
Ni 2	F -1	1.596	0.37	a	?		
Ni 2	Cl -1	2.02	0.37	b	?		
Ni 2	Br -1	2.20	0.37	e	unchecked		
Ni 2	I -1	2.40	0.37	e	unchecked		
Ni 2	N -3	1.70	0.37	e	unchecked		

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Ni 2	N -3	1.647	0.37	j	'from transition metal complexes'		
Ni 3	O -2	1.75	0.37	e	?		
Ni 3	S -2	2.040	0.37	j	'from transition metal complexes'		
Ni 3	F -1	1.58	0.37	e	unchecked		
Ni 3	N -3	1.731	0.37	j	'from transition metal complexes'		
Ni 4	O -2	1.78	0.35	e	unchecked		
Ni 4	F -1	1.61	0.37	e	unchecked		
Ni 9	Br -1	2.16	0.37	b	?		
Ni 9	I -1	2.34	0.37	b	?		
Ni 9	S -2	2.04	0.37	b	?		
Ni 9	Se -2	2.14	0.37	b	?		
Ni 9	Te -2	2.43	0.37	b	?		
Ni 9	N -3	1.75	0.37	b	?		
Ni 9	P -3	2.17	0.37	b	?		
Ni 9	As -3	2.24	0.37	b	?		
Ni 9	H -1	1.40	0.37	b	?		
Np 3	F -1	2.00	0.40	p	?		
Np 3	Cl -1	2.48	0.40	p	?		
Np 3	Br -1	2.62	0.40	p	?		
Np 3	I -1	2.85	0.40	p	?		
Np 4	O -2	2.18	0.37	e	unchecked		
Np 4	O -2	2.11	0.35	p	?		
Np 4	F -1	2.02	0.37	e	unchecked		
Np 4	F -1	1.98	0.40	p	?		
Np 4	Cl -1	2.46	0.40	p	?		
Np 5	O -2	2.09	0.35	p	?		
Np 5	F -1	1.97	0.40	p	?		
Np 5	Cl -1	2.42	0.40	p	?		
Np 6	O -2	2.07	0.35	p	?		
Np 6	F -1	1.97	0.40	p	?		
Np 7	O -2	2.06	0.35	p	?		
O -2	O -2	1.500	0.35	e	unchecked		
Os 4	O -2	1.811	0.37	b	?		
Os 4	S -2	2.21	0.37	e	unchecked		
Os 4	F -1	1.72	0.37	b	?		
Os 4	Cl -1	2.19	0.37	b	?		
Os 4	Br -1	2.37	0.37	e	unchecked		
Os 5	F -1	1.81	0.37	e	unchecked		
Os 6	O -2	2.03	0.37	a	?		
Os 6	F -1	1.80	0.35	e	unchecked		
Os 8	O -2	1.92	0.37	e	unchecked		
P 3	O -2	1.63	0.37	e	unchecked		
P 3	S -2	2.12	0.37	e	unchecked		
P 3	Se -2	2.24	0.37	e	unchecked		
P 3	F -1	1.53	0.35	e	unchecked		
P 4	O -2	1.64	0.37	e	unchecked		
P 4	S -2	2.13	0.35	e	unchecked		
P 4	F -1	1.66	0.37	e	unchecked		
P 5	O -2	1.617	0.37	a	?		
P 5	O -2	1.604	0.37	b	?		
P 5	S -2	2.145	0.37	a	?		
P 5	F -1	1.54	0.37	e	unchecked		
P 5	Cl -1	2.02	0.37	e	?		
P 5	Br -1	2.17	0.40	e	unchecked		
P 5	N -3	1.704	0.37	a	?		
P 9	Br -1	2.15	0.37	b	?		
P 9	I -1	2.40	0.37	b	?		
P 9	S -2	2.11	0.37	b	?		
P 9	Se -2	2.26	0.37	b	?		
P 9	Te -2	2.44	0.37	b	?		
P 9	N -3	1.73	0.37	b	?		
P 9	P -3	2.19	0.37	b	?		
P 9	As -3	2.25	0.37	b	?		
P 9	H -1	1.41	0.37	b	?		
P 5	P 5	2.22	0.35	e	unchecked		
Pa 4	O -2	2.15	0.35	p	?		
Pa 4	F -1	2.02	0.40	p	?		
Pa 4	Cl -1	2.49	0.40	p	?		
Pa 4	Br -1	2.66	0.40	p	?		



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Pa 5	O -2	2.09	0.35	e	unchecked
Pa 5	O -2	2.11	0.35	p	?
Pa 5	F -1	2.04	0.37	e	unchecked
Pa 5	F -1	2.01	0.40	p	?
Pa 5	Cl -1	2.45	0.40	p	?
Pa 5	Br -1	2.58	0.40	p	?
Pb 2	O -2	1.963	0.49	q	?
Pb 2	O -2	2.112	0.37	a	?
Pb 2	S -2	2.541	0.37	a	?
Pb 2	Se -2	2.69	0.37	e	unchecked
Pb 2	F -1	2.03	0.37	b	?
Pb 2	Cl -1	2.53	0.37	b	?
Pb 2	Br -1	2.68	0.37	e	unchecked
Pb 2	I -1	2.83	0.37	e	unchecked
Pb 2	N -3	2.18	0.40	e	unchecked
Pb 4	O -2	2.042	0.37	a	?
Pb 4	F -1	1.94	0.37	b	?
Pb 4	Cl -1	2.43	0.37	b	?
Pb 4	Cl -1	2.36	0.37	e	unchecked
Pb 4	Br -1	3.04	0.35	e	unchecked
Pb 9	Br -1	2.64	0.37	b	?
