Supporting Information: Assessing the Calculation of Exchange Coupling Constants and Spin Crossover Gaps Using the Approximate Projection Model to Improve Density Functional Calculations

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Table S1: J-couplings calculated by B3LYP before and after geometry change made to binuclear transition metal compound 3, 6, 8, 9

Complex	Before	After	Experiment
3	-35.8	-32.6	-15.7
6	100.4	97.8	84
8	12.1	13.3	18.5
9	75.6[1]	71.3	54.4

1 Peralta, J. E.; Melo, J. I. J. Chem. Theory Comput. **2010**, 6, 1894-1899.

Table S2: maximum geometric parameter change from crystal structures to AP optimized structures

Geometric parameter/Complex	1	2	3	4	5	6	7	8	9
Bond length(Å)	1.25	0.19	0.26	0.35	0.04	0.10	0.30	0.07	0.35
Metal-involving bond length(Å)	0.03	0.08	0.26	0.05	0.04	0.10	0.12	0.07	0.09
Angles(°)	8.4	12.2	36.1	16.3	3.2	30.5	16.0	8.2	14.2
Metal-involving angles(°)	6.1	3.4	36.1	2.0	3.2	26.8	16.0	8.2	11.8
Dihedrals(°)	15.8	34.2	89.1	35.2	40.1	30.9	21.4	57.5	63.6
Metal-involving dihedrals(°)	12.8	29.8	75.3	21.3	2.7	28.8	21.4	51.7	63.6

Table S3: Mulliken spin densities on primary spin sites in low-spin (LS) and high-spin (HS) states calculated by B3LYP

Complex	1	2	3	4	5	6	7	8	9
LS Site A	0.614	0.577	4.818	1.150	3.862	0.532	0.657	3.029	3.965
LS Site B	-0.615	-0.577	-0.504	-1.150	-2.731	-0.532	-0.657	-0.536	-0.582
HS Site A	0.615	0.580	4.828	1.158	3.856	0.524	0.650	3.033	4.040
HS Site B	0.615	0.580	0.515	1.158	2.876	0.524	0.650	0.535	0.571

Table S4: J couplings (in wavenumber) calculated by B3LYP

Complex	1	2	3	4	5	6	7	8	9
S_a [1]	0.5	0.5	2.5	0.5	2	0.5	0.5	1.5	2
S_b	0.5	0.5	0.5	0.5	1.5	0.5	0.5	0.5	0.5
CSP[2]	-90.7	-105.9	-32.7	-101.0	-170.1	100.1	130.6	13.3	71.5
CNP	-45.3	-53.0	-27.2	-50.5	-136.1	50.1	65.3	9.9	57.2
CAP	-89.9	-104.7	-32.6	-100.1	-168.6	97.8	130.2	13.3	71.3
LSP	-88.4	-119.0	-43.3	-122.3	-132.9	157.7	113.0	34.4	115.7
LNP	-44.2	-59.5	-36.1	-61.1	-106.3	78.8	56.5	25.8	92.6
LAP	-87.7	-117.7	-43.2	-121.2	-131.7	154.0	112.7	34.4	115.4
HSP	-88.5	-109.9	-39.9	-91.8	-120.9	182.4	119.6	34.8	129.3
HNP	-44.2	-54.9	-33.3	-45.9	-96.7	91.2	59.8	26.1	103.4
HAP	-87.7	-108.7	-39.8	-91.0	-119.8	178.1	119.3	34.8	129.0
ASP	-93.3	-116.1	-44.1	-121.9	-136.4	132.0	116.1	34.2	112.7
ANP	-46.6	-58.1	-36.7	-60.9	-109.1	66.0	58.1	25.6	90.2
AAP	-92.7	-114.8	-43.9	-120.8	-135.2	129.0	115.8	34.2	112.4
Exp	-30.9	-37.4	-15.7	-107	-110	84.0	57.0	18.5	54.4
S^2_{HS} [3]	2.00	2.01	12.01	2.02	15.84	2.01	2.00	6.03	8.83
S^2_{LS}	1.00	0.99	6.99	1.01	3.73	0.98	1.00	3.03	4.82

