Appendix

(Supporting information for chapter 5)

Table 1. The experimental values of the heat of formation (HOF) for all 54 transition metal complexes which are taken in this work (Kcal/mol) are depicted below. These experimental HOF values are taken from the different relevant literatures.

TiS	76.2 ± 2.2[1]	$MnCl_2$	-63.0 ± 0.5[1,2]	NiO	75.0 ± 5.0[1]
TiF_2	-164.5 ± 10.0[2,3]	MnCl	11.3 ± 2.1[1]	NiH	85.6 ± 2.6[1]
TiO	13.7 ± 2.2[1]	MnF_2	-126.2 ± 1.0[1]	NiF_2	-77.8 ± 1.1[1]
TiH	116.4 ± 2.3[4]	MnH	64.2 ± 7.0[1]	NiCl	41.7 ± 1.6[11]
TiF_3	-284.1 ± 10.0[2,3]	MnO	29.6 ± 3.0[1]	$NiCl_2$	-17.4 ± 1.0[11]
TiCl	24.2[1]	MnF	-19.9 ± 3.0[1]	Ni(CO)	35.1 ± 5.8[9]
V2	187.4 ± 5.2[1]	FeF_2	-93.0 ± 3.4[5]	Cu2	113.8 ± 2.6[1]
VS	80.4 ± 3.2[1]	$Fe(CO)_2$	0.2 ± 4.9[9]	CuCl	19.3 ± 2.0[1]
VN	121.0 ± 3.0[1]	Fe(CO)	63.9 ± 3.5[9]	CuF	-3.2 ± 2.0[1]
VO	30.5[2,5]	FeCl	49.5 ± 1.6[10]	CuF_2	-66.0[1]
VCl	37.8 ± 1.5[1]	FeO	61.1 ± 3.0[1]	CuO	76.5 ± 10.0[2]
VF	0.7 ± 15.0[1]	$FeCl_2$	32.8 ± 1.0[10]	CuS	75.1 ± 5.0[2]
CrCl	31.0 ± 0.6[6]	CoH	110.7 ± 1.0[9]	Zn_2	57.7 ± 1.5[1]
$CrCl_2$	-28.1 ± 0.4[6]	CoO	7.0 ± 5.1[1]	$Zn(CH_3)$	26.0 ± 2.5[1]
CrF	3.1 ± 2.4[7]	CoCl	50.3 ± 1.6[10]	$ZnCl_2$	-63.5 ± 0.4[1]
CrO	45.0[2,3,8]	$CoCl_2$	-22.6 ± 1.0[10]	ZnF_2	-118.9 ± 1.1[1]
CrO_2	-18.0[2,3,8]	CoF_2	-87.5[1]	ZnH	62.9 ± 0.5[1]
CrOH	18.9 ± 1.8[6]	$CoCl_3$	-39.1[2,3,8]	ZnO	52.8 ± 0.9[1]

Table 2. This table depicts the experimental values of the ionization potential (IP) for 47 different transition metal complexes estimated in this work (*eV*). These experimental IP values are taken from the different relevant literatures.

TiS	7.1 ± 0.3[3]	$MnCl_2$	11.03 ± 0.01[3]	NiO	9.5 ± 0.2[3]
TiF_2	12.2 ± 0.5[3]	MnCl	8.5 ± 0.3[1]	NiH	8.50 ± 0.10[3]
TiO	6.819 ± 0.006[3]	MnF_2	11.38 ± 0.20[3]	NiF_2	11.5 ± 0.3[3]
TiH	6[3]	MnH	7.8[3]	NiCl	9.28 ± 0.10[1]
TiF_3	10.5 ± 0.5[3]	MnO	8.65 ± 0.20[3]	$NiCl_2$	11.24 ± 0.01[3]
V2	6.357 ± 0.001[3]	MnF	8.51 ± 0.20[3]	Ni(CO)	7.30 ± 0.29[3]
VS	8.4 ± 0.3[3]	FeF_2	11.3 ± 0.3[3]	Cu2	7.9[3]
VN	8.0 ± 1.0[3]	$Fe(CO)_2$	6.68 ± 0.24[7]	CuCl	10.7 ± 0.3[3]
VO	7.2386 ± 0.0006[3]	Fe(CO)	6.66 ± 0.17[7]	CuF	10.90 ± 0.01[3]
CrCl	8.50 ± 0.10[1]	FeCl	8.08 ± 0.10[1]	CuF_2	13.18[3]
$CrCl_2$	9.9[3]	FeO	8.9 ± 0.2[3]	Zn_2	9.0 ± 0.2[3]
CrF	9.3 ± 0.4[3]	$FeCl_2$	10.63 ± 0.10[1]	$ZnCH_3$	7.2[3]
CrO	8.16 ± 0.01[3]	CoH	7.86 ± 0.07[3]	$ZnCl_2$	11.80 ± 0.005[3]
CrO_2	10.3 ± 0.5[3]	CoO	8.9 ± 0.2[3]	ZnF_2	13.91 ± 0.03[3]
CrOH	7.54 ± 0.05[10]	CoCl	8.71 ± 0.10[1]	ZnH	9.4[3]
		$CoCl_2$	10.75 ± 0.10[1]	ZnO	9.34 ± 0.02[12]

In Table 1 and Table 2 the numerical superscripts denote the respective references from where the HOF and IP values are taken. These references are given below-

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Table 3: The group of tables show the ground state gas phase energy of 16 different atoms which are used to form the 54 different TM complexes calculated with 8 different M0X functionals with LANL2DZ basis set along with their respective multiplicities. The energy has the unit a.u.

M05

Atoms	Multiplicity	Energy
H	2	−0.49
C	3	−37.82
N	4	−54.59
O	3	−75.05
F	2	−99.72
S	3	−10.00
Cl	2	−14.85
Ti	3	−57.88
V	6	−71.15
Cr	7	−86.21
Mn	4	−103.81
Fe	3	−123.36
Co	4	−145.02
Ni	3	−169.30
Cu	2	−196.23
Zn	1	−65.74

M05-2X

Atoms	Multiplicity	Energy
H	2	−0.50
C	3	−37.85
N	4	−54.59
O	3	−75.07
F	2	−99.74
S	3	−10.01
Cl	2	−14.86
Ti	3	− 57.90
V	4	−71.16
Cr	5	−86.19
Mn	4	−103.76
Fe	3	−123.30
Co	4	−145.95
Ni	3	−169.21
Cu	2	−196.09
Zn	1	−65.34

M06-L

Atoms	Multiplicity	Energy
H	2	−0.50
C	3	−37.84
N	4	−54.59
O	3	−75.07
F	2	−99.74
S	3	−10.02
Cl	2	−14.89
Ti	3	− 57.95
V	4	−71.21
Cr	7	−86.25
Mn	6	−103.83
Fe	5	−123.38
Co	4	−145.02
Ni	3	−169.25
Cu	2	−196.12
Zn	1	−65.10

M06

Atoms	Multiplicity	Energy
H	2	−0.50
C	3	−37.82
N	4	−54.57
O	3	−75.05
F	2	−99.71
S	3	−10.00
Cl	2	−14.86
Ti	3	−57.91
V	6	−71.18
Cr	7	−86.24
Mn	6	−103.81
Fe	5	−123.34
Co	4	−145.00
Ni	3	−169.26
Cu	2	−196.15
Zn	1	−65.46

M06-2X

Atoms	Multiplicity	Energy
H	2	−0.50
C	3	−37.84
N	4	−54.58
O	3	−75.06
F	2	−99.72
S	3	−9.99
Cl	2	−14.84
Ti	3	−57.89
V	6	−71.16
Cr	5	−86.22
Mn	4	−103.80
Fe	5	−123.33
Co	4	−144.99
Ni	3	−169.26
Cu	2	−196.15
Zn	1	−65.43

M06-HF

Atoms	Multiplicity	Energy
H	2	−0.49
C	3	−37.85
N	4	−54.59
O	3	−75.06
F	2	−99.73
S	3	−9.99
Cl	2	−14.82
Ti	3	−57.88
V	4	−71.13
Cr	7	−86.17
Mn	6	−103.84
Fe	5	−123.29
Co	4	−144.97
Ni	3	−169.23
Cu	2	−196.03
Zn	1	−65.60

M08-SO

Atoms	Multiplicity	Energy
H	2	−0.50
C	3	−37.82
N	4	−54.55
O	3	−75.03
F	2	−99.70
S	3	−10.03
Cl	2	−14.86
Ti	1	−57.80
V	4	−71.04
Cr	7	−86.12
Mn	6	−103.69
Fe	5	−123.20
Co	4	−144.86
Ni	3	−169.13
Cu	2	−196.02
Zn	1	−65.45

M08-HX

Atoms	Multiplicity	Energy
H	2	−0.50
C	3	−37.84
N	4	−54.58
O	3	−75.05
F	2	−99.72
S	3	−10.02
Cl	2	−14.87
Ti	1	−57.84
V	4	−71.15
Cr	7	−86.17
Mn	6	−103.73
Fe	5	−123.26
Co	4	−144.88
Ni	3	−169.11
Cu	2	−195.97
Zn	1	−65.01

Table 4: The computational HOF values of the 54 different TM complexes in 8 different M0X functionals with LANL2DZ basis set along with their respective experimental values taken from the respective literature (the references are given above) and the corresponding error (experiment–theory) values are shown in the following bunch of tables. The HOF results and the errors have the unit Kcal/mole.