Pb 9	I -1	2.78	0.37	b	?
Pb 9	S -2	2.55	0.37	b	?
Pb 9	Se -2	2.67	0.37	b	?
Pb 9	Te -2	2.84	0.37	b	?
Pb 9	N -3	2.22	0.37	b	?
Pb 9	P -3	2.64	0.37	b	?
Pb 9	As -3	2.72	0.37	b	?
Pb 9	H -1	1.97	0.37	b	?
Pd 2	O -2	1.792	0.37	b	?
Pd 2	S -2	2.09	0.37	e	unchecked
Pd 2	F -1	1.74	0.37	b	?
Pd 2	Cl -1	2.05	0.37	b	?
Pd 2	Br -1	2.20	0.37	e	unchecked
Pd 2	I -1	2.36	0.37	e	unchecked
Pd 2	N -3	1.82	0.35	e	unchecked
Pd 2	C -4	1.73	0.37	e	unchecked
Pd 4	S -2	2.30	0.37	e	unchecked
Pd 4	F -1	1.66	0.37	e	unchecked
Pd 9	Br -1	2.19	0.37	b	?
Pd 9	I -1	2.38	0.37	b	?
Pd 9	S -2	2.10	0.37	b	?
Pd 9	Se -2	2.22	0.37	b	?
Pd 9	Te -2	2.48	0.37	b	?
Pd 9	N -3	1.81	0.37	b	?
Pd 9	P -3	2.22	0.37	b	?
Pd 9	As -3	2.30	0.37	b	?
Pd 9	H -1	1.47	0.37	b	?
Pm 3	F -1	1.96	0.40	p	?
Pm 3	Cl -1	2.45	0.40	p	?
Pm 3	Br -1	2.59	0.40	p	?
Pm 3	Cl -1	2.82	0.40	p	?
Po 4	O -2	2.19	0.37	e	unchecked
Po 4	F -1	2.38	0.37	e	unchecked
Pr 3	O -2	2.138	0.37	a	?
Pr 3	O -2	2.098	0.37	ae	'from transition metal complexes'
Pr 3	S -2	2.60	0.37	b	?
Pr 3	Se -1	2.72	0.37	b	?
Pr 3	Te -2	2.90	0.37	b	?
Pr 3	F -1	2.022	0.37	b	?
Pr 3	F -1	1.99	0.40	p	?
Pr 3	Cl -1	2.50	0.37	b	?
Pr 3	Cl -1	2.47	0.40	p	?
Pr 3	Br -1	2.67	0.37	b	?
Pr 3	Br -1	2.63	0.40	p	?
Pr 3	I -1	2.89	0.37	b	?
Pr 3	I -1	2.85	0.40	p	?
Pr 3	N -3	2.215	0.37	ah	?
Pr 3	N -3	2.30	0.37	b	?

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Pr 3	P -3	2.68	0.37	b	?
Pr 3	As -3	2.75	0.37	b	?
Pr 3	H -1	2.02	0.37	b	?
Pt 2	O -2	1.768	0.37	b	?
Pt 2	O -2	1.80	0.37	e	unchecked
Pt 2	S -2	2.16	0.37	e	unchecked
Pt 2	F -1	1.68	0.37	b	?
Pt 2	Cl -1	2.05	0.37	b	?
Pt 2	Br -1	2.20	0.37	e	unchecked
Pt 2	C 2	1.760	0.37	a	?
Pt 2	N -3	1.81	0.37	e	unchecked
Pt 3	O -2	1.87	0.37	e	unchecked
Pt 3	Cl -1	2.30	0.37	e	unchecked
Pt 3	Br -1	2.47	0.35	e	unchecked
Pt 4	O -2	1.879	0.37	a	?
Pt 4	F -1	1.759	0.37	b	?
Pt 4	F -1	2.19	0.37	e	unchecked
Pt 4	Cl -1	2.17	0.37	b	?
Pt 4	Cl -1	2.32	0.37	e	unchecked
Pt 4	Br -1	2.6	0.35	e	unchecked
Pt 9	Br -1	2.18	0.37	b	?
Pt 9	I -1	2.37	0.37	b	?
Pt 9	S -2	2.08	0.37	b	?
Pt 9	Se -2	2.19	0.37	b	?
Pt 9	Te -2	2.45	0.37	b	?
Pt 9	N -3	1.77	0.37	b	?
Pt 9	P -3	2.19	0.37	b	?
Pt 9	As -3	2.26	0.37	b	?
Pt 9	H -1	1.40	0.37	b	?
Pu 3	O -2	2.11	0.37	b	?
Pu 3	O -2	2.14	0.35	p	?
Pu 3	F -1	2.00	0.37	b	?
Pu 3	F -1	1.99	0.40	p	?
Pu 3	Cl -1	2.48	0.37	b	?
Pu 3	Cl -1	2.46	0.40	p	?
Pu 3	Br -1	2.60	0.40	p	?
Pu 3	I -1	2.84	0.40	p	?
Pu 4	O -2	2.09	0.35	p	?
Pu 4	F -1	1.97	0.40	p	?
Pu 4	Cl -1	2.44	0.40	p	?
Pu 5	O -2	2.11	0.37	e	?
Pu 5	O -2	2.08	0.35	p	?
Pu 5	F -1	1.96	0.40	p	?
Pu 6	O -2	2.06	0.35	p	?
Pu 6	F -1	1.96	0.40	p	?
Pu 7	O -2	2.05	0.35	p	?
Rb 1	O -2	2.263	0.37	a	?
