Electronic Supplementary Material (ESI) for CrystEngComm.

SUPPLEMENTARY MATERIAL

Intermolecular Interaction Energies in Transition Metal Coordination Compounds

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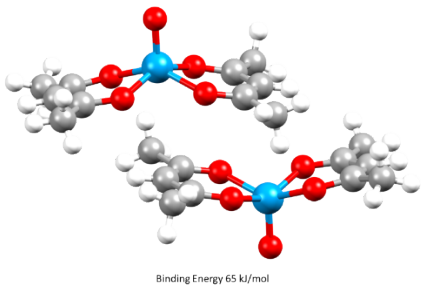
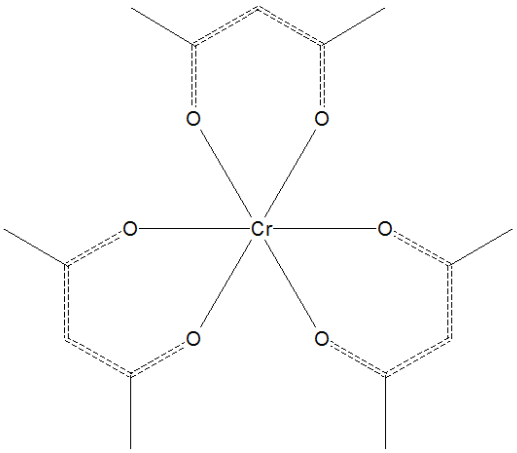
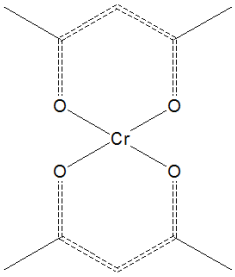
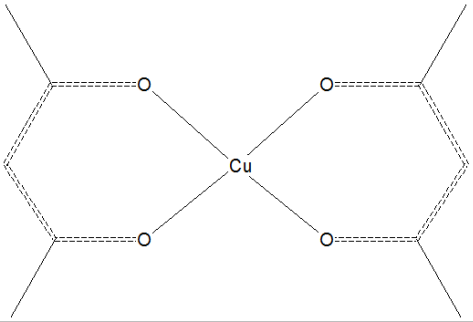
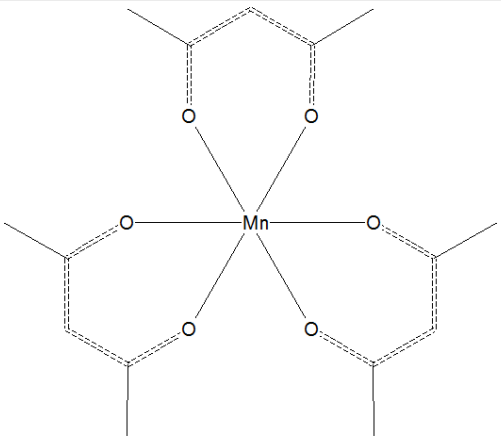
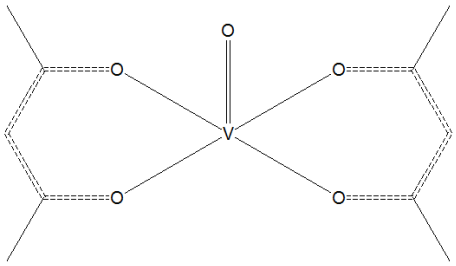
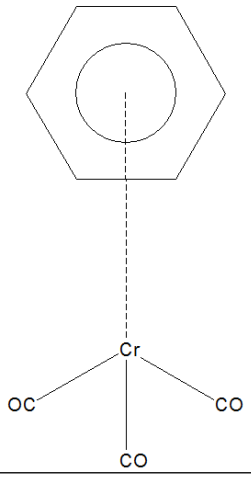
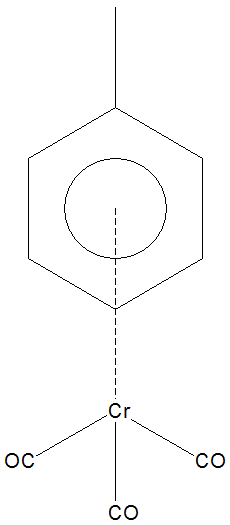
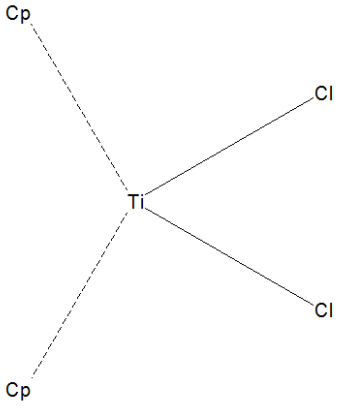
The PIXEL method has been parameterised and validated for transition metals, extending its applicability from ~40% to ~85% of all published crystal structures.