Ti-Series

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
TiS	62.08	76.2	14.12
TiF_2	-129.01	-164.5	-35.49
TiO	13.39	13.7	0.31
TiH	106.74	116.4	9.66
TiF_3	-256.98	-284.1	-27.12
TiCl	32.33	24.2	-8.13

Mean Error (M E) =-7.78
Absolute Error (A E) =15.81

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
TiS	93.77	76.2	-17.57
TiF_2	-107.40	-164.5	-57.10
TiO	46.28	13.7	-32.58
TiH	122.16	116.4	-5.76
TiF_3	-220.76	-284.1	-63.34
TiCl	55.27	24.2	-31.07

Mean Error (M E) =-34.57

Absolute Error (A E) =34.57

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
TiS	54.38	76.2	21.82
TiF_2	-123.90	-164.5	-40.60
TiO	9.36	13.7	4.34
TiH	104.97	116.4	11.43
TiF_3	-263.01	-284.1	-21.09
TiCl	37.50	24.2	-13.30

Mean Error (M E) =-6.23

Absolute Error (A E) =18.76

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
TiS	61.49	76.2	14.71
TiF_2	-122.88	-164.5	-41.62
TiO	17.32	13.7	-3.62
TiH	103.49	116.4	12.91
TiF_3	-251.42	-284.1	-32.68
TiCl	31.36	24.2	-7.16

Mean Error (M E) =-9.58

Absolute Error (A E) =18.78

M06-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
TiS	85.37	76.2	-9.17
TiF_2	-109.03	-164.5	-55.47
TiO	37.21	13.7	-23.51
TiH	112.01	116.4	4.39
TiF_3	-219.44	-284.1	-64.66
TiCl	38.42	24.2	-14.22

Mean Error (M E) =-27.11

Absolute Error (A E) =28.57

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
TiS	113.45	76.2	-37.25
TiF_2	-82.16	-164.5	-82.34
TiO	72.74	13.7	-59.04
TiH	112.16	116.4	4.24
TiF_3	-176.74	-284.1	-107.36
TiCl	50.66	24.2	-26.46

Mean Error (M E) =-51.37

Absolute Error (A E) =52.78

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
TiS	66.19	76.2	10.01
TiF_2	-133.07	-164.5	-31.43
TiO	4.24	13.7	9.46
TiH	76.72	116.4	39.68
TiF_3	-218.86	-284.1	-65.24
TiCl	10.39	24.2	13.81

Mean Error (M E) =-3.95

Absolute Error (A E) =28.27

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
TiS	53.42	76.2	22.78
TiF_2	-152.69	-164.5	11.81
TiO	-0.06	13.7	13.76
TiH	64.29	116.4	52.12
TiF_3	-252.41	-284.1	-31.69
TiCl	4.18	24.2	20.02

Mean Error (M E) =14.7

Absolute Error (A E) =25.36

V-Series

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
V2	191.12	187.4	-3.72
VS	86.73	80.4	-6.33
VN	139.08	121	-18.08
VO	40.77	30.5	-10.27
VCl	51.31	37.8	-13.51
VF	14.21	0.7	-13.51

Mean Error (M E) =-10.90

Absolute Error (A E) =10.90

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
V2	212.98	187.4	-25.58
VS	109.00	80.4	-28.60
VN	171.99	121	-50.99
VO	71.14	30.5	-40.64
VCl	60.51	37.8	-22.71
VF	26.81	0.7	-26.11

Mean Error (M E) =-32.43

Absolute Error (A E) =32.43

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
V2	154.07	187.4	33.33
VS	72.22	80.4	8.18
VN	120.75	121	0.25
VO	29.92	30.5	0.58
VCl	46.88	37.8	-9.08
VF	10.73	0.7	-10.03

Mean Error (M E) =3.86

Absolute Error (A E) =10.24

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
V2	170.28	187.4	17.12
VS	81.18	80.4	-0.78
VN	141.72	121	-20.72
VO	39.27	30.5	-8.77
VCl	47.35	37.8	-9.55
VF	14.57	0.7	-13.87

Mean Error (M E) =-6.10

Absolute Error (A E) =11.80

M06-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
V2	260.17	187.4	-72.77
VS	104.40	80.4	-24.00
VN	167.45	121	-46.45
VO	65.00	30.5	-34.50
VCl	49.30	37.8	-11.50
VF	22.60	0.7	-21.90

Mean Error (M E) =-35.19

Absolute Error (A E) =35.19

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
V2	317.70	187.4	-130.30
VS	122.81	80.4	-42.41
VN	198.03	121	-77.03
VO	96.22	30.5	-65.72
VCl	56.51	37.8	-18.71
VF	31.35	0.7	-30.65

Mean Error (M E) =-60.80

Absolute Error (A E) =60.80

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
V2	22.90	187.4	14.90
VS	92.23	80.4	-11.83
VN	120.96	121	0.041
VO	-16.31	30.5	46.81
VCl	22.90	37.8	14.90
VF	6.13	0.7	-5.43

Mean Error (M E) = 9.90

Absolute Error (A E) = 15.65

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
V2	48.57	187.4	-10.77
VS	117.41	80.4	-37.01
VN	179.19	121	-58.19
VO	102.95	30.5	-72.45
VCl	48.57	37.8	-10.77
VF	27.03	0.7	-26.33

Mean Error (M E) = -35.92

Absolute Error (A E) = 35.92

Cr-Series

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CrCl	35.50	31	-4.50
$CrCl_2$	-11.12	-28.1	-16.98
CrF	6.12	3.1	-3.02
CrO	70.93	45	-25.93
CrO_2	25.95	-18	-43.95
CrOH	35.61	18.9	-16.71

Mean Error (M E) =-18.52
Absolute Error (A E) =18.52

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CrCl	37.26	31	-6.26
$CrCl_2$	15.66	-28.1	-43.76
CrF	12.51	3.1	-9.41
CrO	87.38	45	-42.38
CrO_2	97.09	-18	-115.09
CrOH	39.19	18.9	-20.29

Mean Error (M E) =-39.54
Absolute Error (A E) =39.54

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CrCl	31.50	31	-0.50
$CrCl_2$	-18.59	-28.1	-9.51
CrF	1.11	3.1	1.99
CrO	55.10	45	-10.10
CrO_2	-1.71	-18	-16.29
CrOH	32.43	18.9	-13.53

Mean Error (M E) =-7.99
Absolute Error (A E) =8.65

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CrCl	34.41	31	-3.41
$CrCl_2$	-13.53	-28.1	-14.57
CrF	8.85	3.1	-5.75
CrO	72.19	45	-27.19
CrO_2	31.79	-18	-49.79
CrOH	37.40	18.9	-18.50

Mean Error (M E) =-19.87

Absolute Error (A E) =19.87

M06-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CrCl	33.76	31	-2.76
$CrCl_2$	14.06	-28.1	-42.16
CrF	15.08	3.1	-11.98
CrO	88.94	45	-43.94
CrO_2	105.01	-18	-123.01
CrOH	41.29	18.9	-22.39

Mean Error (M E) =-41.04

Absolute Error (A E) =41.04

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CrCl	26.87	31	4.13
$CrCl_2$	-7.97	-28.1	-20.13
CrF	15.26	3.1	-12.16
CrO	92.30	45	-47.30
CrO_2	129.08	-18	-147.08
CrOH	37.11	18.9	-18.21

Mean Error (M E) =-40.13

Absolute Error (A E) =41.50

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CrCl	34.58	31	-3.58
$CrCl_2$	-7.03	-28.1	-21.07
CrF	14.59	3.1	-11.49
CrO	80.28	45	-35.28
CrO_2	84.19	-18	-102.19
CrOH	23.44	18.9	-4.54

Mean Error (M E) = -29.69

Absolute Error (A E) =29.69

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CrCl	30.47	31	0.53
$CrCl_2$	-19.67	-28.1	-8.43
CrF	4.02	3.1	-0.92
CrO	92.72	45	-47.72
CrO_2	94.88	-18	-112.88
CrOH	18.59	18.9	0.31

Mean Error (M E) = -28.19

Absolute Error (A E) =28.47

Mn Series

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
$MnCl_2$	-84.04	-63	21.04
MnCl	-16.31	11.3	27.61
MnF_2	-148.18	-126.2	21.98
MnH	64.16	64.2	0.04
MnO	16.93	29.6	12.67
MnF	-34.82	-19.9	14.92

Mean Error (M E) =16.38
Absolute Error (A E) =16.38

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
$MnCl_2$	-91.09	-63	28.09
MnCl	-19.89	11.3	31.19
MnF_2	-155.48	-126.2	29.28
MnH	45.41	64.2	18.79
MnO	26.68	29.6	2.92
MnF	-45.42	-19.9	25.52

Mean Error (M E) =22.63
Absolute Error (A E) =22.63

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
$MnCl_2$	-98.55	-63	35.55
MnCl	-14.18	11.3	25.48
MnF_2	-163.04	-126.2	36.84
MnH	38.44	64.2	25.76
MnO	-1.83	29.6	31.43
MnF	-48.86	-19.9	28.96

Mean Error (M E) =30.67
Absolute Error (A E) =30.67

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
$MnCl_2$	-97.25	-63	34.25
MnCl	-23.12	11.3	34.42
MnF_2	-154.29	-126.2	28.09
MnH	59.03	64.2	5.17
MnO	10.34	29.6	19.26
MnF	-42.17	-19.9	22.27