1 Spin quantum number of each spin site

2 The first letter denotes geometry, C stands for crystal, L stands for low spin, H stands for high spin, A stands for AP; the last two letters denote method, SP stands for spin projected, NP stands for non projected, AP stands for approximate projection

3 Spin square expectation value at AP geometry for both HS and LS state

Table S5: J couplings (in wavenumber) calculated by LC-ωPBE

Complex	1	2	3	4	5	6	7	8	9
S_a [1]	0.5	0.5	2.5	0.5	2	0.5	0.5	1.5	2
S_b	0.5	0.5	0.5	0.5	1.5	0.5	0.5	0.5	0.5
CSP[2]	-44.9	-58.8	-16.7	-63.0	-151.9	314.8	118.1	23.7	62.1
CNP	-22.5	-29.4	-13.9	-31.5	-121.5	157.4	59.0	17.8	49.7
CAP	-43.6	-56.9	-16.3	-61.1	-147.3	300.9	115.2	23.2	60.6
LSP	-27.4	-66.9	-16.7	-83.7	-136.6	314.8	107.5	23.7	62.1
LNP	-13.7	-33.4	-13.9	-41.8	-109.3	157.4	53.8	17.8	49.7
LAP	-27.2	-66.1	-16.7	-83.0	-135.4	307.4	107.2	23.7	62.0
HSP	-25.1	-63.6	-16.6	-66.3	-123.5	343.0	109.5	24.2	64.6
HNP	-12.6	-31.8	-13.8	-33.2	-98.8	171.5	54.7	18.2	51.7
HAP	-24.9	-62.9	-16.5	-65.7	-122.3	334.9	109.2	24.2	64.4
ASP	-29.5	-69.4	-16.8	-110.9	-141.4	287.0	105.3	23.6	61.4
ANP	-14.8	-34.7	-14.0	-55.4	-113.1	143.5	52.7	17.7	49.1
AAP	-29.5	-69.2	-16.8	-110.2	-140.3	283.4	105.2	23.6	61.0
Exp	-30.9	-37.4	-15.7	-107	-110	84.0	57.0	18.5	54.4
S^2_{HS} [3]	2.00	2.01	12.01	2.02	15.84	2.01	2.00	6.03	8.83
S^2_{LS}	1.00	0.99	6.99	1.01	3.73	0.98	1.00	3.03	4.82

1 Spin quantum number of each spin site

2 The first letter denotes geometry, C stands for crystal, L stands for low spin, H stands for high spin, A stands for AP; the last two letters denote method, SP stands for spin projected, NP stands for non projected, AP stands for approximate projection

3 Spin square expectation value at AP geometry for both HS and LS state

Table S6: J couplings (in wavenumber) calculated by CAM-B3LYP

Complex	1	2	3	4	5	6	7	8	9
S_a [1]	0.5	0.5	2.5	0.5	2	0.5	0.5	1.5	2
S_b	0.5	0.5	0.5	0.5	1.5	0.5	0.5	0.5	0.5
CSP[2]	-49.5	-60.6	-15.5	-71.8	-143.7	183.8	119.7	10.9	48.1
CNP	-24.8	-30.3	-12.9	-35.9	-115.0	91.9	59.8	8.2	38.5
CAP	-48.0	-58.7	-15.1	-69.7	-139.4	175.7	116.8	10.7	47.0
LSP	-35.9	-73.1	-20.6	-92.8	-122.8	239.8	101.3	25.4	69.6
LNP	-18.0	-36.5	-17.1	-46.4	-98.3	119.9	50.7	19.0	55.6
LAP	-35.6	-72.2	-20.5	-92.0	-121.7	234.2	101.0	25.4	69.4
HSP	-33.6	-69.2	-20.2	-73.8	-113.5	261.1	104.6	25.7	73.0
HNP	-16.8	-34.6	-16.8	-36.9	-90.8	130.6	52.3	19.3	58.4
HAP	-33.3	-68.4	-20.1	-73.2	-112.4	255.0	104.3	25.7	72.8
ASP	-38.9	-75.7	-20.6	-122.9	-125.9	218.5	97.1	25.3	68.7
ANP	-19.5	-37.8	-17.2	-61.5	-100.7	109.2	48.6	19.0	55.0
AAP	-38.9	-75.4	-20.6	-122.2	-125.0	215.6	97.0	25.2	68.3
Exp	-30.9	-37.4	-15.7	-107	-110	84.0	57.0	18.5	54.4
S^2_{HS} [3]	2.00	2.01	12.01	2.02	15.84	2.01	2.00	6.03	8.83
S^2_{LS}	1.00	0.99	6.99	1.01	3.73	0.98	1.00	3.03	4.82