Rb 1	O -2	2.0812	0.415	c	'7 A cut-off'
Rb 1	S -2	2.70	0.37	b	?
Rb 1	S -2	2.2991	0.553	c	'7 A cut-off'
Rb 1	S -2	2.80	0.37	e	unchecked
Rb 1	Se -2	2.81	0.37	b	?
Rb 1	Se -2	2.3886	0.587	c	'7 A cut-off'
Rb 1	Te -2	3.00	0.37	b	?
Rb 1	Te -2	2.4175	0.633	c	'8 A cut-off'
Rb 1	F -1	2.16	0.37	b	?
Rb 1	F -1	1.9718	0.412	c	'6 A cut-off'
Rb 1	F -1	2.20	0.37	e	unchecked
Rb 1	Cl -1	2.652	0.37	a	?
Rb 1	Cl -1	2.2653	0.531	c	'7 A cut-off'
Rb 1	Br -1	2.78	0.37	b	?
Rb 1	Br -1	2.3296	0.578	c	'7 A cut-off'
Rb 1	Br -1	2.86	0.37	e	unchecked
Rb 1	I -1	3.01	0.37	b	?
Rb 1	I -1	2.4509	0.638	c	'7 A cut-off'
Rb 1	I -1	3.12	0.37	e	unchecked
Rb 1	N -3	2.62	0.37	e	unchecked
Rb 1	N -3	2.37	0.37	b	?
Rb 1	P -3	2.76	0.37	b	?

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Rb 1	As	-3	2.87	0.37	b	?	
Rb 1	H	-1	2.26	0.37	b	?	
Re 1	Cl	-1	2.62	0.35	e	unchecked	
Re 3	O	-2	1.9	0.35	e	unchecked	
Re 3	Cl	-1	2.23	0.37	e	unchecked	
Re 4	F	-1	1.81	0.37	e	unchecked	
Re 4	Cl	-1	2.23	0.37	e	unchecked	
Re 4	Br	-1	2.35	0.37	e	unchecked	
Re 5	O	-2	1.86	0.37	e	?	
Re 5	Cl	-1	2.24	0.37	e	unchecked	
Re 6	F	-1	1.79	0.37	e	unchecked	
Re 7	O	-2	1.97	0.37	e	unchecked	
Re 7	F	-1	1.86	0.37	b	?	
Re 7	Cl	-1	2.23	0.37	b	?	
Re 9	Br	-1	2.45	0.37	b	?	
Re 9	I	-1	2.61	0.37	b	?	
Re 9	S	-2	2.37	0.37	b	?	
Re 9	Se	-2	2.50	0.37	b	?	
Re 9	Te	-2	2.70	0.37	b	?	
Re 9	N	-3	2.06	0.37	b	?	
Re 9	P	-3	2.46	0.37	b	?	
Re 9	As	-3	2.54	0.37	b	?	
Re 9	H	-1	1.75	0.37	b	?	
Rh 3	O	-2	1.793	0.37	b	?	
Rh 3	F	-1	1.71	0.37	b	?	
Rh 3	Cl	-1	2.08	0.37	e	unchecked	
Rh 3	Cl	-1	2.17	0.37	b	?	
Rh 3	Br	-1	2.27	0.35	e	unchecked	
Rh 3	N	-3	1.82	0.35	e	unchecked	
Rh 4	F	-1	1.59	0.37	e	unchecked	
Rh 5	F	-1	1.80	0.37	e	unchecked	
Rh 9	Br	-1	2.25	0.37	b	?	
Rh 9	I	-1	2.48	0.37	b	?	
Rh 9	S	-2	2.15	0.37	b	?	
Rh 9	Se	-1	2.33	0.37	b	?	
Rh 9	Te	-2	2.55	0.37	b	?	
Rh 9	N	-3	1.88	0.37	b	?	
Rh 9	P	-3	2.29	0.37	b	?	
Rh 9	As	-3	2.37	0.37	b	?	
Rh 9	H	-1	1.55	0.37	b	?	
Ru 2	Se	-2	2.11	0.35	e	unchecked	
Ru 2	F	-1	1.84	0.35	e	unchecked	
Ru 3	O	-2	1.77	0.37	o	?	
Ru 3	S	-2	2.20	0.35	e	unchecked	
Ru 3	F	-1	2.12	0.37	e	unchecked	
Ru 3	Cl	-1	2.25	0.37	e	unchecked	
Ru 3	N	-3	1.82	0.35	e	unchecked	
Ru 4	O	-2	1.834	0.37	b	?	
Ru 4	S	-2	2.21	0.37	e	unchecked	
Ru 4	F	-1	1.74	0.37	b	?	
Ru 4	Cl	-1	2.21	0.37	b	?	
Ru 5	O	-2	1.90	0.37	o	?	
Ru 5	F	-1	1.82	0.37	e	unchecked	
Ru 5	Cl	-1	2.23	0.35	e	unchecked	
Ru 6	O	-2	1.87	0.35	e	unchecked	
Ru 7	O	-2	1.99	0.37	e	unchecked	
Ru 9	Br	-1	2.26	0.37	b	?	
Ru 9	I	-1	2.48	0.37	b	?	
Ru 9	S	-2	2.16	0.37	b	?	
Ru 9	Se	-2	2.33	0.37	b	?	
Ru 9	Te	-2	2.54	0.37	b	?	
Ru 9	N	-3	1.88	0.37	b	?	
Ru 9	P	-3	2.29	0.37	b	?	
Ru 9	As	-3	2.36	0.37	b	?	
Ru 9	H	-1	1.61	0.37	b	?	
