

Electronic Supplementary Information

**Quantum chemical modeling of magnetically bistable metal coordination compounds.
Synchronization of spin crossover, valence tautomerism and charge transfer induced spin
transition mechanisms**

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Table S1. Spin states (S), total energies without (E, given in a.u.) and with account (E^{ZPE} , given in a.u.) taken for energies of zero harmonic vibrations, relative energies without (ΔE , given in kcal mol⁻¹) and with (ΔE^{ZPE} , given in kcal mol⁻¹) taking into account the energies of zero harmonic vibrations of the low-spin (LS) and the high-spin (HS) isomers of 1,10-phenanthroline-dihydrobis(pyrazolyl)borate Fe^{II} (phen Fe^{II}) and 1,10-phenanthroline-5,6-dione-dihydrobis(pyrazolyl)borate Fe^{II} (phendione Fe^{II}) calculated by the DFT method.

Structure	S	E	ΔE	E^{ZPE}	ΔE^{ZPE}
B3LYP*					
phen Fe ^{II} LS	0	-2789.36694		-2788.90053	
phen Fe ^{II} HS	4/2	-2789.36050	4.0	-2788.89831	1.4
phendione Fe ^{II} LS	0	-2938.56180		-2938.11032	
phendione Fe ^{II} HS	4/2	-2938.55515	4.2	-2938.10762	1.7
TPSSh					
phen Fe ^{II} LS	0	-2790.62692		-2790.15820	
phen Fe ^{II} HS	4/2	-2790.61050	10.3	-2790.14619	7.5
phendione Fe ^{II} LS	0	-2939.88695		-2939.43307	
phendione Fe ^{II} HS	4/2	-2939.87016	10.5	-2939.42087	7.7
OLYP					
phen Fe ^{II} LS	0	-2790.19362		-2789.73281	
phen Fe ^{II} HS	4/2	-2790.19815	-2.8	-2789.74134	-5.4
phendione Fe ^{II} LS	0	-2939.43084		-2938.98520	
phendione Fe ^{II} HS	4/2	-2939.43745	-4.1	-2938.99548	-6.4

Table S2. Total energies without (E) and with (E^{ZPE}) taking into account the energies of zero harmonic vibrations (all energy values are given in a.u.) of the structures of Co^{II} bis-chelates calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure	E	E^{ZPE}
<i>bis</i> -(acetylacetonate)Co ^{II}	-2072.89123	-2072.66825
<i>bis</i> -(trifluoroacetylacetonate)Co ^{II}	-2668.26938	-2668.09245
<i>bis</i> -(hexafluoroacetylacetonate)Co ^{II}	-3263.63635	-3263.50515
<i>bis</i> -(N-phenylsalicylaldiminate)Co ^{II}	-2644.95127	-2644.56118
<i>bis</i> -(N-(<i>p</i> -nitrophenyl)-salicylaldiminate)Co ^{II}	-3053.90136	-3053.50641

