Table 1. Dataset for E_f.

Structure	Metal	E_f	Ref.
C4	Sc	-1.54	[1]
C4	Ti	-1.93	
C4	V	-1.26	
C4	Cr	-0.78	
C4	Mn	-2.43	
C4	Fe	-1.15	
C4	Co	-1.25	
C4	Ni	-1.43	
C4	Cu	-1.84	
C4	Zn	-1.98	
C4	Y	-1.54	
C4	Zr	-1.87	
C4	Nb	-1.15	
C4	Mo	-0.39	
C4	Ru	-1.06	
C4	Rh	-1.42	
C4	Pd	-1.53	
C4	Ag	-0.49	
C4	Cd	-0.38	
C4	Hf	-1.78	
C4	Ta	-1.09	
C4	W	-0.16	
C4	Re	-0.35	
C4	Os	-0.58	
C4	Ir	-1.54	
C4	Pt	-2.07	
C4	Au	-1.79	
N4	Sc	-3.54	
N4	Ti	-2.2	
N4	V	-1.46	
N4	Cr	-1.62	
N4	Mn	-2.99	
N4	Fe	-1.67	
N4	Co	-1.91	
N4	Ni	-2.11	
N4	Cu	-1.3	
N4	Zn	-2.13	
N4	Y	-3.58	
N4	Zr	-1.87	
N4	Nb	0.08	
N4	Mo	1.14	
N4	Ru	0.47	
N4	Rh	-1.05	
N4	Pd	-1.99	
N4	Ag	0.65	
N4	Cd	-0.58	
N4	Hf	-1.98	
N4	Ta	-0.03	
N4	W	1.63	
N4	Re	1.76	
N4	Os	1.34	
N4	Ir	-0.75	
N4	Pt	-1.91	
N4	Au	0.12	
B4	Sc	-0.43	
B4	Ti	0.77	
B4	V	1.41	
B4	Cr	1.68	
B4	Mn	-0.03	
B4	Fe	0.8	
B4	Co	0.37	
B4	Ni	-0.08	
B4	Cu	-0.18	
B4	Zn	-0.08	
B4	Y	-0.89	
B4	Zr	0.74	
B4	Nb	1.88	
B4	Mo	2.22	
B4	Ru	0.72	
B4	Rh	-0.56	
B4	Pd	-0.93	
B4	Ag	0.45	
B4	Cd	0.52	
B4	Hf	1.19	
B4	Ta	2.38	
B4	W	2.91	
B4	Re	2.19	
B4	Os	1.43	
B4	Ir	-0.54	
B4	Pt	-1.19	
B4	Au	-0.39	

N2C2	Sc	-3.8
N2C2	Ti	-3.28
N2C2	V	-2.15
N2C2	Cr	-1.82
N2C2	Mn	-3.53
N2C2	Fe	-2.04
N2C2	Co	-2.25
N2C2	Ni	-2.79
N2C2	Cu	-2.42
N2C2	Zn	-2.4
N2C2	Y	-3.72
N2C2	Zr	-3.29
N2C2	Nb	-1.59
N2C2	Mo	-0.58
N2C2	Ru	-1.05
N2C2	Rh	-1.84
N2C2	Pd	-2.59
N2C2	Ag	-1.22
N2C2	Cd	-1.02
N2C2	Hf	-3.18
N2C2	Ta	-1.63
N2C2	W	-0.21
N2C2	Re	-0.06
N2C2	Os	-0.28
N2C2	Ir	-1.74
N2C2	Pt	-2.73
N2C2	Au	-2.15
B2C2	Sc	0.36
B2C2	Ti	1.56
B2C2	V	1.83
B2C2	Cr	2.18
B2C2	Mn	0.11
B2C2	Fe	0.79
B2C2	Co	0.54
B2C2	Ni	0.06
B2C2	Cu	0.24
B2C2	Zn	0.83
B2C2	Y	-0.01
B2C2	Zr	1.36
B2C2	Nb	2.13
B2C2	Mo	2.28
B2C2	Ru	1.08
B2C2	Rh	-0.07
B2C2	Pd	-0.53
B2C2	Ag	0.97
B2C2	Cd	0.62
B2C2	Hf	1.59
B2C2	Ta	2.39
B2C2	W	2.75
B2C2	Re	2.15
B2C2	Os	1.63
B2C2	Ir	-0.16
B2C2	Pt	-0.86
B2C2	Au	0.13
B2N2	Sc	0.4
B2N2	Ti	0.8
B2N2	V	1.22
B2N2	Cr	1.78
B2N2	Mn	-0.53
B2N2	Fe	0.54
B2N2	Co	0.42
B2N2	Ni	0.12
B2N2	Cu	0.89
B2N2	Zn	0.49
B2N2	Y	0.64
B2N2	Zr	0.83
B2N2	Nb	1.52
B2N2	Mo	1.98
B2N2	Ru	1.3
B2N2	Rh	-0.08
B2N2	Pd	-0.71
B2N2	Ag	1.18
B2N2	Cd	0.48
B2N2	Hf	1.06
B2N2	Ta	1.7
B2N2	W	2.39
B2N2	Re	2.39
B2N2	Os	2.05
B2N2	Ir	0.2
B2N2	Pt	-0.61
B2N2	Au	1.04
g-C3N4(h)	Sc	-1.43
g-C3N4(h)	Ti	0.34
g-C3N4(h)	V	1.59
g-C3N4(h)	Cr	2.17
g-C3N4(h)	Mn	0.58

g-C3N4(h)	Fe	2.47
g-C3N4(h)	Co	2.78
g-C3N4(h)	Ni	2.41
g-C3N4(h)	Cu	1.8
g-C3N4(h)	Zn	1.35
g-C3N4(h)	Y	-2.23
g-C3N4(h)	Zr	-0.28
g-C3N4(h)	Nb	1.82
g-C3N4(h)	Mo	3.85
g-C3N4(h)	Ru	4.08
g-C3N4(h)	Rh	2.87
g-C3N4(h)	Pd	1.95
g-C3N4(h)	Ag	1.34
g-C3N4(h)	Cd	1
g-C3N4(h)	Hf	-0.04
g-C3N4(h)	Ta	2.28
g-C3N4(h)	W	4.57
g-C3N4(h)	Re	5.68
g-C3N4(h)	Os	5.55
g-C3N4(h)	Ir	3.94
g-C3N4(h)	Pt	3.44
g-C3N4(h)	Au	2.43
C3	Sc	-1.72
C3	Ti	-1.91
C3	V	-1.07
C3	Cr	-1.02
C3	Mn	-2.57
C3	Fe	-1.65
C3	Co	-1.92
C3	Ni	-1.19
C3	Cu	0.24
C3	Zn	0.15
C3	Y	-1.63
C3	Zr	-1.53
C3	Nb	-0.23
C3	Mo	0.05
C3	Ru	-1.34
C3	Rh	-2
C3	Pd	-1.49
C3	Ag	1.02
C3	Cd	0.88
C3	Hf	-1.48
C3	Ta	-0.12
C3	W	0.63
C3	Re	0.34
C3	Os	-0.36
C3	Ir	-1.63
C3	Pt	-1.41
C3	Au	0.8
N3	Sc	-1.24
N3	Ti	-0.08
N3	V	0.5
N3	Cr	1.51
N3	Mn	-0.24
N3	Fe	1.12
N3	Co	0.91
N3	Ni	1.14
N3	Cu	0.85
N3	Zn	-0.17
N3	Y	-1.34
N3	Zr	0.73
N3	Nb	2.29
N3	Mo	3.09
N3	Ru	2.62
N3	Rh	2.2
N3	Pd	1.5
N3	Ag	1.08
N3	Cd	0.29
N3	Hf	0.78
N3	Ta	2.72
N3	W	3.98
N3	Re	4.23
N3	Os	4.29
N3	Ir	3.58
N3	Pt	2.96
N3	Au	2.11
B3	Sc	1.33
B3	Ti	2.73
B3	V	3.58
B3	Cr	3.39
B3	Mn	1.53
B3	Fe	2.49
B3	Co	2.02
B3	Ni	1.54
B3	Cu	1.54
B3	Zn	0.74