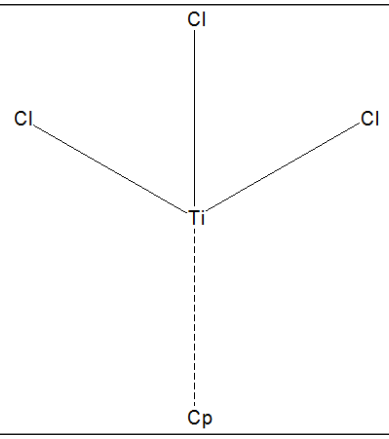
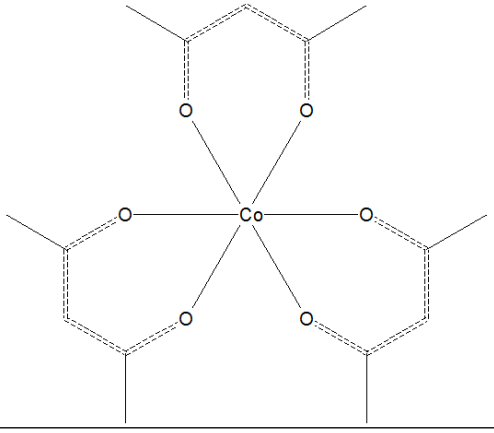
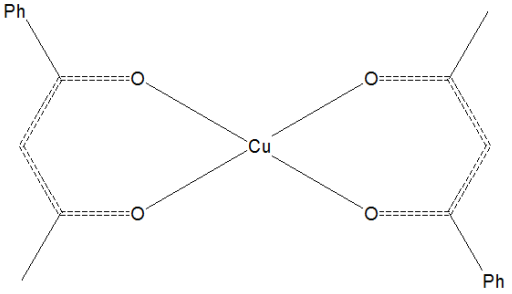
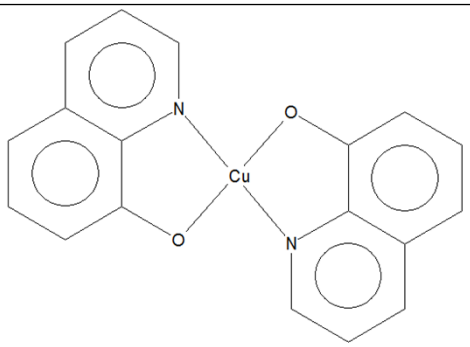


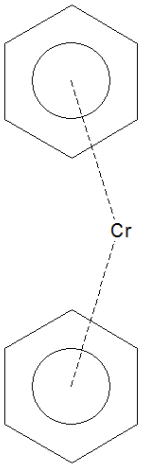
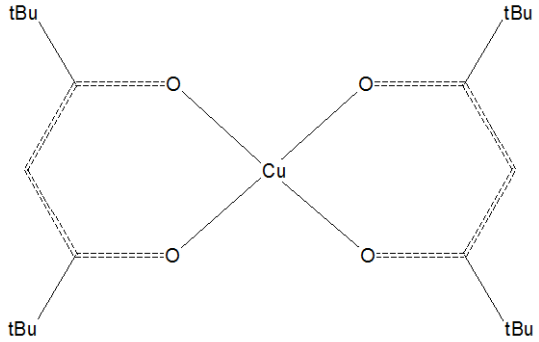
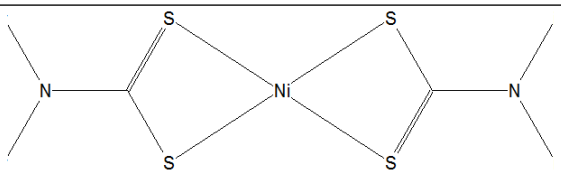
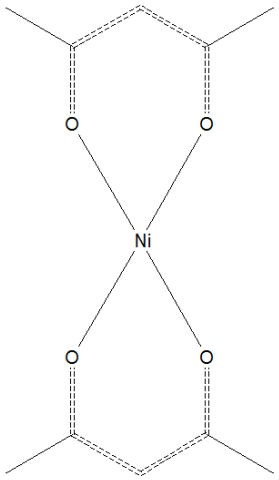
Contents