S 2	O	-2	1.74	0.37	e	unchecked	
S 2	S	-2	2.03	0.37	e	unchecked	
S 2	N	-2	1.597	0.37	a	?	
S 2	N	-3	1.682	0.37	a	?	

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S 2	S	2	2.10	0.35	e	unchecked	
S 4	O	-2	1.644	0.37	a	?	
S 4	F	-1	1.60	0.37	b	?	
S 4	Cl	-1	2.02	0.37	b	?	
S 4	N	-3	1.762	0.37	a	?	
S 6	O	-2	1.624	0.37	a	?	
S 6	F	-1	1.56	0.37	b	?	
S 6	Cl	-1	2.03	0.37	b	?	
S 6	N	-3	1.72	0.37	e	unchecked	
S 9	Br	-1	2.17	0.37	b	?	
S 9	I	-1	2.36	0.37	b	?	
S 9	S	-2	2.07	0.37	b	?	
S 9	Se	-2	2.21	0.37	b	?	
S 9	Te	-2	2.45	0.37	b	?	
S 9	N	-3	1.74	0.37	b	?	
S 9	P	-3	2.15	0.37	b	?	
S 9	As	-3	2.25	0.37	b	?	
S 9	H	-1	1.38	0.37	b	?	
Sb 3	O	-2	1.973	0.37	a	?	
Sb 3	S	-2	2.474	0.37	a	?	
Sb 3	Se	-2	2.60	0.37	e	unchecked	
Sb 3	F	-1	1.883	0.37	a	?	
Sb 3	F	-1	1.90	0.37	b	?	
Sb 3	Cl	-1	2.35	0.37	b	?	
Sb 3	Br	-1	2.51	0.37	e	unchecked	
Sb 3	I	-1	2.76	0.37	e	unchecked	
Sb 3	N	-3	2.108	0.37	d	?	
Sb 5	O	-2	1.942	0.37	a	?	
Sb 5	F	-1	1.797	0.37	a	?	
Sb 5	Cl	-1	2.30	0.37	b	?	
Sb 5	Br	-1	2.48	0.37	e	unchecked	
Sb 5	N	-3	1.99	0.35	e	unchecked	
Sb 9	S	-2	2.45	0.37	b	?	
Sb 9	Se	-2	2.57	0.37	b	?	
Sb 9	Te	-2	2.78	0.37	b	?	
Sb 9	Br	-1	2.50	0.37	b	?	
Sb 9	I	-1	2.72	0.37	b	?	
Sb 9	N	-3	2.12	0.37	b	?	
Sb 9	P	-3	2.52	0.37	b	?	
Sb 9	As	-3	2.60	0.37	b	?	
Sb 9	H	-1	2.77	0.37	b	?	
Sc 3	O	-2	1.849	0.37	a	?	
Sc 3	O	-2	1.877	0.35	o	?	
Sc 3	S	-2	2.321	0.37	a	?	
Sc 3	Se	-2	2.44	0.37	b	?	
Sc 3	Te	-2	2.64	0.37	b	?	
Sc 3	F	-1	1.76	0.37	b	?	
Sc 3	Cl	-1	2.36	0.37	e	unchecked	
Sc 3	Cl	-1	2.23	0.37	b	?	
Sc 3	Br	-1	2.38	0.37	b	?	
Sc 3	I	-1	2.59	0.37	b	?	
Sc 3	N	-3	1.98	0.37	b	?	
Sc 3	P	-3	2.40	0.37	b	?	
Sc 3	As	-3	2.48	0.37	b	?	
Sc 3	H	-1	1.68	0.37	b	?	
Se 2	S	-2	2.21	0.37	e	unchecked	
Se 2	Se	-2	2.33	0.37	e	unchecked	
Se 4	O	-2	1.811	0.37	a	?	
Se 4	F	-1	1.73	0.37	b	?	
Se 4	Cl	-1	2.22	0.37	b	?	
Se 4	Br	-1	2.43	0.37	e	unchecked	
Se 6	O	-2	1.788	0.37	a	?	
Se 6	F	-1	1.69	0.37	b	?	
Se 6	Cl	-1	2.16	0.37	b	?	
Se 6	N	-3	1.90	0.35	e	unchecked	
Se 9	Br	-1	2.33	0.37	b	?	
Se 9	I	-1	2.54	0.37	b	?	
Se 9	S	-2	2.25	0.37	b	?	
Se 9	Se	-2	2.36	0.37	b	?	

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Se 9	Te -2	2.55	0.37	b ?			
Se 9	P -3	2.34	0.37	b ?			
Se 9	As -3	2.42	0.37	b ?			
Se 9	H -1	1.54	0.37	b ?			
Si 4	O -2	1.624	0.37	b ?			
Si 4	O -2	1.640	0.37	a ?			
Si 4	S -2	2.126	0.37	a ?			
Si 4	Se -2	2.26	0.37	b ?			
Si 4	Te -2	2.49	0.37	b ?			
Si 4	F -1	1.58	0.37	b ?			
Si 4	Cl -1	2.03	0.37	b ?			
Si 4	Br -1	2.20	0.37	b ?			
Si 4	I -1	2.41	0.37	b ?			
Si 4	C -4	1.883	0.37	a ?			
Si 4	N -3	1.724	0.37	a ?			
Si 4	N -3	1.77	0.37	b ?			
Si 4	P -3	2.23	0.37	b ?			
Si 4	As -3	2.31	0.37	b ?			
Si 4	H -1	1.47	0.37	b ?			
Sm 2	O -2	2.116	0.37	ai ?			
Sm 3	O -2	2.088	0.37	b ?			