B3	Y	0.84
B3	Zr	2.91
B3	Nb	4.16
B3	Mo	4.95
B3	Ru	2.89
B3	Rh	1.2
B3	Pd	0.3
B3	Ag	1.16
B3	Cd	0.4
B3	Hf	3.31
B3	Ta	4.79
B3	W	5.37
B3	Re	4.49
B3	Os	3.47
B3	Ir	1.25
B3	Pt	0.17
B3	Au	0.88
h-BN	Sc	-6.77
h-BN	Ti	-5.5
h-BN	V	-4.2
h-BN	Cr	-3.9
h-BN	Mn	-4.56
h-BN	Fe	-2.95
h-BN	Co	-3.08
h-BN	Ni	-2.37
h-BN	Cu	-2.11
h-BN	Zn	-3.15
h-BN	Y	-6.69
h-BN	Zr	-5
h-BN	Nb	-2.82
h-BN	Mo	-2.03
h-BN	Ru	-1.57
h-BN	Rh	-2.45
h-BN	Pd	-1.83
h-BN	Ag	-0.79
h-BN	Cd	-1.66
h-BN	Hf	-5.29
h-BN	Ta	-2.66
h-BN	W	-1.24
h-BN	Re	-0.35
h-BN	Os	-0.25
h-BN	Ir	-1.67
h-BN	Pt	-1.18

h-BN	Au	-0.48	
Pc-N4	Al	-6.89	[2]
Pc-N4	Sc	-6.84	
Pc-N4	Ti	-5.47	
Pc-N4	V	-5.03	
Pc-N4	Cr	-5.6	
Pc-N4	Mn	-5.5	
Pc-N4	Fe	-4.84	
Pc-N4	Co	-4.95	
Pc-N4	Ni	-5.19	
Pc-N4	Cu	-3.87	
Pc-N4	Zn	-4.96	
Pc-N4	Ga	-4.64	
Pc-N4	Y	-6.45	
Pc-N4	Zr	-4.97	
Pc-N4	Nb	-3.52	
Pc-N4	Mo	-3.15	
Pc-N4	Ru	-3.33	
Pc-N4	Rh	-4.31	
Pc-N4	Pd	-4.97	
Pc-N4	Ag	-2.24	
Pc-N4	Sn	-4.12	
Pc-N4	Hf	-5.38	
Pc-N4	Ta	-3.74	
Pc-N4	W	-2.68	
Pc-N4	Re	-2.59	
Pc-N4	Os	-2.62	
Pc-N4	Ir	-4.31	
Pc-N4	Pt	-5.46	
Pc-N4	Au	-2.36	
Pc-N4	Bi	-3.09	
Py-N4	Al	-4.85	
Py-N4	Sc	-4.6	
Py-N4	Ti	-3.47	
Py-N4	V	-3.17	
Py-N4	Cr	-3.66	
Py-N4	Mn	-3.77	
Py-N4	Fe	-3.45	
Py-N4	Co	-3.7	
Py-N4	Ni	-3.79	
Py-N4	Cu	-2.41	
Py-N4	Zn	-3.5	
Py-N4	Ga	-2.72	

Py-N4	Y	-4.29
Py-N4	Zr	-2.9
Py-N4	Nb	-1.52
Py-N4	Mo	-0.98
Py-N4	Ru	-1.58
Py-N4	Rh	-2.66
Py-N4	Pd	-3.26
Py-N4	Ag	-0.72
Py-N4	Sn	-2.82
Py-N4	Hf	-3.11
Py-N4	Ta	-1.47
Py-N4	W	-0.34
Py-N4	Re	-0.41
Py-N4	Os	-1.16
Py-N4	Ir	-2.58
Py-N4	Pt	-3.71
Py-N4	Au	-0.18
Py-N4	Bi	-1.13
Pr-N4	Al	-6.81
Pr-N4	Sc	-7.35
Pr-N4	Ti	-5.89
Pr-N4	V	-5.47
Pr-N4	Cr	-6.04
Pr-N4	Mn	-5.48
Pr-N4	Fe	-4.77
Pr-N4	Co	-4.89
Pr-N4	Ni	-5.07
Pr-N4	Cu	-4.17
Pr-N4	Zn	-5.68
Pr-N4	Ga	-4.86
Pr-N4	Y	-7.1
Pr-N4	Zr	-5.57
Pr-N4	Nb	-4.1
Pr-N4	Mo	-4.13
Pr-N4	Ru	-3.71
Pr-N4	Rh	-4.44
Pr-N4	Pd	-5.37
Pr-N4	Ag	-3.43
Pr-N4	Sn	-4.75
Pr-N4	Hf	-5.94
Pr-N4	Ta	-4.25
Pr-N4	W	-3.4
Pr-N4	Re	-3
Pr-N4	Os	-3.02
Pr-N4	Ir	-4.42
Pr-N4	Pt	-5.89
Pr-N4	Au	-2.78
Pr-N4	Bi	-3.53

Table 2. Dataset for ΔG_{*h}.

Structure	Metal	ΔG_{*h}	Ref.
g-C3N4(h)	Fe	0.3	3
g-C3N4(h)	Co	0.31	
g-C3N4(h)	Ni	0.48	
g-C3N4(h)	Cu	0.49	
g-C3N4(h)	Zr	-0.75	
g-C3N4(h)	Mo	-0.29	
g-C3N4(h)	Rh	0.5	
g-C3N4(h)	Ag	0.75	
g-C3N4(h)	Hf	-0.6	
g-C3N4(h)	Ta	-0.6	
g-C3N4(h)	W	-0.61	
g-C3N4(h)	Re	-0.55	
g-C3N4(h)	Os	-0.29	
g-C3N4(h)	Ir	-0.19	
pyridine-4N	Ti	-0.49	4
pyridine-4N	V	-0.12	
pyridine-4N	Cr	0.32	
pyridine-4N	Mn	0.48	
pyridine-4N	Fe	0.32	
pyridine-4N	Co	0.12	
SV-3N	Ti	-0.65	
SV-3N	V	-0.45	
SV-3N	Cr	-0.34	
SV-3N	Mn	-0.31	
SV-3N	Co	0.01	
SV-3N	Ni	0.23	
C2N	Ti	-0.09	5
C2N	V	0.18	
C2N	Zr	-0.46	
pyrrole-4N	Cu	1.9	6
pyrrole-4N	Mn	1.04	
pyrrole-4N	Fe	0.74	
pyrrole-4N	Cr	0.65	
pyrrole-4N	V	0.3	
pyrrole-4N	Co	0.23	
pyrrole-4N	Ru	-0.5	
pyrrole-4N	Ta	-0.64	
SV-3C	Sc	0.94	2
SV-3C	Ti	0.63	
SV-3C	V	0.28	
SV-3C	Cr	0.57	
SV-3C	Mn	0.23	
SV-3C	Fe	0.18	
SV-3C	Co	0.13	
SV-3C	Cu	0.59	
SV-3C	Zn	0.11	
SV-3C	Y	1	
SV-3C	Nb	0.01	
SV-3C	Mo	0.25	
SV-3C	Ru	0.21	
SV-3C	Rh	0	
SV-3C	Ag	0.27	
SV-3C	Ta	-0.52	
SV-3C	W	-0.31	
SV-3C	Re	-0.64	
SV-3C	Os	-0.42	
SV-3C	Ir	-0.66	
SV-3C	Pt	0.11	
SV-3C	Au	-0.07	
pyridine-4N	Sc	-0.22	
pyridine-4N	Ti	-0.28	
pyridine-4N	V	0.16	
pyridine-4N	Cr	0.67	
pyridine-4N	Cu	1.86	
pyridine-4N	Zn	1.01	
pyridine-4N	Y	-0.01	
pyridine-4N	Zr	-0.89	
pyridine-4N	Nb	-0.77	
pyridine-4N	Mo	-0.46	
pyridine-4N	Ru	-0.5	
pyridine-4N	Rh	-0.12	
pyridine-4N	Ag	0.82	
pyridine-4N	Hf	-1.11	
pyridine-4N	Ta	-0.89	
pyridine-4N	W	-0.91	
pyridine-4N	Re	-0.69	
pyridine-4N	Os	-0.57	
pyridine-4N	Ir	-0.27	
pyrrole-4N	Sc	0.8	
pyrrole-4N	Ti	0.02	
pyrrole-4N	Cr	1.04	

pyrrole-4N	Fe	1.12
pyrrole-4N	Co	0.66
pyrrole-4N	Ni	1.65
pyrrole-4N	Y	-0.05
pyrrole-4N	Zr	-0.61
pyrrole-4N	Nb	-0.51
pyrrole-4N	Mo	-0.29
pyrrole-4N	Ru	-0.5
pyrrole-4N	Rh	0.07
pyrrole-4N	Pd	1.55
pyrrole-4N	Cd	1.5
pyrrole-4N	Hf	-0.9
pyrrole-4N	Ta	-0.79
pyrrole-4N	W	-0.66
pyrrole-4N	Re	-0.61
pyrrole-4N	Os	-0.5
pyrrole-4N	Ir	-0.05
pyrrole-4N	Pt	1.07
pyrrole-4N	Au	2.52
DV-4C	Ti	0.43
DV-4C	V	-0.01
DV-4C	Cr	0.24
DV-4C	Co	-0.1
DV-4C	Zr	0.51
DV-4C	Nb	-0.24
DV-4C	Mo	-0.1
DV-4C	Rh	0.06
DV-4C	Cd	1.09
DV-4C	Hf	0.23
DV-4C	Ta	-0.67
DV-4C	W	-0.56
DV-4C	Re	-0.34
DV-4C	Os	-0.06
DV-4C	Ir	-0.21
DV-4C	Pt	-0.09
N1C3	Sc	0.28
N1C3	Ti	0.01
N1C3	V	-0.09
N1C3	Mn	-0.22
N1C3	Y	0.31
N1C3	Zr	0
N1C3	Nb	-0.25
N1C3	Mo	-0.12