Table S3. Spin states (S), total energies without (E, given in a.u.) and with (E^{ZPE} , given in a.u.) taking into account the energies of zero harmonic vibrations, expectation values of the spin-squared (S^2) operator of the electromeric forms in the ground state and broken symmetry (BS) states and values of the lowest frequencies (ω_1 , cm^{-1}) of the adducts **5** ($R_1, R_2 = \text{CH}_3, \text{CF}_3$) and **6** ($R = \text{Ph}, \text{Ph-}p\text{-NO}_2$) calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure		S	E	E^{ZPE}	S^2	ω_1
5 , $R_1 = \text{CH}_3$ $R_2 = \text{CH}_3$	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{II}}$	1/2	-5011.47930	-5010.80072	0.76	16
	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	5/2	-5011.47297	-5010.79881	8.77	11
	BS $_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-5011.47302		4.77	
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{LS}}\text{Fe}^{\text{II}}$	3/2	-5011.45911	-5010.78429	4.13	13
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	7/2	-5011.45242	-5010.78190	16.21	11
	BS $_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-5011.45257		4.21	
5 , $R_1 = \text{CH}_3$ $R_2 = \text{CF}_3$	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{II}}$	1/2	-5606.85491	-5606.22205	0.76	11
	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	5/2	-5606.84901	-5606.22032	8.79	10
	BS $_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-5606.84838		4.80	
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{LS}}\text{Fe}^{\text{II}}$	3/2	-5606.84393	-5606.21505	3.89	8
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	7/2	-5606.83786	-5606.21299	16.10	6
	BS $_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-5606.83845		4.13	
	MECP ₂₋₄		-5606.83714			
	MECP ₆₋₈		-5606.83123			
	MECP ₄₋₆		-5606.83539			
	MECP ₂₋₈		-5606.82627			
5 , $R_1 = \text{CF}_3$ $R_2 = \text{CF}_3$	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{II}}$	1/2	-6202.22208	-6201.63560	0.79	9
	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	5/2	-6202.21702	-6201.63381	8.79	9
	BS $_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-6202.21438		4.81	
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$	5/2	-6202.22567	-6201.64213	8.79	6
	BS1 $_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$		-6202.22564		4.79	
	BS2 $_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$		-6202.22254		4.79	
	BS3 $_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$		-6202.22254		2.78	
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	7/2	-6202.21727	-6201.63780	16.17	6
	BS $_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-6202.21824		4.23	
6 , $R = \text{Ph}$	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{II}}$	1/2	-5583.55901	-5582.71262	0.76	9
	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	5/2	-5583.55286	-5582.71079	8.79	4
	BS $_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-5583.55285		4.80	
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{LS}}\text{Fe}^{\text{II}}$	3/2	-5583.53789	-5582.69540	4.38	8
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	7/2	-5583.53140	-5582.69340	16.44	9
	BS $_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-5583.53160		4.42	
6 , $R = \text{Ph-}p\text{-NO}_2$	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{II}}$	1/2	-5992.49433	-5991.64349	0.76	10
	$_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	5/2	-5992.48834	-5991.64169	8.79	6
	BS $_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-5992.48723		4.81	
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$	5/2	-5992.47886	-5991.63174	8.79	7
	BS1 $_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$		-5992.47884		4.79	
	BS2 $_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$		-5992.47203		4.79	
	BS3 $_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$		-5992.47203		2.79	
	$_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$	7/2	-5992.47081	-5991.62821	16.29	4
	BS $_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}_{\text{HS}}\text{Fe}^{\text{II}}$		-5992.47146		4.24	

^a BS1 corresponds to spin orientation $\alpha\alpha\beta$, BS2 corresponds to spin orientation $\alpha\beta\alpha$, BS3 corresponds to spin orientation $\beta\alpha\alpha$, where α – spin up, β – spin down.