Sm 3	O -2	2.063	0.37	ae	'from transition metal complexes'		
Sm 3	O -2	2.055	0.37	ai	'from transition metal complexes'		
Sm 3	S -2	2.55	0.37	b ?			
Sm 3	Se -2	2.67	0.37	b ?			
Sm 3	Te -2	2.86	0.37	b ?			
Sm 3	F -1	1.94	0.40	p ?			
Sm 3	F -1	2.00	0.37	e	unchecked		
Sm 3	Cl -1	1.977	0.37	b ?			
Sm 3	Cl -1	2.43	0.40	p ?			
Sm 3	Br -1	2.66	0.37	b ?			
Sm 3	Br -1	2.58	0.40	p ?			
Sm 3	I -1	2.84	0.37	b ?			
Sm 3	I -1	2.80	0.40	p ?			
Sm 3	N -3	2.171	0.37	ah ?			
Sm 3	N -3	2.24	0.37	b ?			
Sm 3	P -3	2.63	0.37	b ?			
Sm 3	As -3	2.70	0.37	b ?			
Sm 3	H -1	1.96	0.37	b ?			
Sn 2	O -2	1.94	0.37	b ?			
Sn 2	S -2	2.44	0.37	e	unchecked		
Sn 2	F -1	1.925	0.37	a ?			
Sn 2	Cl -1	2.41	0.37	e	unchecked		
Sn 3	Cl -1	2.36	0.37	b ?			
Sn 2	Br -1	2.53	0.35	d	unchecked		
Sn 2	I -1	2.81	0.37	e	unchecked		
Sn 2	N -3	2.03	0.35	e	unchecked		
Sn 4	O -2	1.905	0.37	a ?			
Sn 4	S -2	2.399	0.37	a ?			
Sn 4	Se -2	2.51	0.37	e	unchecked		
Sn 4	F -1	1.843	0.37	a ?			
Sn 4	Cl -1	2.276	0.37	a ?			
Sn 4	Br -1	2.40	0.37	e	unchecked		
Sn 4	N -3	2.03	0.35	e	unchecked		
Sn 9	Br -1	2.55	0.37	b ?			
Sn 9	I -1	2.76	0.37	b ?			
Sn 9	S -2	2.39	0.37	aa ?			
Sn 9	S -2	2.45	0.37	b ?			
Sn 9	Se -2	2.59	0.37	b ?			
Sn 9	Te -2	2.76	0.37	b ?			
Sn 9	N -3	2.06	0.37	aa ?			
Sn 9	N -3	2.14	0.37	b ?			
Sn 9	P -3	2.45	0.37	b ?			
Sn 9	As -3	2.62	0.37	b ?			
Sn 9	H -1	1.85	0.37	b ?			
Sr 2	O -2	2.118	0.37	a ?			
Sr 2	S -2	2.59	0.37	b ?			
Sr 2	S -2	2.65	0.37	e	unchecked		
Sr 2	Se -2	2.72	0.37	b ?			

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Sr 2	Te -2	2.87	0.37	b ?			
Sr 2	Te -2	2.06	0.37	e	unchecked		
Sr 2	F -1	2.019	0.37	b ?			
Sr 2	Cl -1	2.51	0.37	b ?			
Sr 2	Br -1	2.68	0.37	b ?			
Sr 2	I -1	2.88	0.37	b ?			
Sr 2	N -3	2.23	0.37	b ?			
Sr 2	P -3	2.67	0.37	b ?			
Sr 2	As -3	2.76	0.37	b ?			
Sr 2	H -1	2.01	0.37	b ?			
Ta 4	O -2	2.29	0.37	e	unchecked		
Ta 5	O -2	1.920	0.37	a ?			
Ta 5	S -2	2.47	0.37	e	unchecked		
Ta 5	F -1	1.88	0.37	b ?			
Ta 5	Cl -1	2.30	0.37	b ?			
Ta 9	Br -1	2.45	0.37	b ?			
Ta 9	I -1	2.66	0.37	b ?			
Ta 9	S -2	2.39	0.37	b ?			
Ta 9	Se -2	2.51	0.37	b ?			
Ta 9	Te -2	2.70	0.37	b ?			
Ta 9	N -3	2.01	0.37	b ?			
Ta 9	P -3	2.47	0.37	b ?			
Ta 9	As -3	2.55	0.37	b ?			
Ta 9	H -1	1.76	0.37	b ?			
Tb 3	O -2	2.032	0.37	a ?			
Tb 3	O -2	2.049	0.37	b ?			
Tb 3	O -2	2.013	0.37	ae	'from transition metal complexes'		
Tb 3	S -2	2.51	0.37	b ?			
Tb 3	Se -2	2.63	0.37	b ?			
Tb 3	Te -2	2.82	0.37	b ?			
Tb 3	F -1	1.936	0.37	b ?			
Tb 3	F -1	1.90	0.40	p ?			
Tb 3	Cl -1	2.427	0.37	b ?			
Tb 3	Cl -1	2.39	0.40	p ?			
Tb 3	Br -1	2.58	0.37	b ?			
Tb 3	Br -1	2.54	0.40	p ?			
Tb 3	I -1	2.80	0.37	b ?			
Tb 3	I -1	2.77	0.40	p ?			
Tb 3	N -3	2.130	0.37	ah ?			
Tb 3	N -3	2.20	0.37	b ?			
Tb 3	P -3	2.59	0.37	b ?			
Tb 3	As -3	2.66	0.37	b ?			
Tb 3	H -1	1.91	0.37	b ?			
Tc 4	F -1	1.88	0.40	p ?			