N1C3	Ru	-0.46
N1C3	Rh	0.11
N1C3	Ag	0.03
N1C3	Cd	0.08
N1C3	Hf	-0.33
N1C3	Ta	-0.75
N1C3	W	-0.61
N1C3	Re	-0.61
N1C3	Ir	-0.17
N1C3	Pt	-0.39
N1C3	Au	0.23
N1C3	Hg	0.44
N2C2	Sc	0.46
N2C2	Ti	-0.12
N2C2	V	-0.06
N2C2	Cr	0.3
N2C2	Mn	0.29
N2C2	Fe	-0.07
N2C2	Co	-0.2
N2C2	Ni	0
N2C2	Cu	0.14
N2C2	Zn	-0.06
N2C2	Y	0.45
N2C2	Zr	-0.14
N2C2	Nb	-0.66
N2C2	Mo	-0.46
N2C2	Ru	0.06
N2C2	Rh	-0.06
N2C2	Pd	-0.25
N2C2	Ag	0.17
N2C2	La	0.44
N2C2	Hf	-0.5
N2C2	Ta	-1
N2C2	W	-0.85
N2C2	Re	-0.61
N2C2	Os	-0.45
N2C2	Ir	-0.23
N2C2	Pt	0.03
N2C2	Au	0.3
N3C1	Sc	0.38
N3C1	Ti	-0.54
N3C1	V	-0.21
N3C1	Cr	0.05

N3C1	Mn	0.37		N4	Ir	-0.21	
N3C1	Fe	0.21		N4	Au	1.71	
N3C1	Co	0.12		N4	Co	0.133	
N3C1	Ni	0.27		N4	Fe	0.246	
N3C1	Cu	0.13		N4	Mn	0.389	
N3C1	Zn	-0.25		N4	Rh	-0.185	
N3C1	Y	0.48		N4	V	-0.275	
N3C1	Zr	-0.71		N4	Ir	-0.357	
N3C1	Nb	-0.65		N4	Ru	-0.5785	
N3C1	Mo	-0.48		N4	Hf	-0.696	
N3C1	Ru	-0.51		N4	Os	-0.7061	
N3C1	Rh	-0.19		N4	Re	-0.9186	
N3C1	Pd	0.29		N4	Zr	-0.975	
N3C1	Cd	0.06		N4-G	Sc	0.06	8
N3C1	Hf	-0.98		N4-G	V	0.09	
N3C1	Ta	-0.99		N4-G	Mo	-0.17	
N3C1	W	-0.86		N4-G	Ru	-0.1	
N3C1	Re	-0.78		N4B-G	Sc	0.38	
N3C1	Os	-0.76		N4B-G	V	0.19	
N3C1	Ir	-0.36		N4B-G	Mo	-0.21	
N3C1	Au	0.71		N4B-G	Ru	-0.17	
N4	Sc	-0.34		g-C3N4(t)	Sc	-0.74	9
N4	Ti	-0.53		g-C3N4(t)	Ti	-0.73	
N4	V	-0.13		g-C3N4(t)	V	-0.71	
N4	Cr	0.32		g-C3N4(t)	Cr	-0.41	
N4	Mn	0.53		g-C3N4(t)	Mn	-0.57	
N4	Fe	0.44		g-C3N4(t)	Fe	-0.01	
N4	Co	0.32		g-C3N4(t)	Zr	-0.85	
N4	Cu	1.31		g-C3N4(t)	Nb	-0.82	
N4	Zn	1.15		g-C3N4(t)	Mo	-0.49	
N4	Y	-0.22		g-C3N4(t)	Rh	-0.26	
N4	Zr	-0.9		g-C3N4(t)	Pd	0.24	
N4	Nb	-0.74		g-C3N4(t)	Hf	-0.95	
N4	Mo	-0.37		g-C3N4(t)	Ta	-1.36	
N4	Ru	-0.43		g-CN	Nb	-0.47	10
N4	Rh	-0.07		g-CN	Mo	-0.31	
N4	Pd	1.57		g-CN	Ta	-0.72	
N4	La	0.43		g-CN	W	-0.77	
N4	Hf	-1.09		g-CN	Re	-0.84	
N4	Ta	-1		C3	Mo	0.21	11
N4	W	-0.82		C3	Nb	0.02	
N4	Re	-0.83		C3	V	0.14	
N4	Os	-0.66		C3	Ir	-0.62	

C4	Mo	-0.26	
C4	Nb	-0.42	
C4	Os	0	
C4	Re	-0.28	
C4	V	-0.2	
C4	W	-0.66	
N3	La	-0.01	
N3	Mn	-0.32	
N3	Sc	-0.72	
N3	Ti	-0.66	
N3	Y	-0.55	
N4	Cr	0.36	
N4	Sc	-0.2	
N4	Ti	-0.5	
N4	V	-0.09	
N4	Y	-0.11	
C2N	Ru	-0.5	12
C4	Ti	0.54	1
C4	V	-0.06	
C4	Cr	0.25	
C4	Mn	0.39	
C4	Fe	0.25	
C4	Zr	0.57	
C4	Nb	-0.25	
C4	Mo	-0.18	
C4	Ru	0.16	
C4	Rh	-0.04	
C4	Cd	1.38	
C4	Hf	0.3	
C4	Ta	-0.67	
C4	W	-0.67	
C4	Re	-0.46	
C4	Os	-0.2	
C4	Pt	-0.31	
N4	Sc	-0.28	
N4	Ti	-0.53	
N4	V	-0.15	
N4	Cr	0.28	
N4	Mn	0.39	
N4	Fe	0.28	
N4	Co	0.16	
N4	Ni	1.61	
N4	Cu	1.72	

N4	Y	-0.12
N4	Zr	-0.9
N4	Nb	-0.89
N4	Mo	-0.44
N4	Ru	-0.56
N4	Rh	-0.26
N4	Hf	-1.13
N4	Ta	-1.08
N4	W	-0.93
N4	Re	-0.8
N4	Os	-0.7
N4	Ir	-0.37
N4	Pt	1.51
B4	Sc	0.2
B4	Ti	-0.04
B4	V	0.22
B4	Mn	0.4
B4	Co	-0.13
B4	Ni	-0.23
B4	Zn	-0.1
B4	Y	0.32
B4	Zr	-0.15
B4	Nb	-0.1
B4	Mo	0.17
B4	Rh	0.05
B4	Pd	0.01
B4	Hf	-0.54
B4	Ta	-0.56
B4	W	-0.26
B4	Re	-0.14
B4	Os	-0.09
B4	Ir	-0.22
B4	Pt	-0.22
B4	Au	0.44
N2C2	Ti	-0.1
N2C2	V	-0.08
N2C2	Cr	0.18
N2C2	Mn	0.4
N2C2	Fe	0.32
N2C2	Co	0.06
N2C2	Ni	-0.2
N2C2	Cu	1.29
N2C2	Zn	1.41

N2C2	Zr	-0.06
N2C2	Nb	-0.68
N2C2	Mo	-0.52
N2C2	Ru	-0.02
N2C2	Rh	-0.15
N2C2	Pd	-0.37
N2C2	Ag	1.54
N2C2	Cd	0.85
N2C2	Hf	-0.42
N2C2	Ta	-1.07
N2C2	W	-0.97
N2C2	Re	-0.68
N2C2	Os	-0.54
N2C2	Ir	-0.38
N2C2	Pt	-0.08
N2C2	Au	1.48
B2C2	Ti	-0.2
B2C2	V	0.21
B2C2	Cr	0.31
B2C2	Co	-0.17
B2C2	Ni	0.02
B2C2	Zn	-0.34
B2C2	Zr	-0.06
B2C2	Nb	0.06
B2C2	Mo	0.01
B2C2	Ru	0.19
B2C2	Rh	0.07
B2C2	Pd	-0.03
B2C2	Cd	0.12
B2C2	Hf	-0.23
B2C2	Ta	-0.37
B2C2	W	-0.44
B2C2	Re	-0.12
B2C2	Os	-0.07
B2C2	Ir	-0.12
B2N2	Sc	0.22
B2N2	Ti	0.03
B2N2	V	0.1
B2N2	Cr	0.3
B2N2	Mn	0.51
B2N2	Fe	0.48
B2N2	Zn	0.63
B2N2	Y	-0.21