1 Spin quantum number of each spin site

2 The first letter denotes geometry, C stands for crystal, L stands for low spin, H stands for high spin, A stands for AP; the last two letters denote method, SP stands for spin projected, NP stands for non projected, AP stands for approximate projection

3 Spin square expectation value at AP geometry for both HS and LS state

Table S7: J couplings (in wavenumber) calculated by ωB97XD

Complex	1	2	3	4	5	6	7	8	9
S_a [1]	0.5	0.5	2.5	0.5	2	0.5	0.5	1.5	2
S_b	0.5	0.5	0.5	0.5	1.5	0.5	0.5	0.5	0.5
CSP[2]	-47.9	-60.8	-15.6	-79.1	-148.3	179.7	127.9	13.1	49.9
CNP	-24.0	-30.4	-13.0	-39.6	-118.6	89.9	63.9	9.8	39.9
CAP	-46.5	-58.8	-15.2	-76.8	-143.8	171.7	124.8	12.8	48.7
LSP	-33.7	-63.4	-20.4	-97.9	-128.4	222.5	115.2	27.6	71.9
LNP	-16.9	-31.7	-17.0	-49.0	-102.7	111.3	57.6	20.7	57.5
LAP	-33.4	-62.7	-20.3	-97.1	-127.2	217.3	114.9	27.6	71.7
HSP	-31.7	-61.1	-20.0	-79.8	-118.0	243.0	117.1	28.0	75.2
HNP	-15.9	-30.5	-16.7	-39.9	-94.4	121.5	58.5	21.0	60.2
HAP	-31.4	-60.4	-19.9	-79.1	-116.9	237.2	116.8	28.0	75.1
ASP	-36.1	-65.7	-20.5	-127.3	-132.0	202.7	113.0	27.5	71.1
ANP	-18.0	-32.9	-17.1	-63.6	-105.6	101.3	56.5	20.6	56.9
AAP	-36.0	-65.5	-20.5	-126.3	-131.0	200.1	112.8	27.5	70.7
Exp	-30.9	-37.4	-15.7	-107	-110	84.0	57.0	18.5	54.4
S^2_{HS} [3]	2.00	2.01	12.01	2.02	15.84	2.01	2.00	6.03	8.83
S^2_{LS}	1.00	0.99	6.99	1.01	3.73	0.98	1.00	3.03	4.82

1 Spin quantum number of each spin site
2 The first letter denotes geometry, C stands for crystal, L stands for low spin, H stands for high spin, A stands for AP; the last two letters denote method, SP stands for spin projected, NP stands for non projected, AP stands for approximate projection
3 Spin square expectation value at AP geometry for both HS and LS state

Table S8: errors of spin crossover gaps of a selection of complexes calculated by AP with B3LYP/6-311G* and B3LYP/LACV3P, and by DBLOC (B3LYP/LACV3P)

complex	6-311G*	LACV3P	DBLOC
cr223tetcl2	0.93	0.53	1.82
crcn6	3.36	5.17	5.73
mncn6	0.10	0.92	0.47
fe(3)cn6	4.04	3.43	3.58
col2	10.58	12.56	0.56
coterpy	4.45	3.62	1.89
nibipy3	5.09	9.04	0.95
nidpdpm2h2o2	2.22	6.20	0.20
niphen3	5.09	8.96	6.23
mnen3	3.11	3.64	4.22
MAE	3.90	5.41	2.57