Tc 4	Cl -1	2.21	0.37	e	unchecked		
Tc 7	O -2	1.90	0.37	e	unchecked		
Te 4	O -2	1.977	0.37	a ?			
Te 4	S -2	2.44	0.37	e	unchecked		
Te 4	F -1	1.87	0.37	b ?			
Te 4	Cl -1	2.37	0.37	b ?			
Te 4	Br -1	2.55	0.37	e	unchecked		
Te 4	I -1	2.787	0.37	e	unchecked		
Te 6	O -2	1.917	0.37	a ?			
Te 6	F -1	1.82	0.37	b ?			
Te 6	Cl -1	2.30	0.37	b ?			
Te 9	Br -1	2.53	0.37	b ?			
Te 9	I -1	2.76	0.37	b ?			
Te 9	S -2	2.45	0.37	b ?			
Te 9	Se -2	2.53	0.37	b ?			
Te 9	Te -2	2.76	0.37	b ?			
Te 9	N -3	2.12	0.37	b ?			
Te 9	P -3	2.52	0.37	b ?			
Te 9	As -3	2.60	0.37	b ?			
Te 9	H -1	1.83	0.37	b ?			
Th 4	O -2	2.167	0.37	b ?			
Th 4	O -2	2.18	0.35	p ?			
Th 4	S -2	2.64	0.37	b ?			
Th 4	Se -2	2.76	0.37	b ?			
Th 4	Te -2	2.94	0.37	b ?			

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Th 4	F	-1	2.068	0.37	a	?	
Th 4	F	-1	2.05	0.40	p	?	
Th 4	Cl	-1	2.55	0.37	b	?	
Th 4	Cl	-1	2.52	0.40	p	?	
Th 4	Br	-1	2.71	0.37	b	?	
Th 4	Br	-1	2.68	0.40	p	?	
Th 4	I	-1	2.93	0.37	b	?	
Th 4	I	-1	2.92	0.40	p	?	
Th 4	I	-1	2.96	0.37	e	unchecked	
Th 4	N	-3	2.34	0.37	b	?	
Th 4	P	-3	2.73	0.37	b	?	
Th 4	As	-3	2.80	0.37	b	?	
Th 4	H	-1	2.07	0.37	b	?	
Ti 2	F	-1	2.15	0.37	e	unchecked	
Ti 2	Cl	-1	2.31	0.37	e	unchecked	
Ti 2	Br	-1	2.49	0.37	e	unchecked	
Ti 3	O	-2	1.791	0.37	b	?	
Ti 3	S	-2	2.11	0.37	e	unchecked	
Ti 3	F	-1	1.723	0.37	b	?	
Ti 3	Cl	-1	2.22	0.37	e	unchecked	
Ti 3	Cl	-1	2.17	0.37	b	?	
Ti 3	I	-1	2.52	0.37	e	unchecked	
Ti 4	O	-2	1.815	0.37	a	?	
Ti 4	O	-2	1.78	0.43	o	?	
Ti 4	S	-2	2.29	0.37	e	unchecked	
Ti 4	F	-1	1.76	0.37	b	?	
Ti 4	Cl	-1	2.19	0.37	b	?	
Ti 4	Br	-1	2.36	0.37	e	unchecked	
Ti 9	O	-2	1.790	0.37	k	'from transition metal complexes'	
Ti 9	Cl	-1	2.184	0.37	k	'from transition metal complexes'	
Ti 9	Br	-1	2.32	0.37	b	?	
Ti 9	I	-1	2.54	0.37	b	?	
Ti 9	S	-2	2.24	0.37	b	?	
Ti 9	Se	-2	2.38	0.37	b	?	
Ti 9	Te	-2	2.60	0.37	b	?	
Ti 9	N	-3	1.93	0.37	b	?	
Ti 9	N	-3	1.906	0.37	k	'from transition metal complexes'	
Ti 9	P	-3	2.36	0.37	b	?	
Ti 9	As	-3	2.42	0.37	b	?	
Ti 9	H	-1	1.61	0.37	b	?	
Tl 1	O	-2	2.124	0.37	a	?	
Tl 1	O	-2	2.172	0.37	b	?	
Tl 1	O	-2	1.927	0.50	af	'inorganic and organic compounds'	
Tl 1	S	-2	2.545	0.37	a	?	
Tl 1	F	-1	2.15	0.37	b	?	
Tl 1	Cl	-1	2.56	0.37	b	?	
Tl 1	Cl	-1	2.61	0.37	e	unchecked	
Tl 1	Br	-1	2.69	0.37	e	unchecked	
Tl 1	I	-1	2.822	0.37	a	?	
Tl 3	O	-2	2.003	0.37	b	?	
Tl 3	F	-1	1.88	0.37	b	?	
Tl 3	Cl	-1	2.32	0.37	b	?	
Tl 3	Br	-1	2.65	0.35	e	unchecked	
Tl 9	Br	-1	2.70	0.37	b	?	
Tl 9	I	-1	2.91	0.37	b	?	
Tl 9	S	-2	2.63	0.37	b	?	
Tl 9	Se	-2	2.70	0.37	b	?	
Tl 9	Te	-2	2.93	0.37	b	?	
Tl 9	N	-3	2.29	0.37	b	?	
Tl 9	P	-3	2.71	0.37	b	?	
Tl 9	As	-3	2.79	0.37	b	?	
Tl 9	H	-1	2.05	0.37	b	?	
Tm 3	O	-2	2.000	0.37	b	?	
Tm 3	O	-2	1.968	0.37	ae	'from transition metal complexes'	
Tm 3	O	-2	1.93	0.37	e	unchecked	
Tm 3	S	-2	2.45	0.37	b	?	