B2N2	Zr	0.12
B2N2	Nb	-0.1
B2N2	Mo	0.07
B2N2	Ru	-0.09
B2N2	Pd	-0.1
B2N2	Ag	0.21
B2N2	Cd	0.68
B2N2	Hf	-0.25
B2N2	Ta	-0.44
B2N2	W	-0.31
B2N2	Re	-0.42
B2N2	Os	-0.34
B2N2	Ir	0
B2N2	Pt	-0.02
g-C3N4(h)	Sc	-0.25
g-C3N4(h)	Ti	0.01
g-C3N4(h)	V	0.22
g-C3N4(h)	Cr	0.48
g-C3N4(h)	Mn	0.42
g-C3N4(h)	Fe	0.47
g-C3N4(h)	Co	0.42
g-C3N4(h)	Ni	0.75
g-C3N4(h)	Cu	0.47
g-C3N4(h)	Zn	-0.4
g-C3N4(h)	Y	-0.19
g-C3N4(h)	Zr	-0.44
g-C3N4(h)	Nb	-0.29
g-C3N4(h)	Mo	-0.44
g-C3N4(h)	Ru	-0.35
g-C3N4(h)	Rh	0.54
g-C3N4(h)	Pd	0.44
g-C3N4(h)	Ag	0.66
g-C3N4(h)	Cd	-0.09
g-C3N4(h)	Hf	-0.66
g-C3N4(h)	Ta	-0.55
g-C3N4(h)	W	-0.67
g-C3N4(h)	Re	-0.77
g-C3N4(h)	Os	-0.68
h-B2N2	Sc	-0.42
h-B2N2	Ti	-0.61
h-B2N2	V	-0.3
h-B2N2	Cr	-0.07
h-B2N2	Mn	-0.55

h-B2N2	Fe	-0.1
h-B2N2	Co	-0.52
h-B2N2	Ni	-0.78
h-B2N2	Cu	-0.5
h-B2N2	Y	-0.33
h-B2N2	Zr	-0.63
h-B2N2	Mo	-0.58
h-B2N2	Ru	-0.33
h-B2N2	Hf	-0.98
h-B2N2	W	-1.02
h-B2N2	Re	-0.65
h-B2N2	Os	-0.91
h-B2N2	Ir	-1.24
h-B2N2	Pt	-1.11
h-B2N2	Au	-0.7
C3	Sc	0.94
C3	Ti	0.62
C3	V	0.03
C3	Cr	0.24
C3	Mn	-0.16
C3	Fe	-0.02
C3	Co	-0.04
C3	Ni	0.45
C3	Cu	0.33
C3	Zn	0.06
C3	Y	0.87
C3	Nb	-0.03
C3	Mo	0.21
C3	Ru	0.12
C3	Rh	-0.03
C3	Pd	0.43
C3	Ag	0.09
C3	Cd	-0.13
C3	Ta	-0.52
C3	W	-0.37
C3	Re	-0.68
C3	Os	-0.5
C3	Pt	-0.05
N3	Ti	-0.68
N3	V	-0.49
N3	Cr	-0.45
N3	Mn	0.2
N3	Fe	0.05
N3	Co	-0.01
N3	Ni	-0.03
N3	Cu	0.22
N3	Y	-0.42
N3	Zr	-0.79
N3	Nb	-0.84
N3	Mo	-0.79
N3	Ru	-0.28
N3	Pd	-0.21
N3	Ag	0.55
N3	Hf	-0.99
N3	Ta	-1.15
N3	W	-1.21
N3	Re	-1.12
N3	Os	-0.77
N3	Pt	-1.16
N3	Au	-0.78
B3	Ti	-0.42
B3	Cr	0.35
B3	Mn	0.09
B3	Co	0.38
B3	Ni	0.3
B3	Cu	0.12
B3	Zn	0.15
B3	Zr	-0.48
B3	Nb	-0.2
B3	Pd	0.65
B3	Ag	0.65
B3	Cd	0.46
B3	Ta	-0.8
B3	Os	0.55
B3	Ir	0.4
B3	Pt	0.1
B3	Au	-0.19
h-BN	Ti	-0.77
h-BN	V	-0.49
h-BN	Cr	-0.11
h-BN	Mn	0.2
h-BN	Fe	-0.08
h-BN	Co	0.64
h-BN	Ni	0.8
h-BN	Nb	-0.88
h-BN	Mo	-0.65

h-BN	Ru	-0.55	
h-BN	Pd	0.07	
h-BN	Cd	0.26	
h-BN	Hf	-1.05	
h-BN	Ta	-1.12	
h-BN	W	-1.06	
h-BN	Re	-1.09	
h-BN	Ir	0.03	
h-BN	Pt	-0.64	
h-BN	Au	-0.18	
S2N2	Fe	-0.26	[13]
Pc-C4	Mo	-0.64	

Table 3. Dataset for ΔG_0.

Structure	metal	ΔG_0	Ref.
g-CN	Ti	-1.09	14
g-CN	V	-0.65	
g-CN	Mn	-0.13	
g-CN	Fe	-0.29	
g-CN	Co	-0.13	
g-CN	Ni	0.16	
g-CN	Cu	0.22	
g-CN	Mo	-0.47	
g-CN	Rh	0.14	
g-CN	Hf	-1.7	
g-CN	Re	-0.74	
g-CN	Os	-0.24	
g-CN	Ir	-0.25	
g-CN	Pt	0.06	
g-CN	Ti	-1.54	
g-CN	V	-1.11	
g-CN	Cr	-0.75	
g-CN	Mn	-0.59	
g-CN	Fe	-0.57	
g-CN	Co	-0.41	
g-CN	Ni	-0.07	
g-CN	Cu	0.19	
g-CN	Zr	-1.9	
g-CN	Nb	-1.27	
g-CN	Mo	-0.9	
g-CN	Ru	-0.32	
g-CN	Rh	-0.17	
g-CN	Pd	0.13	
g-CN	Ag	0.97	
g-CN	Hf	-2.12	
g-CN	Ta	-1.44	
g-CN	W	-1.28	
g-CN	Re	-0.86	
g-CN	Os	-0.41	
g-CN	Ir	-0.48	
g-CN	Pt	-0.29	
g-CN	Au	0.32	
pyridine-4N	Ti	-2.12	
pyridine-4N	Zr	-2.69	
pyridine-4N	Pt	1.26	15
pyridine-4N	Re	-1.77	
g-C3N4(t)	Ti	-2.8	16
g-C3N4(t)	V	-3.52	
g-C3N4(t)	Cr	-2.3	
g-C3N4(t)	Mn	-2.72	
g-C3N4(t)	Ni	-1.02	
g-C3N4(t)	Cu	-0.92	
g-C3N4(t)	Zr	-3.97	
g-C3N4(t)	Nb	-2.69	
g-C3N4(t)	Mo	-3.08	
g-C3N4(t)	Pd	-1.55	
g-C3N4(t)	Ag	-1.23	
g-C3N4(t)	Hf	-4.28	
g-C3N4(t)	W	-4.04	
g-C3N4(t)	Re	-4.05	
g-C3N4(t)	Os	-2.85	
g-C3N4(t)	Ir	-2.1	
g-C3N4(t)	Ag	-0.65	
g-C3N4(t)	Ru	-2.44	
g-C3N4(h)	Ti	-2.18	17
g-C3N4(h)	V	-1.82	
g-C3N4(h)	Cr	-1.47	
g-C3N4(h)	Mn	-1.64	
g-C3N4(h)	Fe	-1.58	
g-C3N4(h)	Co	-1.34	
g-C3N4(h)	Ni	-1.06	
g-C3N4(h)	Cu	-1	
g-C3N4(h)	Y	-2.98	
g-C3N4(h)	Nb	-1.76	
g-C3N4(h)	Mo	-1.52	
g-C3N4(h)	Ru	-1.27	
g-C3N4(h)	Pd	-1.22	
g-C3N4(h)	Ag	-0.56	
g-C3N4(h)	Hf	-2.94	
g-C3N4(h)	Ta	-2.22	
g-C3N4(h)	W	-1.81	
g-C3N4(h)	Re	-1.18	
g-C3N4(h)	Os	-1.37	
g-C3N4(h)	Pt	-1.31	
g-C3N4(h)	Au	-1.69	
g-C3N4(h)	Sc	-1.19	

g-C3N4(h)	Ti	-1.64
g-C3N4(h)	V	-1.75
g-C3N4(h)	Cr	-1.25
g-C3N4(h)	Co	-1.24
g-C3N4(h)	Ni	-0.82
g-C3N4(h)	Cu	-0.77
g-C3N4(h)	Y	-2.48
g-C3N4(h)	Zr	-2.19
g-C3N4(h)	Nb	-1.65
g-C3N4(h)	Mo	-1.31
g-C3N4(h)	Ru	-0.63
g-C3N4(h)	Rh	-0.14
g-C3N4(h)	Pd	-0.25
g-C3N4(h)	Ag	-0.23
g-C3N4(h)	Hf	-2.54
g-C3N4(h)	W	-1.42
g-C3N4(h)	Re	-1.03
g-C3N4(h)	Os	-1.11
g-C3N4(h)	Ir	-1.04
g-C3N4(h)	Pt	-0.33
g-C3N4(h)	Au	-1.59
pyridine-4N	Ti	-1.98
pyridine-4N	V	-1.42
pyridine-4N	Cr	-0.51
pyridine-4N	Mn	-0.04
pyridine-4N	Fe	-0.25
pyridine-4N	Co	0.42
pyridine-4N	Ni	1.14
pyridine-4N	Zr	-2.34
pyridine-4N	Nb	-2.02
pyridine-4N	Ru	-0.25
pyridine-4N	Rh	0.37
pyridine-4N	Pd	1.3
pyridine-4N	Ag	0.78
pyridine-4N	Hf	-2.49
pyridine-4N	Ta	-2.16
pyridine-4N	W	-3.59
pyridine-4N	Os	-0.4
pyridine-4N	Pt	1.43
pyridine-4N	Au	0.8
pyridine-4N	Ti	-2.49
pyridine-4N	V	-1.9
pyridine-4N	Cr	-0.55