Table S9: Spin crossover gaps (kcal/mol) on crystal, optimized ground state and optimized AP-corrected ground state geometries calculated by B3LYP/6-311G(d) considering solvent effect and their errors wrt. experiments

complex	G1	G2	G3	G4	exp.	E1	E3	E4	E0
cr(3)f6	24.80	25.40	38.09	38.33	40.37	15.57	2.28	2.04	1.30
cr223tetcl2	24.18	23.78	35.60	36.24	36.53	12.35	0.93	0.29	1.82
crccsime36	20.94	21.49	32.23	32.63	33.52	12.58	1.29	0.89	2.61
crcn6	21.18	22.96	34.36	35.68	31	9.82	3.36	4.68	5.73
crcyclamncs2	23.11	23.22	34.79	35.14	34.54	11.43	0.25	0.60	3.43
cren3	25.38	25.81	38.65	38.83	38.67	13.29	0.02	0.16	1.56
crnh34cl2	25.15	24.86	37.24	37.83	36.95	11.80	0.29	0.88	2.31
crnh36	25.78	25.98	38.92	39.29	39.15	13.37	0.23	0.14	0.82
crox3	23.77	23.86	35.76	36.20	36.53	12.76	0.77	0.33	1.24
mnf6	25.87	25.78	38.57	39.25	41.24	15.37	2.67	1.99	1.31
mn2p2pameth2	11.70	11.45	22.24	22.19	46.55	34.85	24.31	24.36	4.47
mncn6	11.87	12.21	24.20	26.51	24.1	12.23	0.10	2.41	0.47
crf6	13.22	13.15	26.13	25.39	28.09	14.87	1.96	2.70	3.87
vf6	12.68	12.87	25.69	23.97	24.66	11.98	1.03	0.69	1.04
vurea6	12.13	12.24	24.42	24.55	23.99	11.86	0.43	0.56	0.41
fe(3)cn6	62.21	48.95	49.18	57.61	45.14	17.07	4.04	12.47	3.58
feen3	22.62	18.90	19.09	18.81	18.89	3.73	0.20	0.08	2.18
coamn3s3sarh	29.59	31.92	31.92	31.23	33.61	4.02	1.69	2.38	0.42
coamn5ssarh	32.11	31.68	31.68	34.49	32.48	0.37	0.80	2.01	3.85
coen3	37.23	37.20	37.20	36.69	32.33	4.90	4.87	4.36	1.81
coetn4s2amp	31.27	31.88	31.88	31.45	32.62	1.35	0.74	1.17	0.52
col2	34.80	34.32	34.32	34.19	23.74	11.06	10.58	10.45	0.56
con3s3	29.54	31.69	31.69	31.26	34.72	5.18	3.03	3.46	1.16
conh35soch32	28.39	28.94	28.94	28.50	26.22	2.17	2.72	2.28	1.59
conh36	35.78	35.62	35.62	35.30	30.33	5.45	5.29	4.97	0.66
fe(2)cn6	69.80	56.66	56.66	59.57	60.93	8.87	4.27	1.36	3.33
fe2amp3	-13.18	19.59	19.59	19.34	5.26	18.44	14.33	14.08	6.25
febptnncs2	-18.73	22.14	22.14	21.64	0	18.73	22.14	21.64	3.98
fehbpz32	42.83	27.94	27.94	27.78	4.54	38.29	23.40	23.24	6.74
fepapth2	-18.39	20.29	20.29	19.90	3.82	22.21	16.47	16.08	0.05
fephen2ncs2	25.28	23.98	23.98	23.19	0	25.28	23.98	23.19	0.14
fephen2ncse2	26.67	24.57	24.57	23.85	0	26.67	24.57	23.85	0.69
fepybzimh3	-1.63	19.20	19.20	18.73	5.02	6.65	14.18	13.71	0.05
fetacn2	29.48	18.73	18.73	18.67	5.5	23.98	13.23	13.17	10.16
fetpancs2	-1.73	22.88	22.88	22.05	0	1.73	22.88	22.05	2.19
fetpen	38.66	22.87	22.87	22.60	0	38.66	22.87	22.60	5.83
fetppn3	38.88	23.00	23.00	22.72	6.69	32.19	16.31	16.03	3.83
copyimine22	14.35	9.93	9.96	9.74	3.35	11.00	6.61	6.39	3.56