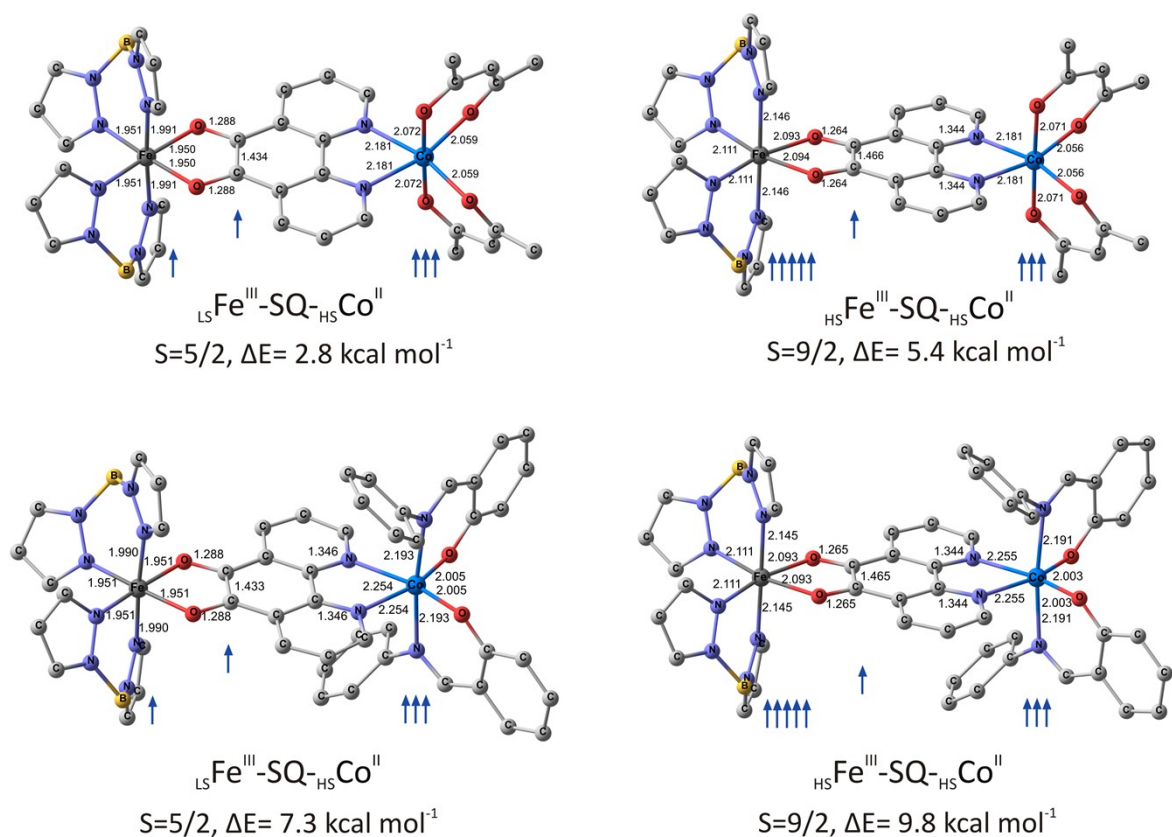


Figure S1. Geometry and energy characteristics of linkage isomers of the adducts **5** ($R_1=R_2=\text{CH}_3$) and **6** ($R=\text{Ph}$) calculated by the DFT B3LYP*/6-311++G(d,p) method. ΔE values are calculated relative to the most energy preferred electromeric forms of adducts **5** ($R_1=R_2=\text{CH}_3$) and **6** ($R=\text{Ph}$).

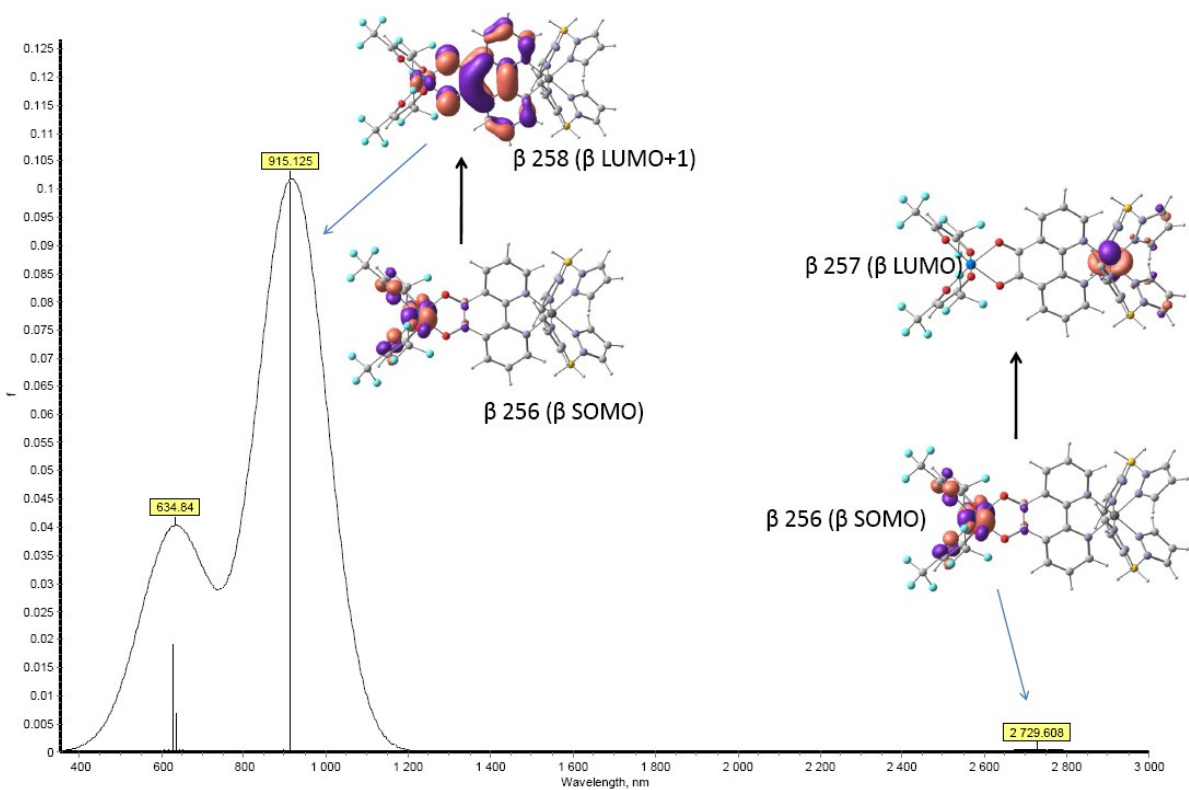


Figure S2. TD-DFT spectrum and the orbitals contributed to the long wave length absorption bands of ${}_{\text{HS}}\text{Co}^{\text{II}}\text{-SQ-}{}_{\text{LS}}\text{Fe}^{\text{III}}$ electromer of adduct **5** ($R_1=R_2=\text{CF}_3$).