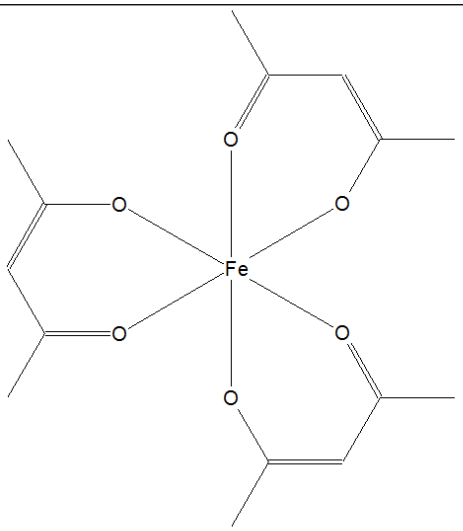
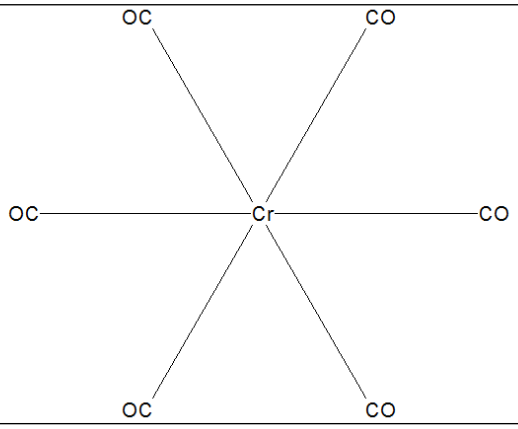
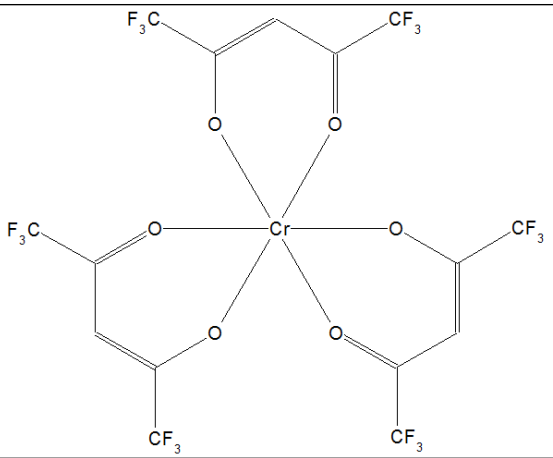
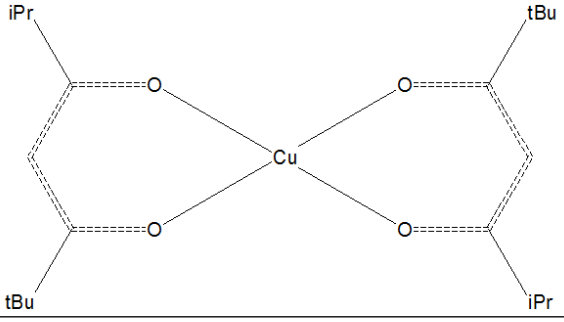
Table S1 Complexes Used for Validation and Parameterisation

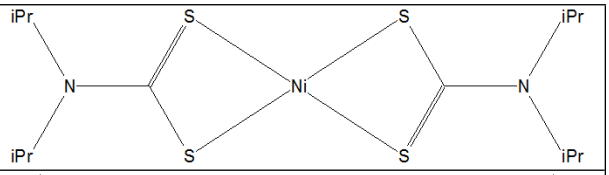
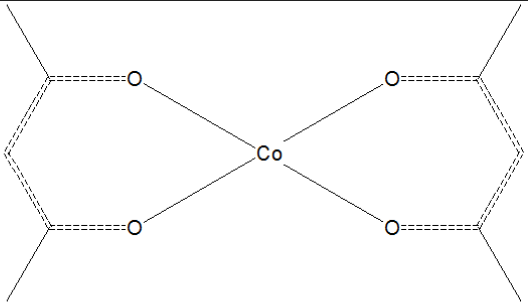
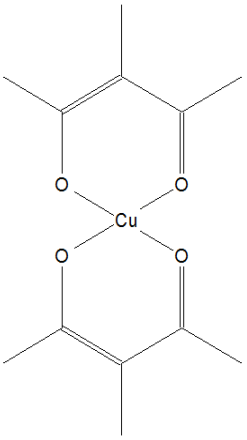
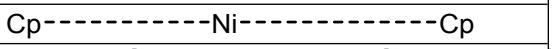
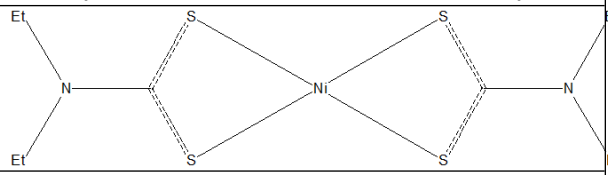
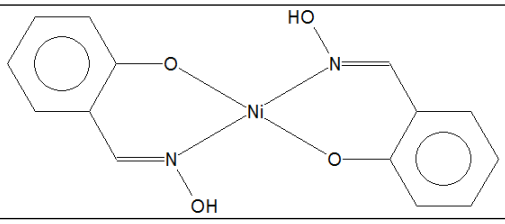
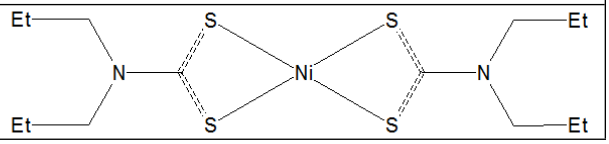
Number	Compound Name	
1	tris(2,4-pentanedionato-O,O')-chromium(iii)	
2	bis(2,4-pentanedionato) chromium	
3	bis(pentane-2,4-dionato)-copper	
4	tris(Acetylacetonato)-manganese(iii)	