Table S9: Spin crossover gaps (kcal/mol) on crystal, optimized ground state and optimized AP-corrected ground state geometries calculated by B3LYP/6-311G(d) considering solvent effect and their errors wrt. experiments

complex	G1	G2	G3	G4	exp.	E1	E3	E4	E0
coterpy	9.47	7.54	7.56	7.38	3.11	6.36	4.45	4.27	1.89
ni2meim6	15.88	15.96	31.90	31.86	28.47	12.59	3.43	3.39	0.72
nibipy3	0.06	15.12	30.20	30.23	25.11	25.05	5.09	5.12	0.95
nibpm2no3	12.54	15.19	30.10	29.99	27.64	15.10	2.46	2.35	0.79
nidmso6	15.68	16.27	32.54	32.32	30.94	15.26	1.60	1.38	2.39
nidpdpm2h2o2	15.52	15.67	31.17	31.23	28.95	13.43	2.22	2.28	0.20
nidpdpm2no3h2o	15.43	15.45	30.76	30.91	28.95	13.52	1.81	1.96	0.64
nidpdpmno32ch3cn	15.23	15.48	30.90	30.81	28.95	13.72	1.95	1.86	3.84
nidpdpmno32	9.44	14.82	29.35	29.51	28.95	19.51	0.40	0.56	0.64
niedta	9.83	15.07	30.11	30.30	27	17.17	3.11	3.30	0.93
nien2scn2	13.20	13.56	26.46	26.44	27.03	13.83	0.57	0.59	0.83
nien3	0.05	15.16	30.31	30.39	26.08	26.03	4.23	4.31	6.89
nif6 (M062x)	18.16	17.77	35.54	35.65	33.72	15.56	1.82	1.93	3.21
nigly3	11.83	15.18	30.10	30.11	28.29	16.46	1.81	1.82	0.22
nih2o6	9.36	17.19	34.38	34.23	33.03	23.67	1.35	1.20	2.95
ninh36	12.55	15.70	31.39	31.51	28.23	15.68	3.16	3.28	0.22
niphen3	1.89	15.08	30.25	30.35	25.16	23.27	5.09	5.19	6.23
nipyrazole6	18.42	15.72	31.42	31.58	28.86	10.44	2.56	2.72	0.25
nitach3mepyr	12.00	14.69	29.35	29.57	23.14	11.14	6.21	6.43	4.59
nitpm2	0.03	15.47	30.91	31.26	27.78	27.75	3.13	3.48	0.85
nitpmno32	11.81	15.40	30.75	30.90	27.58	15.77	3.17	3.32	1.38
feh2o6	17.34	30.11	30.94	30.07	29.19	11.85	1.75	0.88	3.42
fethiocarbamate3	2.97	8.48	9.01	9.18	11.75	8.78	2.74	2.57	0.94
fetrencam	15.29	27.40	27.72	29.01	22.9	7.61	4.82	6.11	3.24
mnden2	20.49	37.99	42.83	42.36	39.05	18.56	3.78	3.31	4.30
mnen	19.07	37.06	41.16	38.70	38.05	18.98	3.11	0.65	4.22
mnh2o6	39.32	42.42	49.19	46.23	47.12	7.80	2.07	0.89	2.45
MAE						14.80	5.83	5.92	2.38
MAE without alpha=1						14.92	3.03	3.22	2.20

1 G1-G4 stand for spin crossover gap on different geometries, G1 is crystal structure, G2 is UDFT geometry, G3 is UDFT//AP, G4 is the AP//AP