Tm 3	Se	-2	2.58	0.37	b	?	
Tm 3	Te	-2	2.77	0.37	b	?	
Tm 3	F	-1	1.842	0.37	b	?	

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Tm 3	F	-1	1.86	0.40	p	?	
Tm 3	F	-1	1.91	0.37	e	unchecked	
Tm 3	Cl	-1	2.38	0.37	b	?	
Tm 3	Cl	-1	2.35	0.40	p	?	
Tm 3	Br	-1	2.53	0.37	b	?	
Tm 3	Br	-1	2.50	0.40	p	?	
Tm 3	I	-1	2.74	0.37	b	?	
Tm 3	I	-1	2.74	0.40	p	?	
Tm 3	N	-3	2.14	0.37	b	?	
Tm 3	P	-3	2.53	0.37	b	?	
Tm 3	As	-3	2.62	0.37	b	?	
Tm 3	H	-1	1.85	0.37	b	?	
U 2	O	-1	2.08	0.37	e	unchecked	
U 3	S	-2	2.54	0.37	e	unchecked	
U 3	F	-1	2.02	0.40	p	?	
U 3	F	-1	2.09	0.37	e	unchecked	
U 3	Cl	-1	2.49	0.40	p	?	
U 3	Br	-1	2.64	0.40	p	?	
U 3	I	-1	2.87	0.40	p	?	
U 4	O	-2	2.112	0.37	b	?	
U 4	O	-2	2.13	0.35	p	?	
U 4	S	-2	2.55	0.37	e	unchecked	
U 4	F	-1	2.038	0.37	a	?	
U 4	F	-1	2.034	0.37	b	?	
U 4	F	-1	2.00	0.40	p	?	
U 4	Cl	-1	2.47	0.40	p	?	
U 4	Br	-1	2.60	0.40	p	?	
U 4	Br	-1	2.61	0.37	e	unchecked	
U 4	I	-1	2.88	0.37	e	unchecked	
U 4	N	-3	2.18	0.37	e	unchecked	
U 5	O	-2	2.075	0.37	b	?	
U 5	O	-2	2.10	0.35	p	?	
U 5	F	-1	1.966	0.37	b	?	
U 5	F	-1	1.99	0.40	p	?	
U 5	Cl	-1	2.46	0.37	b	?	
U 5	Cl	-1	2.43	0.40	p	?	
U 5	Br	-1	2.7	0.35	e	unchecked	
U 6	O	-2	2.051	0.519	r	?	
U 6	O	-2	2.075	0.37	a	?	
U 6	O	-2	2.08	0.35	p	?	
U 6	F	-1	1.98	0.40	p	?	
U 6	Cl	-1	2.42	0.40	p	?	
U 6	N	-3	1.93	0.35	e	unchecked	
U 9	Br	-1	2.63	0.37	b	?	
U 9	I	-1	2.84	0.37	b	?	
U 9	S	-2	2.56	0.37	b	?	
U 9	Se	-2	2.70	0.37	b	?	
U 9	Te	-2	2.86	0.37	b	?	
U 9	N	-3	2.24	0.37	b	?	
U 9	P	-3	2.64	0.37	b	?	
U 9	As	-3	2.72	0.37	b	?	
U 9	H	-1	1.97	0.37	b	?	
V 1	O	-2	1.88	0.37	e	unchecked	
V 1	Cl	-1	2.00	0.35	e	unchecked	
V 2	O	-2	1.70	0.37	e	unchecked	
V 2	S	-2	2.11	0.37	e	unchecked	
V 2	F	-1	2.16	0.37	e	unchecked	
V 2	Cl	-1	2.44	0.37	e	unchecked	
V 3	O	-2	1.743	0.37	a	?	
V 3	O	-2	1.749	0.37	j	'from transition metal complexes'	
V 3	S	-2	2.17	0.37	e	unchecked	
V 3	S	-2	2.185	0.37	j	?	
V 3	F	-1	1.702	0.37	b	?	
V 3	Cl	-1	2.19	0.37	b	?	
V 3	Br	-1	2.33	0.35	e	unchecked	
V 3	N	-3	1.813	0.37	j	'from transition metal complexes'	
V 3	N	-3	1.84	0.35	e	unchecked	
V 4	O	-2	1.784	0.37	a	?	
V 4	O	-2	1.780	0.37	j	'from transition metal complexes'	

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V 4	O	-2	1.735	0.37	j	'vanadyl bond only'	
V 4	S	-2	2.226	0.37	j	'from transition metal complexes'	
V 4	S	-2	2.181	0.37	j	'vanadyl bond only'	
V 4	S	-2	2.24	0.37	e	unchecked	
V 4	F	-1	1.70	0.37	b	?	
V 4	Cl	-1	2.16	0.37	b	?	
V 4	N	-3	1.875	0.37	j	'from transition metal complexes'	
V 5	O	-2	1.803	0.37	a	?	
V 5	O	-2	1.799	0.37	x	?	
V 5	S	-2	2.25	0.37	e	unchecked	
V 5	F	-1	1.70	0.37	e	unchecked	
V 5	Cl	-1	2.16	0.37	b	?	
V 9	O	-2	1.788	0.32	ag	'All oxidation states'	
V 9	O	-2	1.81	0.34	o	?	
V 9	Br	-1	2.30	0.37	b	?	
V 9	I	-1	2.51	0.37	b	?	
V 9	S	-2	2.23	0.37	b	?	
V 9	Se	-2	2.33	0.37	b	?	