Total energies and optimized geometries of the electromeric forms of the adducts 5 (R₁, R₂ = CH₃, CF₃) and 6 (R=Ph, Ph-*p*-NO₂) calculated by DFT B3LYP*/6-311++G(d,p)

LSCo^{III}-SQ-LSFe^{II}, 5 (R₁= CH₃, R₂=CH₃)

E= -5011.47930 a.u., E^{ZPE}= -5010.80072 a.u.

26	3.214329000	-0.000006000	-0.000002000
7	3.217102000	-1.714585000	1.107415000
7	3.756463000	-2.898792000	0.710058000
7	5.034223000	-2.039308000	-1.298309000
7	4.677038000	-0.727027000	-1.199258000
7	4.677027000	0.727057000	1.199239000
7	5.034150000	2.039351000	1.298315000
7	3.756348000	2.898804000	-0.710034000
7	3.217040000	1.714580000	-1.107410000
5	4.172330000	-3.214046000	-0.756313000
1	3.179362000	-3.366924000	-1.432238000
1	4.854869000	-4.208060000	-0.747411000
5	4.172199000	3.214057000	0.756342000
1	3.179223000	3.366869000	1.432271000
1	4.854687000	4.208105000	0.747458000
6	2.843600000	-1.876931000	2.389988000
1	2.411362000	-1.061252000	2.946545000
6	3.134504000	-3.171950000	2.829260000
1	2.957131000	-3.595029000	3.806076000
6	3.716204000	-3.783975000	1.726996000
1	4.097892000	-4.784406000	1.588531000
6	6.176671000	-2.144856000	-2.009417000
1	6.611632000	-3.115876000	-2.193435000
6	6.586667000	-0.873505000	-2.388054000
1	7.462384000	-0.603093000	-2.957824000
6	5.619164000	-0.020002000	-1.848275000
1	5.565854000	1.056908000	-1.881133000
6	5.619188000	0.020061000	1.848237000
1	5.565924000	-1.056852000	1.881080000
6	6.586665000	0.873598000	2.388011000
1	7.462403000	0.603214000	2.957762000
6	6.176606000	2.144938000	2.009404000
1	6.611527000	3.115974000	2.193432000
6	3.716058000	3.783999000	-1.726962000
1	4.097703000	4.784444000	-1.588483000
6	3.134387000	3.171963000	-2.829236000
1	2.956998000	3.595047000	-3.806046000
6	2.843534000	1.876927000	-2.389982000
1	2.411333000	1.061236000	-2.946550000
8	-3.122946000	0.680231000	1.118300000

8	-3.122938000	-0.680192000	-1.118372000
6	-1.982124000	0.371642000	0.617623000
6	-1.982119000	-0.371624000	-0.617675000
6	-0.658478000	1.448568000	2.458131000
6	0.591677000	1.740601000	2.975975000
6	-0.732484000	0.741557000	1.246344000
6	1.742538000	1.340244000	2.285435000
6	0.475049000	0.371417000	0.617480000
7	1.696817000	0.673960000	1.123852000
6	-0.732476000	-0.741556000	-1.246379000
6	0.475053000	-0.371429000	-0.617502000
1	-1.573396000	1.742989000	2.960970000
1	0.700337000	2.282539000	3.909222000
1	2.730545000	1.554566000	2.670572000
6	-0.658464000	-1.448578000	-2.458159000
7	1.696824000	-0.673994000	-1.123852000
6	1.742552000	-1.340288000	-2.285430000
6	0.591694000	-1.740634000	-2.975983000
1	-1.573380000	-1.742988000	-2.961009000
1	2.730559000	-1.554622000	-2.670556000
1	0.700359000	-2.282579000	-3.909225000
27	-4.548130000	-0.000010000	-0.000028000
8	-4.461602000	-1.608836000	1.005220000
8	-5.878061000	-0.596831000	-1.195489000
8	-5.878087000	0.596741000	1.195439000
8	-4.461674000	1.608824000	-1.005269000
6	-5.202765000	-2.625227000	0.808375000
6	-6.173211000	-2.741301000	-0.198881000
6	-6.445570000	-1.739164000	-1.138233000
6	-6.445478000	1.739141000	1.138338000
6	-6.173142000	2.741310000	0.199012000
6	-5.202835000	2.625206000	-0.808373000
1	-6.735014000	-3.664403000	-0.261444000
1	-6.734878000	3.664446000	0.261677000
6	-4.966667000	-3.768309000	1.766202000
1	-5.614993000	-4.621366000	1.557915000
1	-3.919990000	-4.083481000	1.703062000
1	-5.139779000	-3.420883000	2.790040000
6	-7.487127000	-1.966697000	-2.207887000
1	-7.020959000	-1.861489000	-3.192998000
1	-7.948754000	-2.952614000	-2.129102000
1	-8.260656000	-1.195537000	-2.130898000
6	-4.966914000	3.768234000	-1.766308000
1	-3.920187000	4.083302000	-1.703515000
1	-5.140387000	3.420782000	-2.790078000
1	-5.615097000	4.621360000	-1.557859000