2 E1, E3, E4 corresponds to the error wrt. to experiments for G1, G3, G4, and E0 stands for the error of DBLOC method

Table S10: Spin crossover gaps (kcal/mol) on crystal, optimized ground state and optimized AP-corrected ground state geometries calculated by B3LYP/6-311G(d) not considering solvent effect and their errors wrt. experiments

complex	G1	G2	G3	G4	exp.	E1	E3	E4	E0	$\langle S^2 \rangle_{HS}$
cr(3)f6	24.80	25.40	38.09	38.33	40.37	15.57	2.28	2.04	1.30	2.015
cr223tetcl2	24.18	23.78	35.60	36.24	36.53	12.35	0.93	0.29	1.82	3.780
crccsime36	20.94	21.49	32.23	32.63	33.52	12.58	1.29	0.89	2.61	3.788
crcn6	21.18	22.96	34.36	35.68	31	9.82	3.36	4.68	5.73	3.782
crcyclamncs2	22.17	22.10	33.12	33.46	34.54	12.37	1.42	1.08	3.43	3.775
cren3	25.38	25.63	38.36	39.08	38.67	13.29	0.31	0.41	1.56	3.780
crnh34cl2	24.68	23.95	35.50	35.68	36.95	12.27	1.45	1.27	2.31	3.775
crnh36	25.74	26.04	38.99	39.67	39.15	13.41	0.16	0.52	0.82	3.775
crox3	23.79	23.92	35.83	36.21	36.53	12.74	0.70	0.32	1.24	3.769
mnf6	25.87	25.78	38.57	39.25	41.24	15.37	2.67	1.99	1.31	3.786
mn2p2pameth2	11.71	11.33	21.94	21.26	46.55	34.84	24.61	25.29	4.47	2.018
mncn6	11.87	12.56	24.89	24.90	24.1	12.23	0.79	0.80	0.47	2.028
crf6	13.22	13.15	26.13	25.39	28.09	14.87	1.96	2.70	3.87	3.762
vf6	12.68	12.87	25.69	23.97	24.66	11.98	1.03	0.69	1.04	2.005
vurea6	12.13	12.24	24.42	24.55	23.99	11.86	0.43	0.56	0.41	2.007
fe(3)cn6	62.60	42.32	42.55	42.35	45.14	17.46	2.59	2.79	3.58	2.031
feen3	22.62	18.90	19.09	18.81	18.89	3.73	0.20	0.08	2.18	3.797
coamn3s3sarh	29.59	31.92	31.92	31.23	33.61	4.02	1.69	2.38	0.42	2.100
coamn5ssarh	32.11	31.68	31.68	34.49	32.48	0.37	0.80	2.01	3.85	2.093
coen3	37.47	33.73	33.73	41.27	32.33	5.14	1.40	8.94	1.81	2.028
coetn4s2amp	31.27	31.88	31.88	31.45	32.62	1.35	0.74	1.17	0.52	2.074
col2	34.98	34.06	34.06	33.92	23.74	11.24	10.32	10.18	0.56	2.026
con3s3	29.54	31.69	31.69	31.26	34.72	5.18	3.03	3.46	1.16	2.087
conh35soch32	28.91	25.33	25.33	25.18	26.22	2.69	0.89	1.04	1.59	2.021
conh36	36.45	30.96	30.96	30.85	30.33	6.12	0.63	0.52	0.66	2.025
fe(2)cn6	70.36	41.76	41.76	44.52	30.33		11.43	14.19	3.33	3.789
fe2amp3	-13.18	19.59	19.59	19.34	5.26	7.92	14.33	14.08	6.25	6.021
febptnncs2	-18.73	22.14	22.14	21.64	0	18.73	22.14	21.64	3.98	6.074
fehbpz32	42.83	27.94	27.94	27.78	4.54	38.29	23.40	23.24	6.74	6.010
fepapth2	-18.39	20.29	20.29	19.90	3.82	14.57	16.47	16.08	0.05	6.050
fephen2ncs2	25.28	23.98	23.98	23.19	0	25.28	23.98	23.19	0.14	6.228
fephen2ncse2	26.67	24.57	24.57	23.85	0	26.67	24.57	23.85	0.69	6.213
fepybzimh3	-1.63	19.20	19.20	18.73	5.02	3.39	14.18	13.71	0.05	6.070
fetacn2	29.48	18.73	18.73	18.67	5.5	23.98	13.23	13.17	10.16	6.010
fetpancs2	-1.73	22.88	22.88	22.05	0	1.73	22.88	22.05	2.19	6.131
fetpen	38.66	22.87	22.87	22.60	0	38.66	22.87	22.60	5.83	6.025
fetppn3	38.88	23.00	23.00	22.72	6.69	32.19	16.31	16.03	3.83	6.026
copyimine22	14.35	9.93	9.96	9.74	3.35	11.00	6.61	6.39	3.56	3.773