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pyridine-4N	Mn	-0.05
pyridine-4N	Fe	-0.13
pyridine-4N	Co	0.39
pyridine-4N	Ni	1.12
pyridine-4N	Cu	0.85
pyridine-4N	Zr	-2.98
pyridine-4N	Nb	-2.64
pyridine-4N	Mo	-2.05
pyridine-4N	Ru	-0.56
pyridine-4N	Rh	0.4
pyridine-4N	Pd	1.28
pyridine-4N	Ag	0.78
pyridine-4N	Hf	-3.19
pyridine-4N	Ta	-2.93
pyridine-4N	Re	-1.93
pyridine-4N	Os	-0.83
pyridine-4N	Pt	1.37
pyridine-4N	Au	0.65
h-BP	Sc	-0.813
h-BP	Ti	-1.677
h-BP	V	-0.991
h-BP	Cr	-1.082
h-BP	Mn	-1.007
h-BP	Fe	-1.077
h-BP	Co	-0.849
h-BP	Ni	-0.498
h-BP	Cu	0.182
h-BP	Zn	0.458
h-BP	Zr	-1.813
h-BP	Nb	-1.429
h-BP	Mo	-1.285
h-BP	Ru	-0.836
h-BP	Pd	-0.498
h-BP	Ag	0.124
h-BP	Cd	-0.206
h-BP	Hf	-2.142
h-BP	Ta	-1.973
h-BP	W	-1.812
h-BP	Re	-1.653
h-BP	Os	-1.345
h-BP	Ir	-0.695
h-BP	Pt	-0.237
h-BP	Au	0.262

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h-BP	Mn	-0.449	
h-BP	Cu	0.378	
h-BP	Pt	0.062	
C2N	Ti	-1.06	[20]
C2N	V	-0.77	
C2N	Fe	-0.42	
C2N	Co	-0.31	
C2N	Ni	-0.04	
C2N	Zr	-1.03	
C2N	Nb	-1.17	
C2N	Mo	-0.4	
C2N	Ru	-0.02	
C2N	Hf	-1.2	
C2N	Ta	-1.1	
C2N	Re	-0.25	
C2N	Os	-0.14	
C2N	Ti	-1.21	
C2N	V	-1.07	
C2N	Cr	-0.61	
C2N	Mn	-0.52	
C2N	Fe	-0.58	
C2N	Co	-0.48	
C2N	Ni	-0.08	
C2N	Cu	0.01	
C2N	Zr	-1.28	
C2N	Nb	-1.59	
C2N	Mo	-0.3	
C2N	Ru	-0.15	
C2N	Rh	0.04	
C2N	Pd	0.53	
C2N	Ag	0.62	
C2N	Hf	-1.47	
C2N	Ta	-1.54	
C2N	W	-0.65	
C2N	Re	-0.49	
C2N	Os	-0.25	
C2N	Pt	0.6	
C2N	Au	0.68	
g-CN	V	-0.97	
g-CN	Fe	-0.44	
g-CN	Ta	-1.39	
g-CN	W	-0.78	
g-CN	Re	-0.46	
g-CN	Ti	-1.29	
g-CN	Zr	-1.28	
g-CN	Nb	-1.21	
g-CN	Mo	-0.57	
g-CN	Hf	-1.41	
g-CN	Os	-0.26	
N2O2	Cu	-2.02	[21]
Pc-C4	Re	-1.34	
Pc-C4	Mo	-1.44	

Table 4. Dataset for ΔG_1.

Structure	Metal	ΔG_1	Ref.
g-CN	Ti	-0.08	14
g-CN	V	0.24	
g-CN	Cr	0.64	
g-CN	Mn	0.72	
g-CN	Fe	0.92	
g-CN	Co	0.98	
g-CN	Ni	1.11	
g-CN	Zr	-0.19	
g-CN	Nb	0.03	
g-CN	Mo	0.18	
g-CN	Ru	0.68	
g-CN	Rh	0.99	
g-CN	Pd	1.14	
g-CN	Hf	-0.32	
g-CN	Ta	-0.31	
g-CN	W	-0.34	
g-CN	Os	0.44	
g-CN	Ir	0.85	
pyridine-4N	Ti	-0.31	
pyridine-4N	Zr	-0.21	
pyridine-4N	Cu	-0.29	
pyridine-4N	Ag	-0.18	
pyridine-4N	Re	-0.06	
pyridine-4N	Au	-0.01	
h-BP	Sc	0.732	19
h-BP	Ti	0.379	
h-BP	Mn	0.529	
h-BP	Fe	0.58	
h-BP	Co	0.665	
h-BP	Ni	0.749	
h-BP	Y	0.735	
h-BP	Zr	0.499	
h-BP	Nb	-0.67	
h-BP	Tc	0.786	
h-BP	Ru	0.73	
h-BP	Pd	0.41	
h-BP	Cd	0.76	
h-BP	Hf	0.41	
h-BP	Os	0.585	
h-BP	Ir	0.476	
g-C3N4(t)	Ru	-0.15	16
g-C3N4(h)	Ti	0.07	17
g-C3N4(h)	V	0.02	
g-C3N4(h)	Cr	0.87	
g-C3N4(h)	Mn	0.74	
g-C3N4(h)	Fe	0.8	
g-C3N4(h)	Zn	1.1	
g-C3N4(h)	Y	0.84	
g-C3N4(h)	Nb	-0.06	
g-C3N4(h)	Ru	0.68	
g-C3N4(h)	Pd	1.25	
g-C3N4(h)	Ir	1.08	
g-C3N4(h)	Au	1.36	
pyridine-4N	Fe	0.23	
g-C3N4(h)	Ti	-0.12	3
g-C3N4(h)	Co	0.75	
g-C3N4(h)	Zr	-0.4	
g-C3N4(h)	Nb	-0.43	
g-C3N4(h)	Ru	0.66	
g-C3N4(h)	Hf	-0.15	
g-C3N4(h)	Os	0.76	
pyridine-4N	V	-0.76	4
pyridine-4N	Cr	0.68	
pyridine-4N	Mn	0.39	
pyridine-4N	Fe	0.26	
SV-3N	V	-1.59	
SV-3N	Mn	-1.2	
SV-3N	Fe	-0.92	
SV-3N	Ni	-0.69	
DV-4C	Ir	0.27	
DV-4C	Ru	-0.14	
N1C2	Ni	-0.2	
g-C2N	Zr	-0.04	20
g-C2N	Hf	-0.09	
g-CN	Ti	-0.03	
g-CN	Zr	-0.04	
g-CN	Hf	-0.14	
g-C3N4(h)	Ti	-0.07	22
g-C3N4(h)	Zr	-0.18	

C2	Sc	0.81	^{23}(uncorrected)
C2	Ti	0.69	
C2	V	0.58	
C2	Cr	0.71	
C2	Mn	0.48	
C2	Fe	0.35	
C2	Co	0.39	
C2	Y	0.53	
C2	Zr	0.65	
C2	Mo	0.24	
C2	Ru	0.68	
C2	Hf	0.89	
C2	Ta	0.39	
C2	W	-0.1	
C2	Os	0.33	
C2	Ir	0.1	
PD2G1	Sc	1.14	
PD2G1	V	0.11	
PD2G1	Cr	0.38	
PD2G1	Mn	0.41	
PD2G1	Fe	0.57	
PD2G1	Co	0.34	
PD2G1	Y	0.69	
PD2G1	Zr	0.86	
PD2G1	Nb	-0.43	
PD2G1	Mo	-0.35	
PD2G1	Ru	0.52	
PD2G1	Hf	0.76	
PD2G1	Ta	-0.6	
PD2G1	W	-0.63	
PD2G1	Os	-0.45	
PD2G1	Ir	0.71	
PD2G2	Sc	0.92	
PD2G2	Ti	0.47	
PD2G2	V	0.12	
PD2G2	Cr	0.4	
PD2G2	Mn	0.47	
PD2G2	Fe	0.45	
PD2G2	Co	0.2	
PD2G2	Y	0.9	
PD2G2	Zr	0.53	
PD2G2	Nb	-0.51	
PD2G2	Ru	0	
PD2G2	Hf	0.45	
PD2G2	Ta	-0.63	
PD2G2	W	-0.73	
PD2G2	Os	-0.43	
PD2G2	Ir	0.74	
PD2G3	Sc	0.92	
PD2G3	Ti	0.44	
PD2G3	V	0.11	
PD2G3	Cr	0.4	
PD2G3	Mn	0.44	
PD2G3	Fe	0.4	
PD2G3	Co	0.12	
PD2G3	Y	0.7	
PD2G3	Zr	0.57	
PD2G3	Nb	-0.43	
PD2G3	Hf	0.47	
PD2G3	Ta	-0.71	
PD2G3	W	-0.62	
PD2G3	Os	-0.46	
PD2G3	Ir	0.76	
PD2G4	Sc	0.92	
PD2G4	Ti	0.23	
PD2G4	V	0.1	
PD2G4	Cr	0.44	
PD2G4	Fe	0.42	
PD2G4	Co	0.13	
PD2G4	Y	0.69	
PD2G4	Zr	0.4	
PD2G4	Nb	-0.4	
PD2G4	Mo	-0.39	
PD2G4	Ru	0.05	
PD2G4	Hf	0.21	
PD2G4	Ta	-0.67	
PD2G4	Os	-0.39	
PD2G4	Ir	0.78	

Table 5. Dataset for ΔG_5.