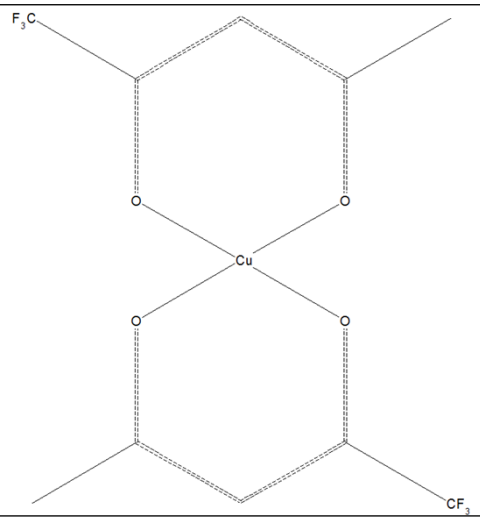
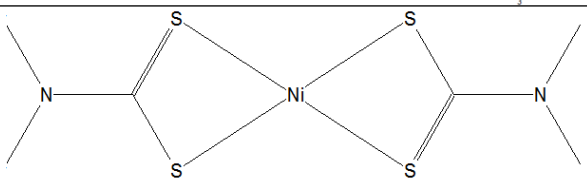
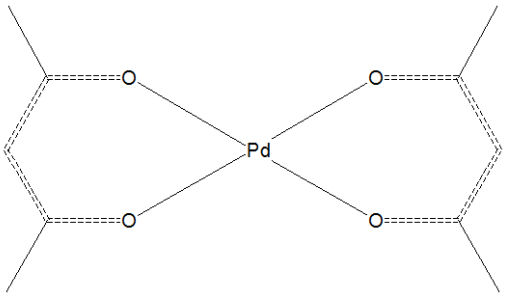
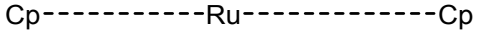
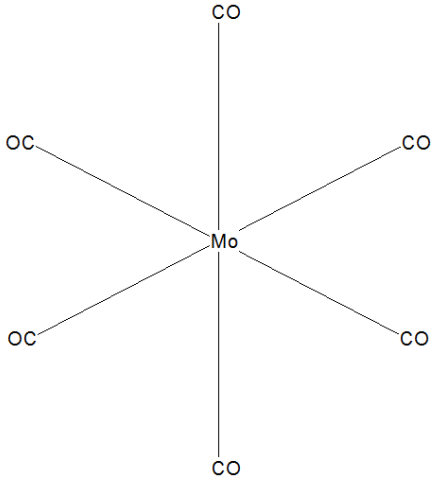
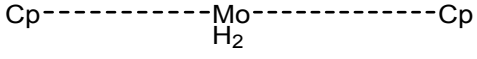
5	bis(Acetylacetonato)-oxo-vanadium(iv)	
6	(η^6-Benzene)-tricarbonyl-chromium	
7	(η^6-Toluene)-tricarbonyl-chromium	
8	bis(η^5-Cyclopentadienyl)-dichloro-titanium	