Mean Error (M E) =23.91
Absolute Error (A E) =23.91

M06-2X

Molecule	HOF(theo)	HOF(expt))	Error(expt–theo)
$MnCl_2$	-100.23	-63	37.23
MnCl	-27.56	11.3	38.86
MnF_2	-153.13	-126.2	26.93
MnH	44.11	64.2	20.09
MnO	24.71	29.6	4.89
MnF	-47.76	-19.9	27.86

Mean Error (M E) =25.98
Absolute Error (A E) =25.98

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
$MnCl_2$	-51.88	-63	-11.12
MnCl	9.58	11.3	1.72
MnF_2	-91.23	-126.2	-34.97
MnH	95.11	64.2	-30.91
MnO	94.15	29.6	-64.55
MnF	125.64	-19.9	-145.54

Mean Error (M E) =-47.56
Absolute Error (A E) =48.13

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
$MnCl_2$	-86.76	-63	23.76
MnCl	-10.17	11.3	21.47
MnF_2	-137.60	-126.2	11.40
MnH	62.33	64.2	1.87
MnO	63.42	29.6	-33.82
MnF	-35.99	-19.9	16.09

Mean Error (M E) = 6.80
Absolute Error (A E) = 18.07

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
$MnCl_2$	-107.24	-63	44.24
MnCl	-28.59	11.3	39.89
MnF_2	-168.33	-126.2	42.13
MnH	32.21	64.2	31.99
MnO	47.95	29.6	-18.35
MnF	-60.29	-19.9	40.39

Mean Error (M E) = 30.05
Absolute Error (A E) = 36.17

Fe-Series

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
FeF_2	-232.08	-93	139.08
$Fe(CO)_2$	44.34	0.2	-44.14
Fe(CO)	95.66	27.91	-67.75
FeCl	48.45	49.5	1.05
FeO	66.51	61.1	-5.41
$FeCl_2$	-184.00	-32.8	151.20

Mean Error (M E) = 29.005
Absolute Error (A E) = 68.105

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
FeF_2	-234.32	-93	141.32
$Fe(CO)_2$	92.76	0.2	-92.56
Fe(CO)	117.33	27.91	-89.42
FeCl	44.80	49.5	4.70
FeO	78.03	61.1	-16.93
$FeCl_2$	-186.12	-32.8	153.32

Mean Error (M E) = 16.738
Absolute Error (A E) = 83.042

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
FeF_2	-235.79	-93	142.79
$Fe(CO)_2$	33.82	0.2	-33.62
Fe(CO)	74.25	27.91	-46.34
FeCl	33.39	49.5	16.11
FeO	54.64	61.1	6.46
$FeCl_2$	-188.56	-32.8	155.76

Mean Error (M E) =40.19
Absolute Error (A E) =66.85

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
FeF_2	-235.57	-93	142.57
$Fe(CO)_2$	29.34	0.2	-29.14
Fe(CO)	87.34	27.91	-59.43
FeCl	44.11	49.5	5.39
FeO	60.69	61.1	0.41
$FeCl_2$	-196.11	-32.8	163.31

Mean Error (M E) =37.19
Absolute Error (A E) =66.71

M06-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
FeF_2	-231.67	-93	138.67
$Fe(CO)_2$	88.94	0.2	-88.74
Fe(CO)	116.36	27.91	-88.45
FeCl	35.64	49.5	13.86
FeO	78.48	61.1	-17.38
$FeCl_2$	-194.83	-32.8	162.03

Mean Error (M E) =20
Absolute Error (A E) =84.67

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
FeF_2	-223.00	-93	130.00
$Fe(CO)_2$	121.27	0.2	-121.07
Fe(CO)	141.49	27.91	-113.58
FeCl	30.86	49.5	18.64
FeO	106.79	61.1	-45.69
$FeCl_2$	-198.36	-32.8	165.56

Mean Error (M E) =5.64
Absolute Error (A E) =99.09

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
FeF_2	-226.93	-93	133.93
$Fe(CO)_2$	93.74	0.2	-93.54
Fe(CO)	133.87	27.91	-105.96
FeCl	21.96	49.5	27.54
FeO	74.80	61.1	-13.70
$FeCl_2$	-193.05	-32.8	160.25

Mean Error (M E) = 18.09
Absolute Error (A E) = 89.15

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
FeF_2	-230.88	-93	137.88
$Fe(CO)_2$	138.92	0.2	-138.72
Fe(CO)	147.43	27.91	-119.52
FeCl	47.96	49.5	1.54
FeO	97.32	61.1	-36.22
$FeCl_2$	-182.71	-32.8	149.91

Mean Error (M E) = -0.86
Absolute Error (A E) = 97.30

Co-Complexes

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CoH	93.01	110.7	17.69
CoO	65.07	74	8.93
CoCl	43.69	50.3	6.61
$CoCl_2$	-23.10	-22.6	0.50
CoF_2	-92.91	-87.5	5.41
$CoCl_3$	-24.70	-39.1	-14.40

Mean Error (M E) =4.12
Absolute Error (A E) =8.92

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CoH	95.55	110.7	15.15
CoO	99.79	74	-25.79
CoCl	40.84	50.3	9.46
$CoCl_2$	-1.33	-22.6	-21.27
CoF_2	-74.83	-87.5	-12.67
$CoCl_3$	3.54	-39.1	-42.64

Mean Error (M E) =-12.96
Absolute Error (A E) =21.16

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CoH	90.70	110.7	20.00
CoO	75.52	74	-1.52
CoCl	36.56	50.3	13.74
$CoCl_2$	-18.58	-22.6	-4.02
CoF_2	-77.69	-87.5	-9.81
$CoCl_3$	-38.21	-39.1	-0.89

Mean Error (M E) =2.92
Absolute Error (A E) =8.33

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CoH	93.23	110.7	17.47
CoO	72.15	74	1.85
CoCl	47.81	50.3	2.49
$CoCl_2$	-23.31	-22.6	0.71
CoF_2	-84.45	-87.5	-3.05
$CoCl_3$	-35.96	-39.1	-3.14

Mean Error (M E) =2.73
Absolute Error (A E) =4.79

M06-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CoH	99.80	110.7	10.90
CoO	102.10	74	-28.10
CoCl	41.05	50.3	9.25
$CoCl_2$	-10.59	-22.6	-12.01
CoF_2	-71.59	-87.5	-15.91
$CoCl_3$	-4.92	-39.1	-34.18

Mean Error (M E) =-11.68
Absolute Error (A E) =18.39

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CoH	105.70	110.7	5.00
CoO	136.94	74	-62.94
CoCl	44.46	50.3	5.84
$CoCl_2$	-5.93	-22.6	-16.67
CoF_2	-57.08	-87.5	-30.42
$CoCl_3$	-61.43	-39.1	22.33

Mean Error (M E) = -12.81
Absolute Error (A E) = 23.87

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CoH	65.02	110.7	45.68
CoO	76.01	74	-2.01
CoCl	35.76	50.3	14.54
$CoCl_2$	-29.80	-22.6	7.20
CoF_2	-88.07	-87.5	0.57

Mean Error (M E) = 13.20
Absolute Error (A E) = 14.0

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
CoH	76.88	110.7	33.82
CoO	102.82	74	-28.82
CoCl	42.21	50.3	8.09
$CoCl_2$	-12.16	-22.6	-10.44
CoF_2	-82.35	-87.5	-5.15

Mean Error (M E) = -0.5
Absolute Error (A E) = 17.26

Ni-Series

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
NiO	84.26	75	-9.26
NiH	92.35	85.6	-6.75
NiF_2	-45.81	-77.8	-31.99
NiCl	45.15	41.7	-3.45
$NiCl_2$	9.85	-17.4	-27.25
NiCO	72.57	35.1	-37.47

Mean Error (M E) = -19.36
Absolute Error (A E) = 19.36

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
NiO	107.18	75	-32.18
NiH	97.49	85.6	-11.89
NiF_2	-53.06	-77.8	-24.74
NiCl	45.80	41.7	-4.10
$NiCl_2$	8.34	-17.4	-25.74
NiCO	112.08	35.1	-76.98

Mean Error (M E) = -29.27
Absolute Error (A E) = 29.27

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
NiO	69.32	75	5.68
NiH	93.73	85.6	-8.13
NiF_2	-65.36	-77.8	-12.44
NiCl	42.41	41.7	-0.71
$NiCl_2$	-9.01	-17.4	-8.39
NiCO	57.13	35.1	-22.03

Mean Error (M E) = -7.67
Absolute Error (A E) = 9.56

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
NiO	87.64	75	-12.64
NiH	94.12	85.6	-8.52
NiF_2	-43.82	-77.8	-33.98
NiCl	44.49	41.7	-2.79
$NiCl_2$	2.98	-17.4	-20.38
NiCO	71.87	35.1	-36.77

Mean Error (M E) = -19.18
Absolute Error (A E) = 19.18

M06-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
NiO	116.15	75	-41.15
NiH	101.97	85.6	-16.37
NiF_2	-39.78	-77.8	-38.02
NiCl	46.41	41.7	-4.71
$NiCl_2$	9.04	-17.4	-26.44
NiCO	115.22	35.1	-80.12

Mean Error (M E) = -34.47
Absolute Error (A E) = 34.47

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
NiO	150.45	75	-75.45
NiH	111.96	85.6	-26.36
NiF_2	-30.39	-77.8	-47.41
NiCl	51.89	41.7	-10.19
$NiCl_2$	50.28	-17.4	-67.68
NiCO	133.79	35.1	-98.69