6	-7.486877000	1.966708000	2.208140000
1	-8.260620000	1.195773000	2.131034000
1	-7.020655000	1.861144000	3.193185000
1	-7.948257000	2.952761000	2.129613000

$\text{LSCo}^{\text{III}}\text{-SQ-HsFe}^{\text{II}}$, **5** ($\text{R}_1 = \text{CH}_3$, $\text{R}_2 = \text{CH}_3$)

$E = -5011.47297$ a.u., $E^{\text{ZPE}} = -5010.79881$ a.u.

26	-3.401940000	-0.004867000	-0.004513000
7	-3.396641000	1.823345000	1.251906000
7	-3.882967000	3.026334000	0.840416000
7	-5.127176000	2.297692000	-1.267918000
7	-4.829881000	0.967176000	-1.314066000
7	-4.841407000	-0.951021000	1.316347000
7	-5.162281000	-2.276218000	1.269683000
7	-3.925542000	-3.026045000	-0.835221000
7	-3.416915000	-1.831982000	-1.246692000
5	-4.163054000	3.362689000	-0.657012000
1	-3.118978000	3.366704000	-1.268981000
1	-4.718453000	4.432239000	-0.700422000
5	-4.213667000	-3.355869000	0.662848000
1	-3.170103000	-3.373257000	1.275779000
1	-4.783504000	-4.417796000	0.706435000
6	-3.168815000	1.935836000	2.571779000
1	-2.793078000	1.092412000	3.132772000
6	-3.499573000	3.216922000	3.025704000
1	-3.427921000	3.607614000	4.029414000
6	-3.954016000	3.873515000	1.886418000
1	-4.318062000	4.880841000	1.748137000
6	-6.278923000	2.525168000	-1.928226000
1	-6.670879000	3.528472000	-2.007218000
6	-6.762781000	1.316447000	-2.420361000
1	-7.664737000	1.148666000	-2.988920000
6	-5.821397000	0.372113000	-2.002578000
1	-5.806799000	-0.697833000	-2.152973000
6	-5.824572000	-0.339349000	2.002067000
1	-5.791786000	0.730081000	2.153023000
6	-6.784051000	-1.267016000	2.416822000
1	-7.684774000	-1.083391000	2.982477000
6	-6.319792000	-2.484049000	1.926611000
1	-6.729203000	-3.480451000	2.004851000
6	-4.004174000	-3.874031000	-1.879369000
1	-4.384054000	-4.875476000	-1.740751000
6	-3.533423000	-3.227374000	-3.018179000
1	-3.463212000	-3.621586000	-4.020609000
6	-3.183549000	-1.951452000	-2.565431000