Table S10: Spin crossover gaps (kcal/mol) on crystal, optimized ground state and optimized AP-corrected ground state geometries calculated by B3LYP/6-311G(d) not considering solvent effect and their errors wrt. experiments

complex	G1	G2	G3	G4	exp.	E1	E3	E4	E0	$\langle S^2 \rangle_{HS}$
coterpy	9.47	7.54	7.56	7.38	3.11	6.36	4.45	4.27	1.89	3.773
ni2meim6	15.88	15.94	31.87	31.88	28.47	12.59	3.40	3.41	0.72	2.011
nibipy3	0.07	15.09	30.16	30.24	25.11	25.04	5.05	5.13	0.95	2.005
nibpm2no3	12.49	15.28	30.48	30.46	27.64	15.15	2.84	2.82	0.79	2.004
nidmso6	15.66	16.22	32.44	32.42	30.94	15.28	1.50	1.48	2.39	2.005
nidpdpm2h2o2	15.36	15.47	30.71	30.80	28.95	13.59	1.76	1.85	0.20	2.004
nidpdpm2no3h2o	15.45	15.59	31.15	30.99	28.95	13.50	2.20	2.04	0.64	2.004
nidpdpmno32ch3cn	15.00	15.11	30.14	30.15	28.95	13.95	1.19	1.20	3.84	2.004
nidpdpmno32	12.27	15.02	30.01	30.20	28.95	16.68	1.06	1.25	0.64	2.004
niedta	8.81	15.23	30.44	30.50	27	18.19	3.44	3.50	0.93	2.003
nien2scn2	13.12	13.57	26.85	26.96	27.03	13.91	0.18	0.07	0.83	2.004
nien3	0.05	15.16	30.31	30.39	26.08	26.03	4.23	4.31	6.89	2.003
nif6 (M062x)	18.16	17.77	35.54	35.65	33.72	15.56	1.82	1.93	3.21	2.003
nigly3	10.73	11.20	20.29	20.41	28.29	17.56	8.00	7.88	0.22	2.003
nih2o6	9.72	17.44	34.87	34.71	33.03	23.31	1.84	1.68	2.95	2.002
ninh36	12.55	15.70	31.39	31.51	28.23	15.68	3.16	3.28	0.22	2.003
niphen3	1.90	15.14	30.25	30.37	25.16	23.26	5.09	5.21	6.23	2.005
nipyrazole6	18.42	15.72	31.42	31.58	28.86	10.44	2.56	2.72	0.25	2.004
nitach3mepyr	12.03	14.76	29.49	29.61	23.14	11.11	6.35	6.47	4.59	2.004
nitpm2	0.03	15.47	30.91	31.26	27.78	27.75	3.13	3.48	0.85	2.004
nitpmno32	10.74	15.12	30.23	30.33	27.58	16.84	2.65	2.75	1.38	2.004
feh2o6	16.84	32.27	34.11	34.11	29.19	12.35	4.92	4.92	3.42	8.754
fethiocarbamate3	3.25	8.60	9.12	9.27	11.75	8.50	2.63	2.48	0.94	8.760
fetrencam	15.29	27.40	27.72	29.01	22.9	7.61	4.82	6.11	3.24	8.757
mnden2	20.10	36.47	36.59	38.07	39.05	18.95	2.46	0.98	4.30	8.753
mnen3	18.78	37.19	37.28	38.97	38.05	19.27	0.77	0.92	4.22	8.753
mnh2o6	39.14	43.25	43.28	47.75	47.12	7.98	3.84	0.63	2.45	8.752
MAE						14.71	5.83	5.92	2.38	
MAE w/o alpha=1						14.98	3.04	2.98	2.20	

1 G1-G4 stand for spin crossover gap on different geometries, G1 is crystal structure, G2 is UDFT geometry, G3 is UDFT//AP, G4 is the AP//AP

2 E1, E3, E4 corresponds to the error wrt. to experiments for G1, G3, G4, and E0 stands for the error of DBLOC method