Mean Error (M E) = -54.30
Absolute Error (A E) = 54.30

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
NiO	100.25	75	-25.25
NiH	90.56	85.6	-4.96
NiF_2	-40.75	-77.8	-32.05
NiCl	42.96	41.7	-1.26
$NiCl_2$	20.46	-17.4	-37.86

Mean Error (M E) = -19.68
Absolute Error (A E) = 19.68

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
NiO	99.49	75	-24.49
NiH	91.22	85.6	-5.62
NiF_2	-61.79	-77.8	-11.01
NiCl	39.32	41.7	2.38
$NiCl_2$	1.53	-17.4	-18.93

Mean Error (M E) = -11.53
Absolute Error (A E) = 12.49

Cu-Complexes

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Cu2	115.20	113.8	-1.40
CuCl	26.14	19.3	-6.84
CuF	9.33	-3.2	-12.53
CuF_2	-27.39	-66	-38.61
CuO	85.22	76.5	-8.72
CuS	87.09	75.1	-11.99

Mean Error (M E) = -13.35
Absolute Error (A E) = 13.35

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Cu2	110.12	113.8	3.68
CuCl	24.37	19.3	-5.07
CuF	8.14	-3.2	-11.34
CuF_2	-30.39	-66	-35.61
CuO	84.14	76.5	-7.64
CuS	87.33	75.1	-12.23

Mean Error (M E) = -11.37
Absolute Error (A E) = 12.60

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Cu2	101.09	113.8	12.71
CuCl	19.70	19.3	-0.40
CuF	0.17	-3.2	-3.37
CuF_2	-53.05	-66	-12.95
CuO	71.49	76.5	5.01
CuS	73.81	75.1	1.29

Mean Error (M E) = 0.38
Absolute Error (A E) = 5.96

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Cu2	109.32	113.8	4.48
CuCl	23.30	19.3	-4.00
CuF	10.44	-3.2	-13.64
CuF_2	-26.95	-66	-39.05
CuO	84.65	76.5	-8.15
CuS	82.86	75.1	-7.76

Mean Error (M E) = -11.35
Absolute Error (A E) = 12.85

M06-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Cu2	118.90	113.8	-5.10
CuCl	24.47	19.3	-5.17
CuF	13.70	-3.2	-16.90
CuF_2	-20.93	-66	-45.07
CuO	89.02	76.5	-12.52
CuS	93.28	75.1	-18.18

Mean Error (M E) = -17.16
Absolute Error (A E) = 17.16

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Cu2	55.18	113.8	58.62
CuCl	-14.14	19.3	33.44
CuF	-17.93	-3.2	14.73
CuF_2	-60.16	-66	-5.84
CuO	59.19	76.5	17.31
CuS	64.03	75.1	11.07

Mean Error (M E) = 21.56
Absolute Error (A E) = 23.50

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Cu2	114.35	113.8	-0.55
CuCl	21.01	19.3	-1.71
CuF	12.27	-3.2	-15.47
CuF_2	-21.48	-66	-44.52
CuO	84.01	76.5	-7.51
CuS	94.65	75.1	-19.55

Mean Error (M E) = -14.89
Absolute Error (A E) = 14.89

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Cu2	115.47	113.8	-1.66
CuCl	18.44	19.3	0.86
CuF	3.13	-3.2	-6.33
CuF_2	-53.82	-66	-12.18
CuO	81.86	76.5	-5.36
CuS	90.82	75.1	-15.72

Mean Error (M E) = -6.73
Absolute Error (A E) = 7.02

Zn-Complexes

M05

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Zn_2	60.37	57.7	-2.67
$ZnCH_3$	-98.29	26	124.29
$ZnCl_2$	-45.93	-63.5	-17.57
ZnF_2	-104.52	-118.9	-14.38
ZnH	68.51	62.9	-5.61
ZnO	76.21	52.8	-23.41

Mean Error (M E) = 10.11
Absolute Error (A E) = 31.32

M05-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Zn_2	61.38	57.7	-3.68
$ZnCH_3$	-92.99	26	118.99
$ZnCl_2$	-41.99	-63.5	-21.51
ZnF_2	-100.47	-118.9	-18.43
ZnH	70.35	62.9	-7.45
ZnO	70.82	52.8	-18.02

Mean Error (M E) = 8.32
Absolute Error (A E) = 49.9

M06-L

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Zn_2	60.11	57.7	-2.41
$ZnCH_3$	-93.68	26	119.68
$ZnCl_2$	-47.47	-63.5	-16.03
ZnF_2	-107.11	-118.9	-11.79
ZnH	68.52	62.9	-5.62
ZnO	63.91	52.8	-11.11

Mean Error (M E) = 12.12
Absolute Error (A E) = 27.77

M06

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Zn_2	58.41	57.7	-0.71
$ZnCH_3$	-94.37	26	120.37
$ZnCl_2$	-46.54	-63.5	-16.96
ZnF_2	-96.29	-118.9	-22.61
ZnH	71.15	62.9	-8.25
ZnO	72.28	52.8	-19.48

Mean Error (M E) = 8.73
Absolute Error (A E) = 31.40

M06-2X

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Zn_2	61.41	57.7	-3.71
$ZnCH_3$	-98.31	26	124.31
$ZnCl_2$	-51.92	-63.5	-11.58
ZnF_2	-98.84	-118.9	-20.06
ZnH	65.30	62.9	-2.40
ZnO	65.09	52.8	-12.29

Mean Error (M E) = 12.38
Absolute Error (A E) = 29.06

M06-HF

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Zn_2	61.70	57.7	-4.00
$ZnCH_3$	-111.41	26	137.41
$ZnCl_2$	-65.37	-63.5	1.87
ZnF_2	-100.82	-118.9	-18.08
ZnH	51.59	62.9	11.31
ZnO	55.89	52.8	-3.09

Mean Error (M E) = 20.90
Absolute Error (A E) = 29.29

M08-SO

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Zn_2	56.70	57.7	1.00
$ZnCH_3$	-146.55	26	172.55
$ZnCl_2$	-55.21	-63.5	-8.29
ZnF_2	-102.23	-118.9	-16.67
ZnH	57.35	62.9	5.55
ZnO	62.10	52.8	-9.30

Mean Error (M E) = 24.15
Absolute Error (A E) = 35.56

M08-HX

Molecule	HOF(theo)	HOF(expt)	Error(expt–theo)
Zn_2	58.03	57.7	-0.33
$ZnCH_3$	-148.22	26	174.22
$ZnCl_2$	-61.80	-63.5	-1.70
ZnF_2	-121.61	-118.9	2.71
ZnH	55.11	62.9	7.79
ZnO	59.77	52.8	-6.97

Mean Error (M E) = 29.29
Absolute Error (A E) = 32.29

Table 5: The IP values of the 47 TM complexes in 6 different M0X functionals with LANL2DZ basis set along with their experimental and the respective error (experiment–theory) values are depicted in the following group of tables. In these following tables the columns heading neural and cation represent the zero point corrected energy of these TM complexes of these states respectively. The multiplicities (M) of these neutral and cationic states are shown in the bracket. The neutral and the cationic energy of a molecule are expressed in a.u., whereas the errors are expressed in eV.

Ti-Series

M05

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
TiS	–68.06213(3)	–67.77894(2)	7.71/7.10	–0.61
TiF_2	–257.76095(3)	–257.26933(4)	13.38/12.20	–1.18
TiO	–133.18073(3)	–132.94747(2)	6.35/6.82	0.47
TiH	–58.46101(2)	–58.23630(3)	6.15/6.00	–0.15
TiF_3	–357.71429(2)	–357.34169(1)	10.14/10.50	0.36

Mean Error (M E) = –0.348
Absolute Error (A E) = 0.680

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
TiS	–68.04347(3)	–67.72918(2)	8.55/7.10	–1.45
TiF_2	–257.78965(3)	–257.36568(2)	11.54/12.20	0.66
TiO	–133.17410(3)	–132.84271(2)	9.02/6.82	–2.20
TiH	–58.46508(4)	–58.23916(3)	6.15/6.00	–0.15
TiF_3	–357.73983(2)	–357.31342(1)	11.60/10.50	–1.10

Mean Error (M E) = –0.848

Absolute Error (A E) = 1.112

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
TiS	–68.17238(3)	–67.92358(2)	6.77/7.10	0.33
TiF_2	–257.85950(3)	–257.40021(4)	12.14/12.20	0.06
TiO	–133.28499(3)	–133.05625(2)	6.22/6.82	0.60
TiH	–58.54990(2)	–58.31764(3)	6.33/6.00	–0.33
TiF_3	–357.84531(2)	–357.49433(1)	9.55/10.50	0.95

Mean Error (M E) = 0.322
Absolute Error (A E) = 0.454

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
TiS	–68.09658(3)	–67.81250(2)	7.73/7.10	–0.63
TiF_2	–257.76899(3)	–257.30774(4)	12.55/12.20	–0.35
TiO	–133.20142(3)	–132.96337(2)	6.48/6.82	0.34
TiH	–58.50154(2)	–58.25807(3)	6.63/6.00	–0.63
TiF_3	–357.71623(2)	–357.34856(1)	10.01/10.50	0.49