V 9	Te	-2	2.57	0.37	b	?	
V 9	N	-3	1.86	0.37	b	?	
V 9	P	-3	2.31	0.37	b	?	
V 9	As	-3	2.39	0.37	b	?	
V 9	H	-1	1.58	0.37	b	?	
W 5	O	-2	1.89	0.37	e	unchecked	
W 6	O	-2	1.917	0.37	a	?	
W 6	O	-2	1.916	0.41	x	?	
W 6	O	-2	1.921	0.37	b	?	
W 6	F	-1	1.83	0.37	b	?	
W 6	Cl	-1	2.27	0.37	b	?	
W 9	Br	-1	2.45	0.37	b	?	
W 9	I	-1	2.66	0.37	b	?	
W 9	S	-2	2.39	0.37	b	?	
W 9	Se	-2	2.51	0.37	b	?	
W 9	Te	-2	2.71	0.37	b	?	
W 9	N	-3	2.06	0.37	b	?	
W 9	P	-3	2.46	0.37	b	?	
W 9	As	-3	2.54	0.37	b	?	
W 9	H	-1	1.76	0.37	b	?	
Xe 2	O	-2	2.05	0.35	e	unchecked	
Xe 2	F	-1	2.02	0.37	e	unchecked	
Xe 4	F	-1	1.93	0.37	e	unchecked	
Xe 6	O	-2	2.00	0.37	e	unchecked	
Xe 6	F	-1	1.89	0.37	e	unchecked	
Xe 8	O	-2	1.94	0.37	e	unchecked	
Y 3	O	-2	2.019	0.37	a	?	
Y 3	O	-2	2.014	0.37	b	?	
Y 3	S	-2	2.48	0.37	b	?	
Y 3	Se	-2	2.61	0.37	b	?	
Y 3	Te	-2	2.80	0.37	b	?	
Y 3	F	-1	1.904	0.37	b	?	
Y 3	F	-1	1.87	0.37	e	unchecked	
Y 3	Cl	-1	2.40	0.37	b	?	
Y 3	Br	-1	2.55	0.37	b	?	
Y 3	I	-1	2.77	0.37	b	?	
Y 3	N	-3	2.17	0.37	b	?	
Y 3	P	-3	2.57	0.37	b	?	
Y 3	As	-3	2.64	0.37	b	?	
Y 3	H	-1	1.86	0.37	b	?	
Yb 3	O	-2	1.965	0.37	a	?	
Yb 3	O	-2	1.985	0.37	b	?	
Yb 3	O	-2	1.954	0.37	ae	'from transition metal complexes'	
Yb 3	S	-2	2.43	0.37	b	?	
Yb 3	Se	-2	2.56	0.37	b	?	
Yb 3	Te	-2	2.76	0.37	b	?	
Yb 3	F	-1	1.875	0.37	b	?	
Yb 3	F	-1	1.85	0.40	p	?	
Yb 3	F	-1	1.90	0.37	e	unchecked	
Yb 3	Cl	-1	2.371	0.37	b	?	
Yb 3	Cl	-1	2.34	0.40	p	?	

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Yb 3	Br	-1	2.451	0.37	b	?	
Yb 3	Br	-1	2.49	0.40	p	?	
Yb 3	I	-1	2.72	0.37	b	?	
Yb 3	I	-1	2.74	0.40	p	?	
Yb 3	N	-3	2.064	0.37	ah	?	
Yb 3	N	-3	2.12	0.37	b	?	
Yb 3	P	-3	2.53	0.37	b	?	
Yb 3	As	-3	2.59	0.37	b	?	
Yb 3	H	-1	1.82	0.37	b	?	
Zn 2	O	-2	1.704	0.37	a	?	
Zn 2	O	-2	1.675	0.39	o	?	
Zn 2	S	-2	2.09	0.37	b	?	
Zn 2	Se	-2	2.22	0.37	b	?	
Zn 2	Te	-2	2.45	0.37	b	?	
Zn 2	F	-1	1.62	0.37	b	?	
Zn 2	F	-1	1.67	0.37	e	unchecked	
Zn 2	Cl	-1	2.01	0.37	b	?	
Zn 2	Br	-1	2.15	0.37	b	?	
Zn 2	I	-1	2.36	0.37	b	?	
Zn 2	N	-3	1.72	0.37	e	unchecked	
Zn 2	P	-3	2.15	0.37	b	?	
Zn 2	As	-3	2.24	0.37	b	?	
Zn 2	H	-1	1.42	0.37	b	?	
Zr 2	O	-2	2.34	0.37	e	unchecked	
Zr 2	F	-1	2.24	0.37	e	unchecked	
Zr 2	Cl	-1	2.58	0.37	e	unchecked	
Zr 4	O	-2	1.928	0.37	a	?	
Zr 4	O	-2	1.937	0.37	b	?	
Zr 4	S	-2	2.41	0.37	b	?	
Zr 4	Se	-2	2.53	0.37	b	?	
Zr 4	Te	-2	2.67	0.37	b	?	
Zr 4	F	-1	1.846	0.37	a	?	
Zr 4	F	-1	1.854	0.37	b	?	
Zr 4	Cl	-1	2.33	0.37	b	?	
Zr 4	Br	-1	2.48	0.37	b	?	
Zr 4	I	-1	2.69	0.37	b	?	
Zr 4	N	-3	2.11	0.37	b	?	
Zr 4	N	-3	2.15	0.37	e	unchecked	
Zr 4	P	-3	2.52	0.37	b	?	
Zr 4	As	-3	2.57	0.37	b	?	
Zr 4	H	-1	1.79	0.37	b	?	
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