Structure	Metal	ΔG_5	Ref.
g-CN	Ti	0.39	14
g-CN	V	0.64	
g-CN	Cr	0.94	
g-CN	Mn	1.19	
g-CN	Fe	1.33	
g-CN	Co	1.35	
g-CN	Ni	1.35	
g-CN	Cu	1.61	
g-CN	Zr	0.25	
g-CN	Nb	0.88	
g-CN	Mo	0.99	
g-CN	Ru	1.27	
g-CN	Rh	1.33	
g-CN	Pd	1.68	
g-CN	Hf	0.16	
g-CN	Ta	0.65	
g-CN	W	0.81	
g-CN	Re	1.09	
g-CN	Os	1.27	
pyridine-4N	Cr	1.07	15
pyridine-4N	Mn	1.25	
pyridine-4N	Fe	0.92	
pyridine-4N	Co	1.35	
pyridine-4N	Ni	1.31	
pyridine-4N	Cu	1.23	
pyridine-4N	Rh	1.33	
pyridine-4N	Pd	1.35	
pyridine-4N	Ag	1.27	
pyridine-4N	Re	0.89	
pyridine-4N	Os	0.61	
pyridine-4N	Pt	1.35	
pyridine-4N	Au	1.24	
pyridine-4N	Cr	0.8	
pyridine-4N	Mn	0.85	
pyridine-4N	Co	0.62	
pyridine-4N	Rh	0.66	
pyridine-4N	Pd	0.61	
pyridine-4N	Ag	0.21	
pyridine-4N	Re	0.94	
pyridine-4N	Ir	0.74	
pyridine-4N	Pt	0.72	
pyridine-4N	Au	0.24	
g-C2N	Ti	0.4	20
g-C2N	V	0.42	
g-C2N	Cr	0.74	
g-C2N	Mn	1.03	
g-C2N	Fe	1.07	
g-C2N	Co	1.26	
g-C2N	Ni	1.22	
g-C2N	Zr	0.28	
g-C2N	Nb	0.82	
g-C2N	Mo	1	
g-C2N	Hf	0.27	
g-C2N	Ta	0.76	
g-C2N	W	0.87	
g-C2N	Re	0.82	
h-BP	Sc	-0.434	19
h-BP	Ti	0.103	
h-BP	Cr	0.669	
h-BP	Mn	0.559	
h-BP	Fe	0.61	
h-BP	Co	0.584	
h-BP	Ni	0.968	
h-BP	Y	-0.609	
h-BP	Nb	0.128	
h-BP	Mo	0.731	
h-BP	Ru	0.644	
h-BP	Pd	1.061	
h-BP	Cd	0.741	
h-BP	Hf	0.041	
h-BP	W	0.507	
h-BP	Re	0.604	
h-BP	Os	0.489	
h-BP	Ir	0.233	
h-BP	Sc	-0.519	
h-BP	Ti	0.266	
h-BP	Cr	0.126	
h-BP	Mn	0.298	
h-BP	Fe	0.051	
h-BP	Ni	0.327	
h-BP	Y	-0.478	

h-BP	Nb	0.046	
h-BP	Mo	0.514	
h-BP	Re	-0.327	
h-BP	Sc	-1.044	
h-BP	Ti	-0.788	
h-BP	V	-0.545	
h-BP	Cr	-0.225	
h-BP	Mn	-0.131	
h-BP	Fe	-0.074	
h-BP	Ni	-0.061	
h-BP	Y	-0.569	
h-BP	Zr	-0.909	
h-BP	Mo	-0.095	
h-BP	Hf	-0.664	
h-BP	Ta	-1	
h-BP	Re	-0.467	
g-C3N4(h)	Ti	0.46	17
g-C3N4(h)	Ti	0.42	
g-C3N4(h)	V	0.95	
g-C3N4(h)	V	0.4	
g-C3N4(h)	V	0.94	
g-C3N4(h)	V	-0.18	
g-C3N4(h)	Nb	1.05	
g-C3N4(h)	Co	1.04	
g-C3N4(h)	Cu	0.92	
g-C3N4(t)	V	0.53	16
g-C3N4(t)	Cr	0.67	
g-C3N4(t)	Mn	0.86	
g-C3N4(t)	Mo	0.76	
g-C3N4(t)	Pd	1.09	
g-C3N4(t)	Pt	0.91	
g-C3N4(h)	Ti	0.3	3
g-C3N4(h)	V	1.06	
g-C3N4(h)	Co	0.82	
g-C3N4(h)	Zr	-0.03	
g-C3N4(h)	Nb	0.94	
g-C3N4(h)	Mo	0.79	
g-C3N4(h)	Hf	0.24	
g-C3N4(h)	Ta	0.67	
g-C3N4(h)	W	0.87	
g-C3N4(h)	Re	1.06	
C2	Ru	0.27	23
PD2G1	Ru	0.54	
PD2G2	Ru	0.48	
PD2G3	Ru	0.47	
PD2G4	Ru	0.47	
C2	Ir	0.27	
PD2G1	Ir	0.44	
PD2G2	Ir	0.45	
PD2G3	Ir	0.39	
PD2G4	Ir	0.56	
pyrrole-4N	Mn	-0.21	6
pyrrole-4N	Ni	0.65	
pyrrole-4N	Fe	-0.59	
pyrrole-4N	Cr	-0.56	
pyrrole-4N	Co	-0.02	
pyrrole-4N	Rh	-0.36	
pyridine-4N	Ti	-0.76	4
pyridine-4N	V	-0.21	
pyridine-4N	Cr	0.81	
pyridine-4N	Mn	0.85	
SV-3N	V	-0.24	
SV-3N	Mn	0.21	
SV-3N	Co	0.65	
N1C2	Ni	0.21	
g-C2N	Ti	0.35	5
g-C2N	V	0.42	
g-C2N	Cr	0.91	
g-C2N	Mn	1.17	
g-C2N	Zr	0.2	
g-C2N	Hf	0.12	
g-C2N	Ti	-0.11	
g-C2N	V	0.29	
g-C2N	Cr	0.47	
g-C2N	Mn	0.57	
g-C2N	Zr	-0.2	
g-C2N	Hf	-0.43	
N3/BP	Sc	-0.287	24
N3/BP	Ti	-0.436	
N3/BP	Cr	0.972	
N3/BP	Fe	0.713	
N3/BP	Co	0.384	
N3/BP	Ni	0.563	
N3/BP	Cu	0.539	
N3/BP	Y	-0.255	
N3/BP	Zr	-0.746	

N3/BP	Nb	0.631
N3/BP	Mo	1.128
N3/BP	Ru	0.246
N3/BP	Rh	0.119
N3/BP	Pd	0.403
N3/BP	Re	0.643
N3/BP	Os	0.457
N3/BP	Ir	-0.006
N3/BP	Pt	0.21
N3/BP	Au	0.416
N3/BP	Ti	0.037
N3/BP	V	0.395
N3/BP	Cr	0.636
N3/BP	Mn	0.556
N3/BP	Co	0.964
N3/BP	Ni	1.245
N3/BP	Zr	0.11
N3/BP	Ru	0.615
N3/BP	Pd	1.243
N3/BP	Hf	0.059
N3/BP	Ta	-0.337
N3/BP	W	1.083
N3/BP	Re	0.776
N3/BP	Os	0.703
N3/BP	Ir	0.449
N3/BP	Pt	0.885
N3/BP	Sc	-0.772
N3/BP	Ti	-0.548
N3/BP	V	-0.352
N3/BP	Y	-0.491
N3/BP	Zr	-0.815
N3/BP	Nb	-0.55
N3/BP	Mo	-0.049
N3/BP	Hf	-0.912
N3/BP	Ta	-0.852
N3/BP	W	-0.019
N3/BP	Sc	0.396
N3/BP	Ti	0.367
N3/BP	Y	0.74
N3/BP	Nb	0.139
N3/BP	Mo	0.097
N3/BP	W	0.158
g-C3N4(h)	Sc	0.29

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g-C3N4(h)	Ti	0.28
g-C3N4(h)	V	0.98
g-C3N4(h)	Cr	0.99
g-C3N4(h)	Mn	0.8
g-C3N4(h)	Fe	0.85
g-C3N4(h)	Y	0.52
g-C3N4(h)	Zr	0.2
g-C3N4(h)	Nb	1
g-C3N4(h)	Mo	1.08
g-C3N4(h)	Ru	0.67
g-C3N4(h)	Rh	0.68
g-C3N4(h)	Pd	1.1
g-C3N4(h)	Cd	0.5
g-C3N4(h)	Hf	0.11
g-C3N4(h)	Ta	0.58
g-C3N4(h)	Re	0.67
g-C3N4(h)	Os	0.45
g-C3N4(h)	Pt	0.77
g-C3N4(h)	Au	0.15
h-BP	Ti	0.52
h-BP	V	0.26
h-BP	Cr	0.67
h-BP	Fe	0.56
h-BP	Co	0.39
h-BP	Ni	0.95
h-BP	Cu	0.9
h-BP	Mo	1.02
h-BP	Rh	0.38
h-BP	Pd	0.83
h-BP	Ag	0.82
h-BP	Re	0.55
h-BP	Os	0.41
h-BP	Ir	0.21
h-BP	Pt	0.88
h-BP	Au	0.63
h-BP	Ti	-0.02
h-BP	V	0.02
h-BP	Cr	0.3
h-BP	Fe	0.55
h-BP	Co	0.2
h-BP	Ni	0.56
h-BP	Cu	-0.02
h-BP	Mo	0.6