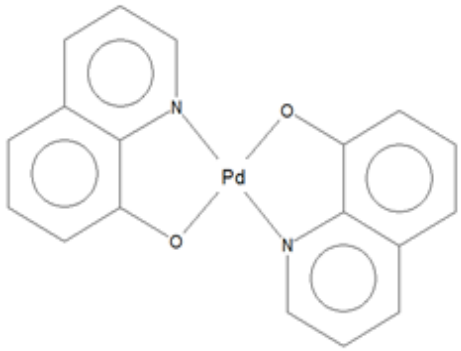
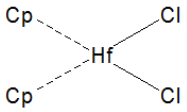
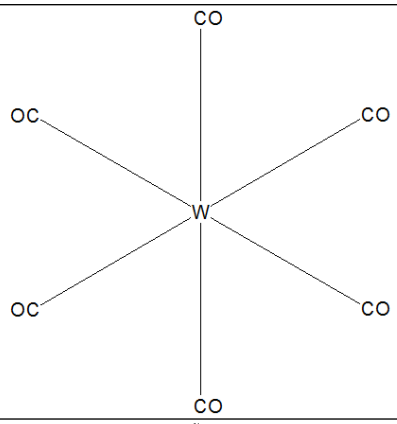
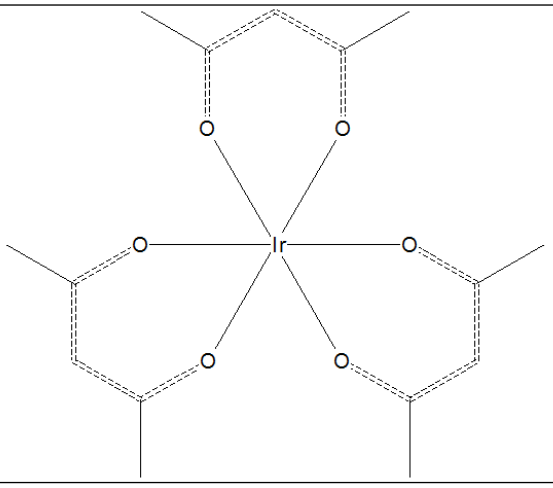
9	Trichloro-(η^5-cyclopentadienyl)-titanium(iv)	
10	tris(Pentane-2,4-dionato-κ^2O,O')-cobalt(iii)	
11	bis(η^5-Cyclopentadienyl)-vanadium	Cp----------V----------Cp
12	bis(Benzoylacetone)-copper(ii)	
13	bis(8-Hydroxyquinolinato-N,O)-copper(ii)	

14	bis(η^6-Benzene)-chromium(0)	
15	bis(η^5-Cyclopentadienyl)-cobalt	Cp----------Cr----------Cp
16	bis(2,2,6,6-Tetramethyl-3,5-heptanedionato)-copper(ii)	
17	bis(N,N-Dimethyldithiocarbamate)-copper(ii)	
18	bis(Acetylacetonato- κ^2O,O')-nickel(ii)	

19	tris(Acetylacetonato-O,O')-iron(iii)	
20	bis(η^5-Cyclopentadienyl)-iron	Cp----------Fe----------Cp
21	Hexacarbonyl-chromium	
22	tris(1,1,1,5,5,5-Hexafluoroacetylacetonato-O,O')-chromium	
23	bis(2,2,6-Trimethylheptane-3,5-dionato)-copper(ii)	

24	bis(N,N-Di-isopropyldithiocarbamato-S,S')-nickel(ii)	
25	bis(2,4-Pentanedionato-O,O')-cobalt(ii)	
26	Copper(ii) 3-methylpentane-2,4-dionate	
27	bis(Cyclopentadienyl)-nickel	
28	bis(N,N-Diethyldithiocarbamato-S,S')-nickel(ii)	
29	bis(Salicylaldoximato-N,O)-nickel(ii)	
30	bis(Di-n-propyldithiocarbamato)-nickel(ii)	

31	trans-bis(1,1,1-Trifluoropentan-2,4-dionato)-copper(ii)	
32	bis(N,N-Dimethyldithiocarbamato)-nickel(ii)	
33	bis(2,4-Pentanedionato)-palladium(ii)	
34	bis(η^5-Cyclopentadienyl)-ruthenium	
35	Hexacarbonyl-molybdenum	
36	Dihydrido-bis(cyclopentadienyl) molybdenum	

37	8-Hydroxyquinolinato palladium(ii)	
38	Dichloro-bis(η^5-cyclopentadienyl)-hafnium	
39	Hexacarbonyl-tungsten	
40	tris(2,4-Pentanedionato)-iridium(iii)	

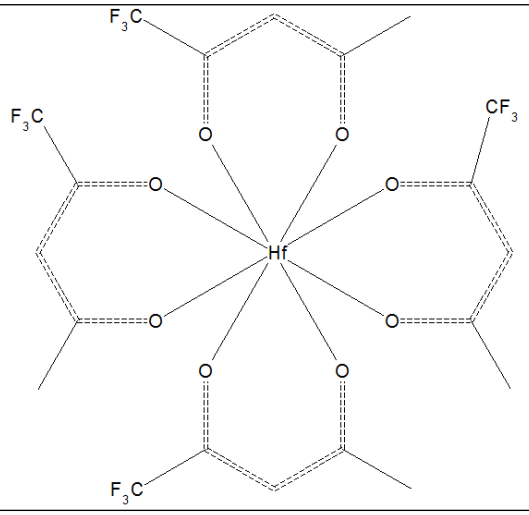
41	tetrakis(Trifluoroacetylacetonato)-hafnium(iv)	
42	bis(η^5-Cyclopentadienyl)-dihydrido-tungsten	Cp----------W(H$_2$)----------Cp
43	bis(η^5-Cyclopentadienyl)-osmium	Cp----------Os----------Cp

Table S2: Sources of van der Waals radii (*RAVDW*), polarisabilities (*POLZE*) and electronegativities (*ELNEG*) for different parameter sets. In the *POLZE* column, CM stands for Claussius-Mossotti and SK stands for Slater-Kirkwood. *m* and *R* are gradients and correlation coefficients of the straight-line fits for all, 1st row only and 2nd/3rd row only transition metal complexes. Gradients are in kJ mol^{-1}.