Mean Error (M E) = –0.156
Absolute Error (A E) = 0.488

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
TiS	–68.03129(3)	–67.72224(2)	8.41/7.10	–1.31
TiF_2	–257.73941(3)	–257.31580(2)	11.53/12.20	0.67
TiO	–133.158801(3)	–132.82922(2)	8.97/6.82	–2.15
TiH	–58.46698(4)	–58.18975(3)	7.54/6.00	–1.54
TiF_3	–357.66313(2)	–357.24670(1)	11.33/10.50	–0.83

Mean Error (M E) = –1.032
Absolute Error (A E) = 1.30

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
TiS	–67.96414(3)	–67.64195(4)	8.76/7.10	–1.66
TiF_2	–257.69695(3)	–257.25506(2)	12.03/12.20	0.17
TiO	–133.09595(3)	–132.75148(2)	9.37/6.82	–2.55
TiH	–58.44952(2)	–58.19113(3)	7.03/6.00	–1.03
TiF_3	–357.60408(2)	–357.12900(1)	12.93/10.50	–2.43

Mean Error (M E) = –1.50
Absolute Error (A E) = 1.568

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
TiS	-67.99357 (3)	-67.68630 (2)	8.36/7.10	-1.26
TiF_2	-257.66622 (3)	-257.31846 (2)	9.46/12.20	2.74
TiO	-133.08429 (3)	-132.82884(2)	6.95/6.82	-0.13
TiH	-58.42186 (2)	-58.17636 (3)	6.68/6.00	-0.68
TiF_3	-357.54128 (2)	-357.15061 (1)	10.63/10.50	-0.13

Mean Error (M E) = 0.108
Absolute Error (A E) = 0.988

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
TiS	-68.0594(3)	-67.78051 (2)	7.59/7.10	-0.49
TiF_2	-257.75535 (3)	-257.41704(2)	9.21/12.20	2.99
TiO	-133.15922 (3)	-132.90480 (2)	6.92/6.82	-0.10
TiH	-58.49120 (4)	-58.24747(3)	6.63/6.00	-0.63
TiF_3	-357.65811 (2)	-357.25556(1)	10.95/10.50	-0.45

Mean Error (M E) = 0.264
Absolute Error (A E) = 0.932

V-Series
M05

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
V2	–142.39054(3)	–142.18723(4)	5.36/6.36	0.83
VS	–81.31479(4)	–81.01502(3)	8.16/8.40	0.24
VN	–125.87598(3)	–125.58023(4)	8.05/8.00	–0.05
VO	–146.42902(4)	–146.18137(3)	6.74/7.24	0.50

Mean Error (M E) = 0.380
Absolute Error (A E) = 0.405

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
V2	–142.35868(7)	–142.1310(4)	6.19/6.36	0.17
VS	–81.28662(4)	–80.94635(3)	9.26/8.40	–0.86
VN	–125.84760(3)	–125.59635(2)	6.84/8.00	1.16
VO	–146.40192(4)	–146.07208(3)	8.98/7.24	–1.74

Mean Error (M E) = –0.318
Absolute Error (A E) = 0.983

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
V2	–142.56242(3)	–142.33801(4)	6.11/6.36	0.25
VS	–81.41437(4)	–81.13793(3)	7.52/8.40	0.88
VN	–125.98490(3)	–125.73963(2)	6.67/8.00	1.33
VO	–146.52263(4)	–146.26489(3)	7.01/7.24	0.23

Mean Error (M E) = 0.673
Absolute Error (A E) = 0.673

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
V2	–142.47364(3)	–142.23179(4)	6.58/6.36	0.58
VS	–81.35009(4)	–81.03831(3)	8.48/8.40	–0.08
VN	–125.89482(3)	–125.64537(2)	6.79/8.00	–0.27
VO	–146.45132(4)	–146.19158(3)	7.07/7.24	0.17

Mean Error (M E) = 0.10
Absolute Error (A E) = 0.275

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
V2	–142.29239(7)	–142.07824(8)	5.82/6.36	0.54
VS	–81.28589(4)	–80.97817(3)	8.37/8.40	0.03
VN	–125.84787(3)	–125.58766(2)	7.08/8.00	0.92
VO	–146.39945(4)	–146.07116(1)	8.93/7.24	–1.69

Mean Error (M E) = – 0.05
Absolute Error (A E) = 0.795

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
V2	–142.15559(7)	–141.95538(8)	5.45/6.36	0.91
VS	–81.22480(4)	–80.90518(5)	8.70/8.40	–0.30
VN	–125.78190(3)	–125.46374(2)	8.65/8.00	–0.65
VO	–146.33410(4)	–145.99436(3)	9.24/7.24	–2.00

Mean Error (M E) = –0.51
Absolute Error (A E) = 0.965

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
V2	-142.16396(1)	-141.93424(4)	6.25/6.36	0.11
VS	-81.21290(4)	-80.94070(3)	7.41/8.40	0.99
VN	-125.76396(3)	-125.45015(4)	8.54/8.00	-0.54
VO	-146.38493(4)	-146.10981(3)	7.49/7.24	-0.25

Mean Error (M E) = 0.078
Absolute Error (A E) = 0.473

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
V2	-142.21024(1)	-142.0088(4)	5.48/6.36	0.88
VS	-81.27824(4)	-80.98257(3)	8.05/8.40	0.35
VN	-125.80643(3)	-125.51519(4)	7.92/8.00	0.08
VO	-146.32273(4)	-146.04761(3)	7.49/7.24	-0.25

Mean Error (M E) = 0.265
Absolute Error (A E) = 0.39

Cr-Series

M05

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CrCl	–101.20560(6)	–100.89935(5)	8.33/8.50	0.17
$CrCl_2$	–116.17603(5)	–115.77705(4)	10.86/9.90	–0.96
CrF	–186.10261(6)	–185.81227(5)	7.90/9.30	1.40
CrO	–161.39602(5)	–161.11832(4)	7.56/8.16	0.60
CrO_2	–236.61280(3)	–236.22768(2)	10.48/10.30	–0.18
CrOH	–162.02722(6)	–161.75490(5)	7.41/7.54	0.13

Mean Error (M E) = 0.193
Absolute Error (A E) = 0.573

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CrCl	–101.19015(6)	–100.82929(5)	9.82/8.50	–1.32
$CrCl_2$	–116.12818(5)	–115.70593(4)	11.49/9.90	–1.59
CrF	–186.09065(6)	–185.76705(5)	8.81/9.30	0.49
CrO	–161.36900(5)	–161.06997(4)	8.14/8.16	0.02
CrO_2	–236.52012(5)	–236.05300(2)	12.71/10.30	–2.41
CrOH	–162.02360(6)	–161.74374(5)	7.62/7.54	–0.08

Mean Error (M E) = –0.815

Absolute Error (A E) = 0.985

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CrCl	–101.28768(6)	–100.97753(5)	8.44/8.50	0.06
$CrCl_2$	–116.30232(5)	–115.94268(4)	9.79/9.90	0.11
CrF	–186.16204(6)	–185.87004(5)	7.95/9.30	1.35
CrO	–161.47803(5)	–161.19095(4)	7.81/8.16	0.35
CrO_2	–236.73353(3)	–236.32495(2)	11.19/10.30	–0.89
CrOH	–162.09710(6)	–161.82976(5)	7.28/7.54	0.26

Mean Error (M E) = 0.207
Absolute Error (A E) = 0.503

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CrCl	–101.24026(6)	–100.91847(5)	8.76/8.50	–0.26
$CrCl_2$	–116.22236(5)	–115.81287(4)	11.14/9.90	–1.24
CrF	–186.11430(6)	–185.81054(5)	8.27/9.30	1.03
CrO	–161.41191(5)	–161.11840(4)	7.99/8.16	0.17
CrO_2	–236.61604(3)	–236.22574(2)	10.62/10.30	–0.32
CrOH	–162.04534(6)	–161.76330(5)	7.68/7.54	–0.14

Mean Error (M E) = –0.127
Absolute Error (A E) = 0.527

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CrCl	–101.20783(6)	–100.83224(5)	10.22/8.50	–1.72
$CrCl_2$	–116.12464(5)	–115.75010(4)	10.19/9.90	–0.29
CrF	–186.09718(6)	–185.76146(5)	9.14/9.30	0.16
CrO	–161.38083(5)	–161.07764(4)	8.25/8.16	–0.09
CrO_2	–236.50468(5)	–236.05836(6)	12.14/10.30	–1.84
CrOH	–162.03302(6)	–161.74384(5)	7.87/7.54	–0.33

Mean Error (M E) = –0.685
Absolute Error (A E) = 0.738

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CrCl	–101.14248(6)	–100.76304(5)	9.72/8.50	–1.18
$CrCl_2$	–116.06271(5)	–115.61589(6)	12.15/9.90	–2.25
CrF	–186.04902(6)	–185.72680(5)	8.77/9.30	0.53
CrO	–161.32715(5)	–160.99854(6)	8.94/8.16	–0.78
CrO_2	–236.42523(5)	–235.99254(6)	11.77/10.30	–1.47
CrOH	–161.98755(6)	–161.70440(5)	7.71/7.54	–0.17

Mean Error (M E) = –1.128

Absolute Error (A E) = 1.063

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CrCl	-101.11260(6)	-100.77343(5)	9.23/8.50	-0.73
$CrCl_2$	-116.07634(5)	-115.64768(4)	11.66/9.90	-1.76
CrF	-185.98527(6)	-185.67754(5)	8.37/9.30	0.93
CrO	-161.25885(5)	-160.96230(4)	8.07/8.16	0.09
CrO_2	-236.37573(5)	-235.94612(8)	11.69/10.30	-1.39
CrOH	-161.90945(6)	-161.63013(5)	7.6/7.54	-0.06