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h-BP	Ru	0.24
h-BP	Rh	0.06
h-BP	Pd	0.18
h-BP	Ag	-0.13
h-BP	W	0.32
h-BP	Os	0.25
h-BP	Ir	0.09
h-BP	Pt	0.35
h-BP	Au	-0.12
Pc-N1C3	Os	0.423823
O1C3	Os	0.275196

Table 6. Dataset for $\Delta G_{9(N\text{-}end)}$.

structure	metal	$\Delta G_{9(N\text{-}end)}$	Ref.
g-CN	Ti	0.08	14
g-CN	V	-0.3	
g-CN	Cr	-0.73	
g-CN	Mn	-0.87	
g-CN	Fe	-0.77	
g-CN	Co	-0.91	
g-CN	Ni	-1.2	
g-CN	Cu	-1.46	
g-CN	Zr	0.41	
g-CN	Nb	0.15	
g-CN	Mo	0.01	
g-CN	Ru	-0.54	
g-CN	Rh	-1.16	
g-CN	Pd	-1.3	
g-CN	Hf	0.67	
g-CN	Ta	0.35	
g-CN	W	0.22	
g-CN	Re	0.06	
g-CN	Os	-0.54	
g-CN	Ir	-0.93	
pyridine-4N	Ti	0.73	
pyridine-4N	Zr	1.2	
pyridine-4N	Cu	-1.56	15
pyridine-4N	Zr	1.14	
pyridine-4N	Nb	1.3	
pyridine-4N	Hf	1.4	
pyridine-4N	Ta	1.51	
pyridine-4N	Re	0.89	
h-BP	Sc	-1.395	19
h-BP	Ti	-0.378	
h-BP	V	-1.029	
h-BP	Mn	-0.59	
h-BP	Fe	-0.593	
h-BP	Co	-0.957	
h-BP	Ni	-1.038	
h-BP	Y	-1.427	
h-BP	Zr	-0.555	
h-BP	Nb	-0.475	
h-BP	Mo	-0.754	
h-BP	Ru	-0.599	
h-BP	Pd	-1.325	
h-BP	Hf	-0.326	
h-BP	Ta	-0.18	
h-BP	W	-0.427	
h-BP	Re	-0.472	
h-BP	Os	-0.053	
h-BP	Ir	-0.88	
g-C3N4(t)	Cr	0.6	16
g-C3N4(t)	Mn	-0.24	
g-C3N4(t)	Mo	1.44	
g-C3N4(t)	Rh	-0.46	
g-C3N4(t)	Pd	-0.59	
g-C3N4(t)	Hf	2.96	
g-C3N4(t)	Os	0.71	
g-C3N4(t)	Pt	-0.38	
g-C3N4(h)	Ti	0.09	
g-C3N4(h)	V	0.01	
g-C3N4(h)	Zr	0.89	
g-C3N4(h)	Nb	0.4	
g-C3N4(h)	Hf	1.23	
g-C3N4(h)	Ta	0.84	
pyridine-4N	Fe	-0.58	
pyridine-4N	Os	0.33	
g-C3N4(h)	Ti	0.28	3
g-C3N4(h)	V	0.05	
g-C3N4(h)	Fe	-0.24	
g-C3N4(h)	Co	-0.44	
g-C3N4(h)	Zr	0.91	
g-C3N4(h)	Nb	0.47	
g-C3N4(h)	Ru	-0.19	
g-C3N4(h)	Ag	-0.85	
g-C3N4(h)	Hf	0.93	
g-C3N4(h)	W	0.44	
g-C3N4(h)	Os	0.31	
PD2G1	Ru	0.11	23
PD2G2	Ru	0.01	
PD2G3	Ru	0.12	
PD2G4	Ru	0.07	
C2	Ir	-0.17	
PD2G1	Ir	0.01	
PD2G2	Ir	0.04	

PD2G3	Ir	-0.01	
PD2G4	Ir	-0.02	
pyridine-4N	Mn	-0.52	[4]
pyridine-4N	Fe	-0.4	
pyrrole-4N	Cu	-1.91	[6]
pyrrole-4N	Mn	-0.83	
pyrrole-4N	Ni	-1.38	
pyrrole-4N	Fe	-0.74	
pyrrole-4N	Cr	-0.52	
pyrrole-4N	Co	-0.96	
C2N	Ti	-0.49	[20]
C2N	V	-0.71	
C2N	Cr	-1.1	
C2N	Mn	-1.38	
C2N	Fe	-1.2	
C2N	Co	-1.33	
C2N	Ni	-1.59	
C2N	Zr	-0.34	
C2N	Nb	-0.42	
C2N	Mo	-0.56	
C2N	Hf	-0.29	
C2N	Ta	-0.35	
C2N	W	-0.26	
C2N	Re	-0.54	
C2N	Os	-1.02	
pyridine-4N	Sc	0.3	[8]
N4B-G	Sc	-0.051	
pyridine-4N	Ti	0.77	
N4B-G	Ti	0.54	
pyridine-4N	V	0.51	
N4B-G	V	0.285	
pyridine-4N	Cr	-0.18	
N4B-G	Cr	-0.32	
pyridine-4N	Zr	1.17	
N4B-G	Zr	0.92	
pyridine-4N	Nb	1.47	
N4B-G	Nb	1.28	
pyridine-4N	Mo	0.86	
N4B-G	Mo	0.53	
pyridine-4N	Ru	-0.26	
N4B-G	Ru	-0.27	
pyridine-4N	Hf	1.53	
N4B-G	Hf	1.29	

g-C9N10	Mn	-0.811	[26]
g-C3N4(t)	Rh	-0.07	[9]
g-C3N4(t)	Os	0.26	
g-C3N4(t)	Fe	0.535	
N2C2	Os	0.19	[27]
N2C2	Cr	0.4	
DV-4C	Mn	-0.17	
DV-4C	Os	0.47	
DV-4C	Cr	0.45	
SV-3N	Ti	0.77	
SV-3N	Y	0.97	
SV-3C	Fe	-0.39	[28]
N1C2	Fe	0.24	
N2C1	Fe	0.27	
P3	Fe	-0.27	
N1C2	Mo	0.53	[29]
SV-3C	Nb	0.51	[30]
SV-3C	Re	0.32	
N1C2	V	0.15	
N1C2	Nb	0.41	
N1C2	Mo	0.54	
pyridine-4N	V	0.51	
N1C2	Ru	0.19	
N3C1	V	0.54	
SV-3C	W	0.37	
N1C2	Zr	0.55	
pyridine-4N	Fe	-0.42	[31]
pyridine-4N	Co	-0.38	
pyridine-4N	Mo	0.67	
pyridine-4N	W	1.08	
pyridine-4N	Ru	-0.28	
pyridine-4N	Rh	-0.47	
g-CN	Sc	0.08	[10]
g-CN	Ti	0.08	
g-CN	V	-0.3	
g-CN	Fe	-0.77	
g-CN	Co	-0.91	
g-CN	Ni	-1.2	
g-CN	Cu	-1.46	
g-CN	Y	0.09	
g-CN	Zr	0.41	
g-CN	Ru	-0.54	
g-CN	Rh	-1.16	

g-CN	Pd	-1.3
g-CN	Hf	0.55
g-CN	Os	-0.54
g-CN	Ir	-0.93
g-CN	Pt	-1.45
g-CN	Nb	0.15
g-CN	Mo	0.01
g-CN	Ta	0.35
g-CN	W	0.22
g-CN	Re	0.06	
B1C2	Hf	0.34	[32]
B3C1	Ti	0.507725	
B3C1	W	0.641811	
B3C1	Hf	0.937480	
N3O1	Cr	0.479654	
Pc-N1C3	Os	0.282884	

Table 7. Dataset for $\Delta G_{9(O\text{-}end)}$.