Set	***RAVDW***	***POLZE***	***ELNEG***	m_{all}	R_{all}	$m_{1st\ row}$	$R_{1st\ row}$	$m_{2nd/3rd}$	$R_{2nd/3rd}$
1	Batsanov	CM	Pauling	1.01(1)	0.92	1.00(2)	0.92	1.06(3)	0.92
2	Batsanov	SK	Pauling	1.01(2)	0.92	0.99(2)	0.92	1.09(3)	0.93
3	Nag	SK	Pauling	1.02(2)	0.92	1.01(2)	0.92	1.06(4)	0.91
4	Nag	CM	Pauling	1.01(1)	0.92	0.99(1)	0.92	1.06(3)	0.93
5	Batsanov	CM	Allred-Rochow	0.99(1)	0.92	0.99(2)	0.92	1.02(3)	0.92

Table S3 Transition Metal Parameters for Different Data Sets

Set 1

Atom	*DIFA*	*RAVDW*	*RINTER*	*ZTOT*	*ZVAL*	*POLZE*	*ELNEG*	*POTIO*	*WEIGHT*
Ti	0.4	2.15	1.32	22	4	4.18	1.5	0.251	47.88
V	0.4	2.05	1.22	23	5	3.31	1.6	0.248	50.94
Cr	0.4	2.05	1.17	24	6	2.86	1.6	0.249	52.00
Mn	0.4	2.05	1.17	25	7	2.93	1.5	0.273	54.94
Fe	0.4	2.05	1.16	26	8	2.81	1.8	0.289	55.85
Co	0.4	2.00	1.16	27	9	2.62	1.8	0.289	58.93
Ni	0.4	2.00	1.15	28	10	2.61	1.8	0.281	58.69
Cu	0.4	2.00	1.35	29	11	2.81	1.9	0.284	63.55
Zn	0.4	2.10	1.31	30	12	3.63	1.6	0.345	65.38
Zr	0.4	2.30	1.45	40	12	5.56	1.33	0.251	91.22
Nb	0.4	2.15	1.34	41	13	4.30	1.60	0.253	92.91
Mo	0.4	2.10	1.29	42	14	3.72	2.16	0.261	95.94
Tc	0.4	2.05	1.23	43	15	3.41	1.90	0.267	98.91
Ru	0.4	2.05	1.24	44	16	3.23	2.20	0.271	101.07
Rh	0.4	2.00	1.25	45	17	3.29	2.28	0.274	102.91
Pd	0.4	2.05	1.28	46	18	3.51	2.20	0.307	106.42
Ag	0.4	2.10	1.34	47	19	4.07	1.93	0.278	107.87
Cd	0.4	2.20	1.41	48	20	5.15	1.69	0.330	112.41
Hf	0.4	2.35	1.44	72	12	5.32	1.30	0.251	178.49
Ta	0.4	2.20	1.34	73	13	4.31	1.50	0.277	180.95
W	0.4	2.10	1.30	74	14	3.78	2.36	0.289	183.85
Re	0.4	2.05	1.28	75	15	3.51	1.90	0.288	186.21
Os	0.4	2.00	1.26	76	16	3.34	2.20	0.310	190.20
Ir	0.4	2.00	1.26	77	17	3.40	2.20	0.330	192.22
Pt	0.4	2.05	1.29	78	18	3.61	2.28	0.329	195.08
Au	0.4	2.10	1.34	79	19	4.04	2.54	0.339	196.97
Hg	0.4	2.05	1.44	80	20	5.87	2.00	0.384	200.59