Mean Error (M E) = –0.487
Absolute Error (A E) = 0.827

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CrCl	-101.18510(6)	-100.85293(5)	9.04/8.50	-0.54
$CrCl_2$	-116.17204(5)	-115.73415(4)	11.92/9.90	-2.02
CrF	-186.06204(6)	-185.76687(5)	8.03/9.30	1.27
CrO	-161.31378(5)	-161.04311(4)	7.37/8.16	0.79
CrO_2	-236.45201(5)	-236.033(8)	11.4/10.30	-1.10
CrOH	-161.99146(6)	-161.72585(5)	7.52/7.54	0.02

Mean Error (M E) = –0.263
Absolute Error (A E) = 0.957

Mn-Series

M05

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
$MnCl_2$	–133.84734(6)	–133.44409(5)	10.97/11.03	0.06
MnCl	–118.84234(5)	–118.55901(6)	7.71/8.50	0.79
MnF_2	–303.65422(6)	–303.21135(5)	12.05/11.38	–0.67
MnH	–104.39165(5)	–104.15779(6)	6.36/7.80	1.44
MnO	–179.03790(6)	–178.72627(5)	8.48/8.65	0.17
MnF	–203.72374(7)	–203.46117(6)	7.15/8.51	1.36

Mean Error (M E) = 0.525
Absolute Error (A E) = 0.748

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
$MnCl_2$	–133.82815(6)	–133.40428(5)	11.53/11.03	–0.50
MnCl	–118.80858(5)	–118.51330(6)	8.04/8.50	0.46
MnF_2	–303.65641(6)	–303.17590(5)	13.08/11.38	–1.70
MnH	–104.37663(7)	–104.11759(6)	7.05/7.80	0.75
MnO	–178.99462(6)	–178.62020(5)	10.18/8.65	–1.53
MnF	–203.71100(7)	–203.42537(6)	7.77/8.51	0.74

Mean Error (M E) = –0.297
Absolute Error (A E) = 0.947

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
$MnCl_2$	–133.96468(6)	–133.56618(5)	10.84/11.03	0.19
MnCl	–118.79842(5)	–118.45070(8)	9.46/8.50	0.96
MnF_2	–303.72264(6)	–303.31761(5)	11.02/11.38	0.36
MnH	–104.45650(5)	–104.18610(6)	7.36/7.80	0.44
MnO	–179.10353(6)	–178.78553(5)	8.65/8.65	0.00
MnF	–203.77634(5)	–203.49784(6)	7.58/8.51	–0.07

Mean Error (M E) = 0.313
Absolute Error (A E) = 0.337

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
$MnCl_2$	–133.88871(6)	–133.47583(5)	11.24/11.30	–0.21
MnCl	–118.86434(5)	–118.57298(6)	7.93/8.50	0.57
MnF_2	–303.64977(6)	–303.19774(5)	12.30/11.38	–0.92
MnH	–104.40442(7)	–104.15965(6)	6.66/7.80	1.14
MnO	–179.04459(6)	–178.72451(5)	8.71/8.65	–0.06
MnF	–203.72979(7)	–203.45158(6)	7.57/8.51	0.94

Mean Error (M E) = 0.243
Absolute Error (A E) = 0.640

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
$MnCl_2$	–133.84101(6)	–133.41339(5)	11.64/11.03	–0.61
MnCl	–118.83792(5)	–118.53510(6)	8.24/8.50	0.26
MnF_2	–303.64780(6)	–303.16924(5)	13.02/11.38	–1.64
MnH	–104.41349(7)	–104.15099(6)	7.14/7.80	0.66
MnO	–179.01711(6)	–178.71127(5)	8.32/8.65	0.33
MnF	–203.73139(7)	–203.43479(6)	8.07/8.51	0.44

Mean Error (M E) = –0.093
Absolute Error (A E) = 0.657

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
$MnCl_2$	–133.76475(6)	–133.31654(5)	12.20/11.03	–1.17
MnCl	–118.80056(5)	–118.47298(6)	8.90/8.50	–0.40
MnF_2	–303.60698(6)	–303.09217(5)	14.01/11.38	–2.63
MnH	–104.37118(7)	–104.11075(6)	7.09/7.80	0.71
MnO	–178.95652(4)	–178.66967(5)	7.81/8.65	–0.16
MnF	–203.50530(7)	–203.21518(8)	7.89/8.51	–0.62

Mean Error (M E) = –0.712
Absolute Error (A E) = 0.948

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
$MnCl_2$	-133.73428(6)	-133.28663(7)	12.18/11.03	-1.15
MnCl	-118.71340(7)	-118.42489(6)	7.85/8.50	0.65
MnF_2	-303.49917(6)	-303.04255(5)	12.43/11.38	-1.05
MnH	-104.27061(5)	-104.03271(6)	6.47/7.80	1.33
MnO	-178.81785(8)	-178.53766(7)	7.62/8.65	1.03
MnF	-203.59679(7)	-203.30549(6)	7.93/8.51	0.58

Mean Error (M E) = 0.232
Absolute Error (A E) = 0.965

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
$MnCl_2$	-133.82113(6)	-133.39587(5)	11.57/11.03	-0.54
MnCl	-118.78722(7)	-118.49836(6)	7.86/8.50	0.64
MnF_2	-303.59147(6)	-303.13692(5)	12.37/11.38	-0.99
MnH	-104.35302(5)	-104.09524(6)	7.01/7.80	0.79
MnO	-178.89544(8)	-178.6118(7)	7.72/8.65	0.93
MnF	-203.67416(7)	-203.38442(6)	7.88/8.51	0.63

Mean Error (M E) = 0.243
Absolute Error (A E) = 0.753

Fe-Series

M05

Molecule	Neutral(M)	Cation(M)	I.P.(Theo)/I.P.(Expt)	Error(Expt–Theo)
FeF_2	–323.17464(5)	–322.7560(6)	11.39/11.30	–0.09
$Fe(CO)_2$	–349.92686(3)	–349.64031(4)	7.80/6.68	–1.12
Fe(CO)	–236.60356(3)	–236.36637(4)	6.45/6.66	0.21
FeCl	–138.33650(4)	–138.06096(5)	7.50/8.08	0.58
FeO	–198.55624(5)	–198.25594(6)	8.17/8.90	0.73
$FeCl_2$	–153.36239(5)	–152.97253(6)	10.61/10.63	0.02

Mean Error (M E) = 0.055
Absolute Error (A E) = 0.458

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
FeF_2	–323.15660(5)	–322.68585(6)	12.81/11.30	–1.51
$Fe(CO)_2$	–349.88156(3)	–349.648123(4)	6.35/6.68	0.38
Fe(CO)	–236.55729(3)	–236.32935(4)	6.16/6.66	0.50
FeCl	–138.29076(6)	–137.99462(5)	8.06/8.08	0.02
FeO	–198.49805(6)	–198.17188(6)	8.88/8.90	0.02
$FeCl_2$	–153.32240(5)	–152.88989(4)	11.76/10.63	–1.13

Mean Error (M E) = –0.287
Absolute Error (A E) = 0.593

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
FeF_2	–323.22768(5)	–322.81445(6)	11.25/11.30	0.05
$Fe(CO)_2$	–350.03896(3)	–349.77287(4)	7.25/6.68	–0.56
Fe(CO)	–236.69488(3)	–236.43441(4)	7.09/6.66	–0.43
FeCl	–138.41747(4)	–138.11276(5)	8.29/8.08	–0.21
FeO	–198.61331(5)	–198.29543(6)	8.65/8.90	0.25
$FeCl_2$	–153.46522(5)	–153.07825(6)	10.53/10.63	0.10

Mean Error (M E) = –0.133
Absolute Error (A E) = –0.267

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
FeF_2	–323.14989(5)	–322.72976(6)	11.43/11.30	–0.13
$Fe(CO)_2$	–349.92134(3)	–349.62914(4)	7.95/6.68	–1.27
Fe(CO)	–236.59464(3)	–236.34582(4)	6.77/6.66	–0.11
FeCl	–138.33712(6)	–138.05367(5)	7.71/8.08	0.37
FeO	–198.54425(5)	–198.23517(6)	8.41/8.90	0.49
$FeCl_2$	–153.38501(5)	–152.99294(6)	10.67/10.63	–0.04

Mean Error (M E) = –0.115
Absolute Error (A E) = 0.402

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
FeF_2	–323.14347(5)	–322.68328(6)	12.52/11.30	–1.22
$Fe(CO)_2$	–349.86512(3)	–349.63597(4)	6.24/6.68	0.44
Fe(CO)	–236.56190(3)	–236.331979(4)	6.26/6.66	0.40
FeCl	–138.31843(6)	–138.01244(5)	8.33/ 8.08	0.25
FeO	–198.51263(5)	–198.19274(6)	8.71/8.90	0.19
$FeCl_2$	–153.33025(5)	–152.89777(6)	11.77/10.63	–1.14