Structure	Metal	$\Delta G_{9(O\text{-}end)}$	Ref.
h-BP	Sc	-0.377	19
h-BP	Ti	0.41	
h-BP	V	-0.219	
h-BP	Cr	0.756	
h-BP	Mn	-0.024	
h-BP	Fe	0.017	
h-BP	Zr	0.374	
h-BP	Nb	0.449	
h-BP	Mo	0.107	
h-BP	Hf	0.697	
h-BP	Ta	0.522	
h-BP	W	0.37	
pyridine-4N	Cr	0.11	4
SV-3N	Ti	2.16	
SV-3N	V	1.9	
SV-3N	Cr	1.77	
SV-3N	Mn	1.07	
SV-3N	Fe	0.83	
SV-3N	Ni	0.49	
N1C2	Ni	0.25	
SV-3N	Cu	-0.21	
DV-4C	Pt	-1.11	33
N1C3	Pt	-1.35	
N3C1	Pt	-1.89	
pyridine-4N	Pt	-2.22	
O1C3	Pt	-1.3	
B3C1	Pt	-0.15	
B4	Pt	0	
C2N	Sc	1.714	34
C2N	Ru	0.007	
C2N	Ti	1.607	
C2N	Rh	-0.558	
C2N	V	0.864	
C2N	Pd	-0.828	
C2N	Cr	0.223	
C2N	Ag	-1.915	
C2N	Mn	0.578	
C2N	Cd	-0.532	
C2N	Fe	0.18	
C2N	La	1.157	
C2N	Co	-0.061	
C2N	Hf	2.179	
C2N	Ni	-0.52	
C2N	Ta	1.391	
C2N	Cu	-0.721	
C2N	Zn	0.482	
C2N	Y	1.622	
C2N	Os	0.231	
C2N	Zr	1.904	
C2N	Ir	-0.09	
C2N	Nb	1.532	
C2N	Pt	-0.095	
C2N	Mo	0.689	
C2N	Au	-0.989	
S1N3	Fe	0.209	35
pyridine-4N	Cr	0.143	36
N4P-G	Cr	0.296	
N4S-G	Cr	0.176	
pyridine-4N	Mn	-0.309	
N4P-G	Mn	-0.126	
N4S-G	Mn	-0.187	
pyridine-4N	Fe	-0.523	
N4P-G	Fe	-0.386	
N4S-G	Fe	-0.453	
N4P-G	Co	-1.053	
N4S-G	Co	-0.975	
N4P-G	Ni	-1.722	
N4S-G	Ni	-1.794	
N4P-G	Cu	-1.791	
N4S-G	Cu	-1.646	
pyridine-4N	Zn	-0.852	
N4P-G	Ru	-0.114	
N4S-G	Ru	-0.17	
pyridine-4N	Rh	-1.07	
N4P-G	Rh	-0.973	
N4S-G	Rh	-1.12	
pyridine-4N	Pd	-2.372	
N4P-G	Pd	-2.284	
N4S-G	Pd	-2.474	
N4P-G	Ag	-1.278	
N4S-G	Ag	-1.333	

pyridine-4N	Ir	-1.098	
N4P-G	Ir	-0.879	
N4S-G	Ir	-1.05	
pyridine-4N	Pt	-2.385	
N4P-G	Pt	-2.169	
N4S-G	Pt	-2.357	
pyridine-4N	Au	-2.21	
N4P-G	Au	-2.199	
N4S-G	Au	-2.189	
g-C3N4(h)	Sc	2.36	37
g-C3N4(h)	Ti	1.61	
g-C3N4(h)	V	1.11	
g-C3N4(h)	Cr	0.91	
g-C3N4(h)	Mn	0.89	
g-C3N4(h)	Fe	0.64	
g-C3N4(h)	Co	0.56	
g-C3N4(h)	Ni	0.41	
g-C3N4(h)	Cu	0.69	
g-C3N4(h)	Zn	1.54	
g-C3N4(h)	Y	2.55	
g-C3N4(h)	Zr	2.31	
g-C3N4(h)	Nb	1.22	
g-C3N4(h)	Mo	0.68	
g-C3N4(h)	Ru	0.13	
g-C3N4(h)	Rh	0.73	
g-C3N4(h)	Pd	0.13	
g-C3N4(h)	Ag	-0.31	
g-C3N4(h)	Cd	0.52	
g-C3N4(h)	Hf	2.61	
g-C3N4(h)	Ta	1.61	
g-C3N4(h)	W	0.93	
g-C3N4(h)	Os	0.75	
g-C3N4(h)	Ir	0.48	
g-C3N4(h)	Pt	0.97	
C2N	Sc	1.54	
C2N	Ti	1.13	
C2N	V	0.78	
C2N	Cr	0.34	
C2N	Mn	0.18	
C2N	Fe	0.15	
C2N	Co	0	
C2N	Ni	-0.44	
C2N	Cu	-0.75	
C2N	Zn	0.35	
C2N	Y	1.47	
C2N	Zr	1.78	
C2N	Nb	1.09	
C2N	Mo	0.54	
C2N	Ru	-0.13	
C2N	Rh	-0.6	
C2N	Pd	-1.04	
C2N	Ag	-1.85	
C2N	Cd	-0.55	
C2N	Hf	2.08	
C2N	Ta	1.46	
C2N	W	1.21	
C2N	Re	0.9	
C2N	Os	0.15	
C2N	Ir	-0.05	
C2N	Pt	-0.18	
C2N	Au	-0.91	
Pc	Sc	1.94	
Pc	Ti	1.68	
Pc	Cr	-0.27	
Pc	Mn	-0.75	
Pc	Co	-1.39	
Pc	Y	2.99	
Pc	Zr	2.51	
Pc	Mo	0.66	
Pc	Rh	-0.91	
Pc	Pd	-2.58	
Pc	Cd	-1.71	
Pc	Ta	1.97	
Pc	W	1.09	
Pc	Re	0.25	
Pc	Os	-0.08	
Pc	Ir	-0.96	
Pc	Pt	-2.54	
pyridine-4N	Cr	-0.11	
DV-4C	Fe	0.1	
DV-4C	Co	0.16	
SV-3C	Sc	2.23	2
SV-3C	Ti	2.02	
SV-3C	V	1.29	
SV-3C	Cr	1.05	
SV-3C	Mn	1.22	

SV-3C	Fe	0.73
SV-3C	Co	0.42
SV-3C	Ni	0.19
SV-3C	Cu	-0.22
SV-3C	Zn	0.03
SV-3C	Y	2.15
SV-3C	Zr	1.62
SV-3C	Nb	1.57
SV-3C	Mo	0.88
SV-3C	Ru	-0.06
SV-3C	Rh	0.08
SV-3C	Pd	-0.48
SV-3C	Ag	-0.61
SV-3C	Cd	-0.38
SV-3C	Hf	1.91
SV-3C	Ta	1.8
SV-3C	W	1.29
SV-3C	Re	1.12
SV-3C	Os	0.47
SV-3C	Ir	0.25
SV-3C	Pt	-0.09
SV-3C	Au	-1.25
DV-4C	Sc	2.13
DV-4C	Ti	1.53
DV-4C	V	1.23
DV-4C	Mn	0.28
DV-4C	Fe	-0.05
DV-4C	Co	-0.39
DV-4C	Zn	-1.26
DV-4C	Y	1.96
DV-4C	Zr	1.66
DV-4C	Nb	1.06
DV-4C	Mo	0.47
DV-4C	Ru	-0.37
DV-4C	Ag	-1.19
DV-4C	Cd	-1.39
DV-4C	Hf	1.51
DV-4C	Ta	1.31
DV-4C	W	0.91
DV-4C	Re	0.59
DV-4C	Os	-0.07
DV-4C	Ir	-0.36
DV-4C	Pt	-0.76

pyridine-4N	Sc	2.29
pyridine-4N	Ti	1.56
pyridine-4N	V	1.15
pyridine-4N	Cr	-0.03
pyridine-4N	Mn	-0.15
pyridine-4N	Y	2.07
pyridine-4N	Zr	1.29
pyridine-4N	Nb	0.86
pyridine-4N	Mo	-0.29
pyridine-4N	Rh	-1.34
pyridine-4N	Pd	-2.54
pyridine-4N	Ag	-1.6
pyridine-4N	Cd	-1.89
pyridine-4N	Hf	1.5
pyridine-4N	Ta	1.19
pyridine-4N	W	0.52
pyridine-4N	Re	0.27
pyridine-4N	Os	-0.55
pyridine-4N	Pt	-1.94
pyrrole-4N	Sc	2.13
pyrrole-4N	Ti	1.49
pyrrole-4N	V	1.02
pyrrole-4N	Cr	-0.43
pyrrole-4N	Mn	-0.64
pyrrole-4N	Fe	-0.95
pyrrole-4N	Co	-1.5
pyrrole-4N	Ni	-2.08
pyrrole-4N	Cu	-2.72
pyrrole-4N	Zn	-2.68
pyrrole-4N	Y	2.34
pyrrole-4N	Zr	1.53
pyrrole-4N	Ru	-1.49
pyrrole-4N	Rh	-2.14
pyrrole-4N	Pd	-3.12
pyrrole-4N	Ag	-3.05
pyrrole-4N	Cd	-3
pyrrole-4N	Hf	1.64
pyrrole-4N	Ta	1.16
pyrrole-4N	W	0.17
pyrrole-4N	Re	-0.55
pyrrole-4N	Os	-0.97
pyrrole-4N	Ir	-1.33
pyrrole-4N	Au	-3.34

S2C1	Ru	0.303825	
Pc-N4	Os	-0.201649	
Py-N1C3	Os	0.885342	

Pc-C4	Re	1.873181	

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