Set 2

Atom	*DIFA*	*RAVDW*	*RINTER*	*ZTOT*	*ZVAL*	*POLZE*	*ELNEG*	*POTIO*	*WEIGHT*
Ti	0.4	2.15	1.32	22	4	3.69	1.5	0.251	47.88
V	0.4	2.05	1.22	23	5	3.05	1.6	0.248	50.94
Cr	0.4	2.05	1.17	24	6	3.05	1.6	0.249	52.00
Mn	0.4	2.05	1.17	25	7	3.05	1.5	0.273	54.94
Fe	0.4	2.05	1.16	26	8	3.05	1.8	0.289	55.85
Co	0.4	2.00	1.16	27	9	2.76	1.8	0.289	58.93
Ni	0.4	2.00	1.15	28	10	2.76	1.8	0.281	58.69
Cu	0.4	2.00	1.35	29	11	2.76	1.9	0.284	63.55
Zn	0.4	2.10	1.31	30	12	3.36	1.6	0.345	65.38
Zr	0.4	2.30	1.45	40	12	4.84	1.33	0.251	91.22
Nb	0.4	2.15	1.34	41	13	3.69	1.60	0.253	92.91
Mo	0.4	2.10	1.29	42	14	3.36	2.16	0.261	95.94
Tc	0.4	2.05	1.23	43	15	3.05	1.90	0.267	98.91
Ru	0.4	2.05	1.24	44	16	3.05	2.20	0.271	101.07
Rh	0.4	2.00	1.25	45	17	2.76	2.28	0.274	102.91
Pd	0.4	2.05	1.28	46	18	3.05	2.20	0.307	106.42
Ag	0.4	2.10	1.34	47	19	3.36	1.93	0.278	107.87
Cd	0.4	2.20	1.41	48	20	4.05	1.69	0.330	112.41
Hf	0.4	2.35	1.44	72	12	5.27	1.30	0.251	178.49
Ta	0.4	2.20	1.34	73	13	4.05	1.50	0.277	180.95
W	0.4	2.10	1.30	74	14	3.36	2.36	0.289	183.85
Re	0.4	2.05	1.28	75	15	3.05	1.90	0.288	186.21
Os	0.4	2.00	1.26	76	16	2.76	2.20	0.310	190.20
Ir	0.4	2.00	1.26	77	17	2.76	2.20	0.330	192.22
Pt	0.4	2.05	1.29	78	18	3.05	2.28	0.329	195.08
Au	0.4	2.10	1.34	79	19	3.36	2.54	0.339	196.97
Hg	0.4	2.05	1.44	80	20	3.05	2.00	0.384	200.59

Set 3

Atom	*DIFA*	*RAVDW*	*RINTER*	*ZTOT*	*ZVAL*	*POLZE*	*ELNEG*	*POTIO*	*WEIGHT*
Ti	0.4	2.07	1.32	22	4	3.17	1.5	0.251	47.88
V	0.4	2.06	1.22	23	5	3.11	1.6	0.248	50.94
Cr	0.4	2.06	1.17	24	6	3.11	1.6	0.249	52.00
Mn	0.4	2.04	1.17	25	7	2.99	1.5	0.273	54.94
Fe	0.4	2.02	1.16	26	8	2.88	1.8	0.289	55.85
Co	0.4	1.91	1.16	27	9	2.30	1.8	0.289	58.93
Ni	0.4	1.98	1.15	28	10	2.65	1.8	0.281	58.69
Cu	0.4	1.92	1.35	29	11	2.35	1.9	0.284	63.55
Zn	0.4	1.98	1.31	30	12	2.65	1.6	0.345	65.38
Zr	0.4	2.19	1.45	40	12	3.97	1.33	0.251	91.22
Nb	0.4	2.17	1.34	41	13	3.83	1.60	0.253	92.91
Mo	0.4	2.16	1.29	42	14	3.76	2.16	0.261	95.94
Tc	0.4	2.16	1.23	43	15	3.76	1.90	0.267	98.91
Ru	0.4	2.17	1.24	44	16	3.83	2.20	0.271	101.07
Rh	0.4	2.04	1.25	45	17	2.99	2.28	0.274	102.91
Pd	0.4	2.09	1.28	46	18	3.30	2.20	0.307	106.42
Ag	0.4	2.10	1.34	47	19	3.36	1.93	0.278	107.87
Cd	0.4	2.17	1.41	48	20	3.83	1.69	0.330	112.41
Hf	0.4	2.19	1.44	72	12	3.97	1.30	0.251	178.49
Ta	0.4	2.18	1.34	73	13	3.90	1.50	0.277	180.95
W	0.4	2.18	1.30	74	14	3.90	2.36	0.289	183.85
Re	0.4	2.16	1.28	75	15	3.76	1.90	0.288	186.21
Os	0.4	2.17	1.26	76	16	3.83	2.20	0.310	190.20
Ir	0.4	2.09	1.26	77	17	3.30	2.20	0.330	192.22
Pt	0.4	2.09	1.29	78	18	3.30	2.28	0.329	195.08
Au	0.4	2.10	1.34	79	19	3.36	2.54	0.339	196.97
Hg	0.4	2.24	1.44	80	20	4.35	2.00	0.384	200.59