Mean Error (M E) = –0.18
Absolute Error (A E) = 0.607

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
FeF_2	–323.10426(5)	–322.59831(6)	13.77/11.30	–2.47
$Fe(CO)_2$	–349.81303(5)	–349.59754(4)	5.86/6.68	082
Fe(CO)	–236.50153(7)	–236.31722(4)	5.02/6.66	1.64
FeCl	–138.26482(6)	–137.95164(5)	8.52/8.08	–0.44
FeO	–198.43447(5)	–198.13905(6)	8.04/8.90	0.86
$FeCl_2$	–153.25359(5)	–152.76533(6)	13.29/10.63	–2.66

Mean Error (M E) = –0.375
Absolute Error (A E) = 1.482

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
FeF_2	-322.98566(5)	-322.32397(8)	18.01/11.30	-6.71
$Fe(CO)_2$	-349.60638(1)	-349.37589(2)	6.27/6.68	0.41
Fe(CO)	-236.34235(1)	-236.18822(4)	4.19/6.66	2.47
FeCl	-138.21711(4)	-137.89732(5)	8.70/8.08	-0.62
FeO	-198.35345(3)	-197.95282(2)	10.90/8.90	-2.00
$FeCl_2$	-153.21581(5)	-152.69099(2)	14.28/10.63	-3.65

Mean Error (M E) = 1.683
Absolute Error (A E) = 2.643

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
FeF_2	-323.06130(5)	-322.39615(8)	18.10/11.30	-6.80
$Fe(CO)_2$	-349.67467(1)	-349.49725(2)	4.83/6.68	1.85
Fe(CO)	-236.41939(3)	-236.26486(4)	4.21/6.66	2.45
FeCl	-138.24618(6)	-137.95115(5)	8.03/8.08	0.05
FeO	-198.39894(3)	-197.98698(2)	11.21/8.90	-2.31
$FeCl_2$	-153.27947(5)	-152.86001(6)	11.41/10.63	-0.78

Mean Error (M E) = –0.923
Absolute Error (A E) = 2.373

Co-Complexes

M05

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CoH	–145.60625(3)	–145.29226(2)	8.54/7.86	–0.68
CoO	–220.22177(4)	–219.89630(5)	8.86/8.90	0.04
CoCl	–160.00731(3)	–159.70661(4)	8.18/8.71	0.53
$CoCl_2$	–175.01184(4)	–174.60302(5)	11.12/10.75	–0.37

Mean Error (M E) = –0.120
Absolute Error (A E) = 0.405

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CoH	–145.53921(3)	–145.22497(4)	8.55/7.86	–0.69
CoO	–220.12058(4)	–219.80796(5)	8.51/8.90	0.39
CoCl	–159.95430(3)	–159.59780(4)	9.71/8.71	–1.00
$CoCl_2$	–174.92784(4)	–174.50328(5)	11.55/10.75	–0.80

Mean Error (M E) = –0.525

Absolute Error (A E) = 0.720

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CoH	–145.61831(3)	–145.29588(2)	8.77/7.86	–0.91
CoO	–220.22529(4)	–219.92950(5)	8.05/8.90	0.85
CoCl	–160.05764(3)	–159.73119(4)	8.88/8.71	–0.17
$CoCl_2$	–175.08236(4)	–174.70091(5)	10.38/10.75	0.37

Mean Error (M E) = 0.035
Absolute Error (A E) = 0.575

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CoH	–145.58906(3)	–145.27053(4)	8.67/7.86	–0.81
CoO	–220.18524(4)	–219.85295(5)	9.04/8.90	–0.14
CoCl	–159.99046(3)	–159.67737(4)	8.52/8.71	0.19
$CoCl_2$	–175.01157(4)	–174.60055(5)	11.18/10.75	–0.43

Mean Error (M E) = –0.298
Absolute Error (A E) = 0.393

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CoH	–145.57214(3)	–145.25930(4)	8.51/7.86	–0.65
CoO	–220.14113(4)	–219.82586(5)	8.58/8.90	0.32
CoCl	–159.97596(3)	–159.62490(4)	9.55/8.71	–0.84
$CoCl_2$	–174.94551(4)	–174.51315(5)	11.77/10.75	–1.02

Mean Error (M E) = –0.548
Absolute Error (A E) = 0.708

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CoH	–145.53179(2)	–145.23423(4)	8.10/7.86	–0.24
CoO	–220.06575(4)	–219.78416(5)	7.66/8.90	1.24
CoCl	–159.92249(3)	–159.56212(4)	9.81/8.71	–1.10
$CoCl_2$	–174.86898(4)	–174.38120(5)	13.27/10.75	–2.52

Mean Error (M E) = 0.655
Absolute Error (A E) = 1.275

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CoH	-145.45154(3)	-145.15417(4)	8.09/7.86	-0.23
CoO	-220.01236(4)	-219.63150(3)	10.36/8.90	-1.46
CoCl	-159.85585(3)	-159.53574(4)	8.71/8.71	0.00
$CoCl_2$	-174.85906(4)	-174.40189(3)	12.44/10.75	-1.69

Mean Error (M E) = –0.845
Absolute Error (A E) = 0.845

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
CoH	-145.45880(3)	-145.16520(4)	7.99/7.86	-0.13
CoO	-220.01655(4)	219.63180(3)	10.47/8.90	-1.57
CoCl	-159.88413(3)	-159.54137(4)	9.33/8.71	-0.62
$CoCl_2$	-174.87904(4)	-174.44221(3)	11.89/10.75	-1.14

Mean Error (M E) = –0.865
Absolute Error (A E) = 0.865

Ni-Series

M05

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
NiO	–244.47808(3)	–244.16127(4)	8.62/9.50	0.88
NiH	–169.8941792)	–169.56710(3)	8.90/8.50	–0.40
NiF_2	–369.03858(3)	–368.61511(4)	11.52/11.50	–0.02
NiCl	–184.29184(2)	–183.85512(3)	11.02/9.28	–1.74
$NiCl_2$	–199.24630(3)	–198.82214(4)	11.54/11.24	–0.30
NiCO	–282.59610(1)	–282.29501(2)	8.19/7.30	0.89

Mean Error (M E) = –0.115
Absolute Error (A E) = 0.705

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
NiO	–244.36405(3)	–244.01205(4)	9.58/9.50	–0.08
NiH	–169.79136(2)	–169.46740(3)	8.82/8.50	–0.32
NiF_2	–368.99062(3)	–368.47946(4)	13.91/11.50	–2.41
NiCl	–184.20161(2)	–183.75973(3)	12.02/9.28	–2.74
$NiCl_2$	–199.16772(3)	–198.73267(4)	11.84/11.24	–0.60
NiCO	–282.48160(1)	–282.22624(2)	6.94/7.30	0.36

Mean Error (M E) = –0.965
Absolute Error (A E) = 1.085

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
NiO	–244.46808(3)	–244.13818(4)	8.98/9.50	0.52
NiH	–169.84639(2)	–169.53818(3)	8.39/8.50	0.11
NiF_2	–369.04480	–368.61324(4)	11.74/11.50	–0.24
NiCl	–184.28120(2)	–183.94821(3)	9.06/9.28	0.22
$NiCl_2$	–199.29999(3)	–198.88208(4)	11.37/11.24	–0.13
NiCO	–282.60548	–282.30513(2)	8.17/7.30	–0.87

Mean Error (M E) = –0.065
Absolute Error (A E) = 0.552

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
NiO	–244.42051(3)	–244.08761(4)	9.06/9.50	0.44
NiH	–169.84758(2)	–169.51249(3)	9.12/8.50	–0.62
NiF_2	–368.97402(3)	–368.53409(4)	11.97/11.50	–0.47
NiCl	–184.25567(2)	–183.83903(1)	11.33/9.28	–2.05
$NiCl_2$	–199.22962(3)	–198.79485(4)	11.83/11.24	–0.59
NiCO	–282.54369(1)	–282.23473(2)	8.41/7.30	–1.11

Mean Error (M E) = –0.733
Absolute Error (A E) = 0.88

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
NiO	–244.38381(3)	–244.06510(4)	8.67/9.50	0.83
NiH	–169.83374(2)	–169.50897(3)	8.84/8.50	–0.34
NiF_2	–368.97930(3)	–368.47952(4)	13.60/11.50	–2.10
NiCl	–184.23247(2)	–183.78927(3)	12.06/9.28	–2.78
$NiCl_2$	–199.17932(3)	–198.73846(4)	12.00/11.24	–0.76
NiCO	–282.50018(1)	–282.24600(2)	6.92/7.30	0.38

Mean Error (M E) = –0.795
Absolute Error (A E) = 1.198

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
NiO	–244.30688(3)	–243.92367(4)	10.43/9.50	–0.93
NiH	–169.78455(2)	–169.45866(3)	8.87/8.50	–0.37
NiF_2	–368.94976(3)	–368.39010(4)	15.23/11.50	–3.73
NiCl	–184.17336(2)	–183.74873(3)	11.56/9.28	–2.28
$NiCl_2$	–199.04228(3)	–198.64213(4)	10.89/11.24	0.35
NiCO	–282.46233(3)	–282.20172(2)	7.09/7.30	0.21

Mean Error (M E) = – 1.125
Absolute Error (A E) = 1.312

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
NiO	-244.24743(3)	-243.92533(4)	8.76/9.50	0.74
NiH	-169.71266(2)	-169.38010(3)	9.05/8.50	-0.55
NiF_2	-368.83140(3)	-368.30351(2)	14.36/11.50	-2.86
NiCl	-184.11626(2)	-183.72908(3)	10.54/9.28	-1.26
$NiCl_2$	-199.04865(3)	-198.61061(4)	11.92/11.24	-0.68