1	-2.789939000	-1.115852000	-3.125840000
8	3.259086000	0.674372000	-1.120668000
8	3.260610000	-0.679344000	1.121186000
6	2.119856000	0.364687000	-0.617719000
6	2.120654000	-0.372651000	0.617765000
6	0.813337000	1.434300000	-2.461181000
6	-0.421892000	1.742478000	-2.999695000
6	0.868397000	0.727943000	-1.246100000
6	-1.580642000	1.344992000	-2.317201000
6	-0.350701000	0.363217000	-0.629916000
7	-1.546942000	0.673050000	-1.166570000
6	0.870139000	-0.739696000	1.245240000
6	-0.349508000	-0.377096000	0.629154000
1	1.740071000	1.719635000	-2.947994000
1	-0.510363000	2.289192000	-3.932339000
1	-2.568233000	1.578202000	-2.700730000
6	0.816226000	-1.448814000	2.459272000
7	-1.544651000	-0.692113000	1.165341000
6	-1.577805000	-1.367265000	2.313521000
6	-0.417875000	-1.762639000	2.996157000
1	1.743669000	-1.732191000	2.945908000
1	-2.565021000	-1.605894000	2.694678000
1	-0.505121000	-2.311964000	3.927369000
27	4.686362000	-0.001189000	0.000046000
8	4.600408000	-1.613917000	-0.998842000
8	6.016399000	-0.592364000	1.197369000
8	6.014899000	0.592132000	-1.197866000
8	4.598168000	1.611349000	0.998882000
6	5.343514000	-2.628416000	-0.799584000
6	6.315090000	-2.739394000	0.207250000
6	6.586082000	-1.733866000	1.143350000
6	6.582177000	1.734878000	-1.144623000
6	6.309522000	2.740197000	-0.208805000
6	5.338937000	2.627404000	0.798797000
1	6.878629000	-3.661250000	0.272376000
1	6.871031000	3.663243000	-0.274608000
6	5.102376000	3.773751000	1.752516000
1	4.054938000	4.086525000	1.690428000
1	5.278416000	3.430737000	2.777352000
1	5.748546000	4.627230000	1.539521000
6	7.623523000	1.958872000	-2.215197000
1	8.083715000	2.945766000	-2.140890000
1	8.398137000	1.189186000	-2.134427000
1	7.157665000	1.848359000	-3.199861000
6	7.628475000	-1.956093000	2.213273000
1	7.163002000	-1.846648000	3.198230000

1	8.090530000	-2.942079000	2.138471000
1	8.401578000	-1.184916000	2.132181000
6	5.108486000	-3.775182000	-1.753198000
1	5.758249000	-4.626461000	-1.542329000
1	4.062356000	-4.091798000	-1.688290000
1	5.280391000	-3.431110000	-2.778368000

$\text{HS-Co}^{\text{II}}\text{-BQ-Ls-Fe}^{\text{II}}$, **5** ($\text{R}_1 = \text{CH}_3$, $\text{R}_2 = \text{CH}_3$)

$E = -5011.45911$ a.u., $E^{\text{ZPE}} = -5010.78429$ a.u.

26	-3.321386000	-0.000005000	0.000004000
7	-3.326875000	1.800958000	0.959990000
7	-3.847475000	2.951374000	0.452742000
7	-5.121768000	1.927999000	-1.476810000
7	-4.780208000	0.626459000	-1.253954000
7	-4.780244000	-0.626422000	1.253967000
7	-5.121853000	-1.927948000	1.476819000
7	-3.847574000	-2.951370000	-0.452727000
7	-3.326923000	-1.800974000	-0.959968000
5	-4.247255000	3.136494000	-1.039670000
1	-3.246024000	3.210939000	-1.717552000
1	-4.913196000	4.136716000	-1.130556000
5	-4.247396000	-3.136482000	1.039679000
1	-3.246178000	-3.211002000	1.717571000
1	-4.913391000	-4.136669000	1.130537000
6	-2.971439000	2.070808000	2.229871000
1	-2.556537000	1.303333000	2.863044000
6	-3.255193000	3.401310000	2.550224000
1	-3.087659000	3.906216000	3.489076000
6	-3.813534000	3.920601000	1.389836000
1	-4.182618000	4.908790000	1.159748000
6	-6.264421000	1.978834000	-2.193463000
1	-6.688595000	2.932937000	-2.468522000
6	-6.690237000	0.682215000	-2.448986000
1	-7.570151000	0.369545000	-2.989827000
6	-5.732098000	-0.127880000	-1.831839000
1	-5.691365000	-1.203618000	-1.762654000
6	-5.732162000	0.127951000	1.831761000
1	-5.691390000	1.203687000	1.762567000
6	-6.690366000	-0.682108000	2.448853000
1	-7.570309000	-0.369404000	2.989627000
6	-6.264570000	-1.978742000	2.193376000
1	-6.688786000	-2.932830000	2.468422000
6	-3.813626000	-3.920607000	-1.389811000
1	-4.182739000	-4.908784000	-1.159726000
6	-3.255227000	-3.401345000	-2.550184000