Set 4

Atom	*DIFA*	*RAVDW*	*RINTER*	*ZTOT*	*ZVAL*	*POLZE*	*ELNEG*	*POTIO*	*WEIGHT*
Ti	0.4	2.07	1.32	22	4	4.18	1.5	0.251	47.88
V	0.4	2.06	1.22	23	5	3.31	1.6	0.248	50.94
Cr	0.4	2.06	1.17	24	6	2.86	1.6	0.249	52.00
Mn	0.4	2.04	1.17	25	7	2.93	1.5	0.273	54.94
Fe	0.4	2.02	1.16	26	8	2.81	1.8	0.289	55.85
Co	0.4	1.91	1.16	27	9	2.62	1.8	0.289	58.93
Ni	0.4	1.98	1.15	28	10	2.61	1.8	0.281	58.69
Cu	0.4	1.92	1.35	29	11	2.81	1.9	0.284	63.55
Zn	0.4	1.98	1.31	30	12	3.63	1.6	0.345	65.38
Zr	0.4	2.19	1.45	40	12	5.56	1.33	0.251	91.22
Nb	0.4	2.17	1.34	41	13	4.30	1.60	0.253	92.91
Mo	0.4	2.16	1.29	42	14	3.72	2.16	0.261	95.94
Tc	0.4	2.16	1.23	43	15	3.41	1.90	0.267	98.91
Ru	0.4	2.17	1.24	44	16	3.23	2.20	0.271	101.07
Rh	0.4	2.04	1.25	45	17	3.29	2.28	0.274	102.91
Pd	0.4	2.09	1.28	46	18	3.51	2.20	0.307	106.42
Ag	0.4	2.10	1.34	47	19	4.07	1.93	0.278	107.87
Cd	0.4	2.17	1.41	48	20	5.15	1.69	0.330	112.41
Hf	0.4	2.19	1.44	72	12	5.32	1.30	0.251	178.49
Ta	0.4	2.18	1.34	73	13	4.31	1.50	0.277	180.95
W	0.4	2.18	1.30	74	14	3.78	2.36	0.289	183.85
Re	0.4	2.16	1.28	75	15	3.51	1.90	0.288	186.21
Os	0.4	2.17	1.26	76	16	3.34	2.20	0.310	190.20
Ir	0.4	2.09	1.26	77	17	3.40	2.20	0.330	192.22
Pt	0.4	2.09	1.29	78	18	3.61	2.28	0.329	195.08
Au	0.4	2.10	1.34	79	19	4.04	2.54	0.339	196.97
Hg	0.4	2.24	1.44	80	20	5.87	2.00	0.384	200.59

Set 5 (Recommended)

Atom	*DIFA*	*RAVDW*	*RINTER*	*ZTOT*	*ZVAL*	*POLZE*	*ELNEG*	*POTIO*	*WEIGHT*
Ti	0.4	2.15	1.32	22	4	4.18	1.32	0.251	47.88
V	0.4	2.05	1.22	23	5	3.31	1.45	0.248	50.94
Cr	0.4	2.05	1.17	24	6	2.86	1.56	0.249	52.00
Mn	0.4	2.05	1.17	25	7	2.93	1.60	0.273	54.94
Fe	0.4	2.05	1.16	26	8	2.81	1.64	0.289	55.85
Co	0.4	2.00	1.16	27	9	2.62	1.70	0.289	58.93
Ni	0.4	2.00	1.15	28	10	2.61	1.75	0.281	58.69
Cu	0.4	2.00	1.35	29	11	2.81	1.75	0.284	63.55
Zn	0.4	2.10	1.31	30	12	3.63	1.66	0.345	65.38
Zr	0.4	2.30	1.45	40	12	5.56	1.33	0.251	91.22
Nb	0.4	2.15	1.34	41	13	4.30	1.60	0.253	92.91
Mo	0.4	2.10	1.29	42	14	3.72	2.16	0.261	95.94
Tc	0.4	2.05	1.23	43	15	3.41	1.90	0.267	98.91
Ru	0.4	2.05	1.24	44	16	3.23	2.20	0.271	101.07
Rh	0.4	2.00	1.25	45	17	3.29	2.28	0.274	102.91
Pd	0.4	2.05	1.28	46	18	3.51	2.20	0.307	106.42
Ag	0.4	2.10	1.34	47	19	4.07	1.93	0.278	107.87
Cd	0.4	2.20	1.41	48	20	5.15	1.69	0.330	112.41
Hf	0.4	2.35	1.44	72	12	5.32	1.23	0.251	178.49
Ta	0.4	2.20	1.34	73	13	4.31	1.33	0.277	180.95
W	0.4	2.10	1.30	74	14	3.78	1.40	0.289	183.85
Re	0.4	2.05	1.28	75	15	3.51	1.46	0.288	186.21
Os	0.4	2.00	1.26	76	16	3.34	1.52	0.310	190.20
Ir	0.4	2.00	1.26	77	17	3.40	1.55	0.330	192.22
Pt	0.4	2.05	1.29	78	18	3.61	1.44	0.329	195.08
Au	0.4	2.10	1.34	79	19	4.04	1.42	0.339	196.97
Hg	0.4	2.05	1.44	80	20	5.87	1.44	0.384	200.59