Mean Error (M E) = –0.922
Absolute Error (A E) = 1.218

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
NiO	-244.25453(3)	-243.93265(4)	8.76/9.50	0.74
NiH	-169.69905(2)	-169.38188(3)	8.63/8.50	-0.13
NiF_2	-368.86150(3)	-368.30389(2)	15.17/11.50	-3.67
NiCl	-184.11985(2)	-183.75262(3)	9.99/9.28	-0.71
$NiCl_2$	-199.08872(3)	-198.61061(4)	13.01/11.24	-1.77

Mean Error (M E) = –1.108
Absolute Error (A E) = 1.404

Cu-Complexes

M05

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Cu2	–392.52365(1)	–392.24986(2)	7.45/7.90	0.45
CuCl	–211.20999(1)	–210.84353(2)	9.97/10.70	0.73
CuF	–296.08868(1)	–295.70459(2)	10.45/10.90	0.45
CuF_2	–395.89882(2)	–395.42547(3)	12.88/13.18	0.30

Mean Error (M E) = 0.483
Absolute Error (A E) = 0.483

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Cu2	–392.26378(1)	–391.98220(2)	7.66/7.90	0.24
CuCl	–211.08707(1)	–210.71418(2)	10.15/10.70	0.55
CuF	–295.97569(1)	–295.57584(2)	10.88/10.90	0.02
CuF_2	–395.80827(2)	–395.28317(3)	14.29/13.18	–1.11

Mean Error (M E) = -0.075
Absolute Error (A E) = 0.48

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Cu2	–392.32527(1)	–392.04287(2)	7.69/7.90	0.21
CuCl	–211.14849(1)	–210.78163(2)	9.98/10.70	0.72
CuF	–296.00731(1)	–295.62593(2)	10.38/10.90	0.52
CuF_2	–395.85876(2)	–395.40228(3)	12.42/13.18	0.76

Mean Error (M E) = 0.553
Absolute Error (A E) = 0.553

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Cu2	–392.37541(1)	–392.08044(2)	8.03/7.90	–0.13
CuCl	–211.14535(1)	–210.76129(2)	10.45/10.70	0.25
CuF	–296.00093(1)	–295.60046(2)	10.90/10.90	0.00
CuF_2	–395.80561(2)	–395.31909(3)	13.24/13.18	–0.06

Mean Error (M E) = -0.015
Absolute Error (A E) = 0.11

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Cu2	–392.36500(1)	–392.08944(2)	7.50/7.90	0.40
CuCl	–211.12544(1)	–210.74606(2)	10.32/10.70	0.38
CuF	–296.00387(1)	–295.60496(2)	10.86/10.90	0.04
CuF_2	–395.80971(2)	–395.28820(3)	14.19/13.18	–1.01

Mean Error (M E) = -0.048
Absolute Error (A E) = 0.458

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Cu2	–392.22573(1)	–391.98291(2)	6.61/7.90	1.29
CuCl	– 211.04551(1)	–210.66928(2)	10.24/10.70	0.46
CuF	–295.94129(1)	–295.52292(2)	11.38/10.90	–0.48
CuF_2	–395.76656(2)	–395.17660(3)	16.05/13.18	–2.87

Mean Error (M E) = -0.4
Absolute Error (A E) = 1.275

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Cu2	-392.09953(1)	-391.82578(2)	7.45/7.90	0.45
CuCl	-211.00595(1)	-210.62906(2)	10.26/10.70	0.44
CuF	-295.86248(1)	-295.46030(2)	10.94/10.90	-0.04
CuF_2	-395.65778(2)	-395.20424(1)	12.34/13.18	0.84

Mean Error (M E) = 0.423
Absolute Error (A E) = 0.443

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Cu2	-391.99845(1)	-391.72784(2)	7.36/7.90	0.54
CuCl	-210.97084(1)	-210.13573(2)	22.72/10.70	-12.02
CuF	-295.83194(1)	-295.44143(2)	10.63/10.90	0.27
CuF_2	-395.66947(2)	-395.18926(1)	13.07/13.18	0.11

Mean Error (M E) = –2.775
Absolute Error (A E) = 3.235

Zn-Complexes

M05

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Zn_2	–131.48769(1)	–131.21171(2)	7.51/9.00	1.49
$ZnCH_3$	–105.51983(2)	–105.27486(1)	6.67/7.20	0.53
$ZnCl_2$	–95.66124(1)	–95.24782(2)	11.25/11.80	0.55
ZnF_2	–265.45820(1)	–264.98826(2)	12.79/13.91	1.12
ZnH	–66.25818(2)	–65.99196(1)	7.24/9.40	2.16
ZnO	–140.81694(1)	–140.51711(2)	8.16/9.34	1.18

Mean Error (M E) = 1.172
Absolute Error (A E) = 1.172

M05-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Zn_2	–130.68995(1)	–130.40313(2)	7.81/9.00	1.19
$ZnCH_3$	–105.14762(2)	–104.88942(1)	7.03/7.20	0.17
$ZnCl_2$	–95.27331(1)	–94.84012(2)	11.79/11.80	0.01
ZnF_2	–265.09180(1)	–264.58855(2)	13.69/13.91	0.22
ZnH	–65.85998(2)	–65.57990(1)	7.62/9.40	1.78
ZnO	–140.44756(1)	–140.12187(2)	8.86/9.34	0.48

Mean Error (M E) = 0.642
Absolute Error (A E) = 0.642

M06-L

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Zn_2	–130.20734(1)	–129.93107(2)	7.52/9.00	1.48
$ZnCH_3$	–104.91490(2)	–104.66198(1)	6.88/7.20	0.32
$ZnCl_2$	–95.10063(1)	–94.69195(2)	11.12/11.80	0.68
ZnF_2	–265.32264(1)	–264.79053(2)	14.48/13.91	–0.57
ZnH	–65.62252(2)	–65.35193(1)	7.63/9.40	1.77
ZnO	–140.21614(1)	–139.90115(2)	8.57/9.34	0.77

Mean Error (M E) = 0.742
Absolute Error (A E) = 0.932

M06

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Zn_2	–130.92934(1)	–130.63692(2)	7.96/9.00	1.24
$ZnCH_3$	–105.24085(2)	–104.98174(1)	7.05/7.20	0.15
$ZnCl_2$	–95.40075(1)	–94.97627(2)	11.55/11.80	0.25
ZnF_2	–265.14999(1)	–264.67371(2)	12.96/13.91	0.95
ZnH	–65.97630(2)	–65.69488(1)	7.66/9.40	1.74
ZnO	–140.53731(1)	–140.21115(2)	8.88/9.34	0.46

Mean Error (M E) = 0.798
Absolute Error (A E) = 0.798

M06-2X

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Zn_2	–130.86416(1)	–130.59157(2)	7.42/9.00	1.58
$ZnCH_3$	–105.22848(2)	–104.96699(1)	7.12/7.20	0.08
$ZnCl_2$	–95.33812(1)	–94.90339(2)	11.83/11.80	–0.03
ZnF_2	–265.13526(1)	–264.64046(2)	13.46/13.91	0.45
ZnH	–65.95377(2)	–65.66963(1)	7.73/9.40	1.67
ZnO	–140.52693(1)	–140.19692(2)	8.98/9.34	0.36

Mean Error (M E) = 0.685
Absolute Error (A E) = 0.695

M06-HF

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Zn_2	–131.20259(1)	–130.95452(2)	6.75/9.00	2.25
$ZnCH_3$	–105.41959(2)	–105.15215(1)	7.28/7.20	–0.08
$ZnCl_2$	–95.48692(1)	–95.03112(2)	12.40/11.80	–0.60
ZnF_2	–265.32264(1)	–264.79053(2)	14.48/13.91	–0.57
ZnH	–66.14115(2)	–65.85066(1)	7.91/9.40	1.49
ZnO	–140.71806(1)	–140.38462(2)	9.07/9.34	0.27

Mean Error (M E) = 0.46
Absolute Error (A E) = 0.877

M08-SO

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Zn_2	-130.90932(1)	-130.63109(2)	7.57/9.00	1.43
$ZnCH_3$	-105.24509(2)	-104.98641(1)	7.04/7.20	0.16
$ZnCl_2$	-95.38503(1)	-94.91956(2)	12.67/11.80	-0.87
ZnF_2	-265.14278(1)	-264.57646(2)	15.41/13.91	-1.50
ZnH	-65.97973(2)	-65.70251(1)	7.54/9.40	1.86
ZnO	-140.52146(3)	-140.19968(2)	8.76/9.34	0.58

Mean Error (M E) = 0.277
Absolute Error (A E) = 1.067

M08-HX

Molecule	Neutral(M)	Cation(M)	I.P(Theo)/I.P(Expt)	Error(Expt–Theo)
Zn_2	-130.01575(1)	-129.74383(2)	7.40/9.00	1.60
$ZnCH_3$	-104.82281(2)	-104.56793(1)	6.94/7.20	0.26
$ZnCl_2$	-94.96992(1)	-54.50502(2)	12.65/11.80	-0.85
ZnF_2	-264.73854(1)	-264.18503(2)	15.06/13.91	-1.15
ZnH	-65.53737(2)	-65.26244(1)	7.48/9.40	1.92
ZnO	-140.09833(3)	-139.78189(2)	8.61/9.34	0.73

Mean Error (M E) = 0.418
Absolute Error (A E) = 1.085