1	-3.087677000	-3.906267000	-3.489024000
6	-2.971469000	-2.070842000	-2.229841000
1	-2.556535000	-1.303379000	-2.863009000
8	2.997326000	-0.540237000	1.193151000
8	2.997324000	0.540303000	-1.193092000
6	1.888029000	-0.315305000	0.678062000
6	1.888028000	0.315331000	-0.678020000
6	0.540280000	-1.222239000	2.588627000
6	-0.714022000	-1.468518000	3.125518000
6	0.617073000	-0.628813000	1.321711000
6	-1.856371000	-1.132342000	2.394178000
6	-0.581025000	-0.317544000	0.651590000
7	-1.804630000	-0.572820000	1.173411000
6	0.617070000	0.628806000	-1.321681000
6	-0.581027000	0.317514000	-0.651567000
1	1.454720000	-1.467362000	3.118658000
1	-0.828303000	-1.922995000	4.103476000
1	-2.847464000	-1.305562000	2.791372000
6	0.540273000	1.222237000	-2.588593000
7	-1.804631000	0.572777000	-1.173390000
6	-1.856377000	1.132314000	-2.394152000
6	-0.714032000	1.468507000	-3.125487000
1	1.454709000	1.467382000	-3.118619000
1	-2.847475000	1.305537000	-2.791338000
1	-0.828312000	1.922997000	-4.103439000
27	4.676854000	0.000007000	0.000024000
8	4.648119000	1.760653000	0.971650000
8	6.012442000	0.802410000	-1.258772000
8	6.012407000	-0.802485000	1.258785000
8	4.648030000	-1.760620000	-0.971632000
6	5.476854000	2.721940000	0.876863000
6	6.490145000	2.815623000	-0.093684000
6	6.689066000	1.869961000	-1.115879000
6	6.689009000	-1.870042000	1.115853000
6	6.490053000	-2.815667000	0.093629000
6	5.476753000	-2.721927000	-0.876901000
1	7.129773000	3.689769000	-0.078582000
1	7.129679000	-3.689815000	0.078473000
6	5.309561000	3.830904000	1.891892000
1	4.295834000	4.239183000	1.817952000
1	5.416661000	3.413053000	2.898735000
1	6.033807000	4.637185000	1.756648000
6	7.764514000	2.104881000	-2.153798000
1	8.465120000	1.263039000	-2.143257000
1	7.305623000	2.129406000	-3.148007000
1	8.313223000	3.034247000	-1.986211000

6	7.764423000	-2.105047000	2.153788000
1	7.305402000	-2.130256000	3.147926000
1	8.313491000	-3.034135000	1.985834000
1	8.464693000	-1.262927000	2.143768000
6	5.309447000	-3.830828000	-1.891996000
1	6.033578000	-4.637201000	-1.756695000
1	4.295659000	-4.238979000	-1.818205000
1	5.416734000	-3.412945000	-2.898806000

$\text{HS-Co}^{\text{II}}\text{-BQ-HS-Fe}^{\text{II}}$, **5** ($\text{R}_1 = \text{CH}_3$, $\text{R}_2 = \text{CH}_3$)

$E = -5011.45242$ a.u., $E^{\text{ZPE}} = -5010.78190$ a.u.

26	-3.472692000	-0.000066000	-0.000050000
7	-3.485868000	1.973830000	1.044500000
7	-4.022508000	3.106249000	0.515872000
7	-5.235477000	2.115594000	-1.499824000
7	-4.881776000	0.799921000	-1.419347000
7	-4.881956000	-0.799640000	1.419246000
7	-5.235929000	-2.115227000	1.499849000
7	-4.023093000	-3.106345000	-0.515689000
7	-3.486381000	-1.974029000	-1.044458000
5	-4.312079000	3.272652000	-1.008571000
1	-3.265141000	3.241141000	-1.616229000
1	-4.900568000	4.311877000	-1.167703000
5	-4.312749000	-3.272534000	1.008756000
1	-3.265841000	-3.241173000	1.616465000
1	-4.901467000	-4.311615000	1.167982000
6	-3.210647000	2.245194000	2.331592000
1	-2.789100000	1.485026000	2.973438000
6	-3.564070000	3.562359000	2.646469000
1	-3.466376000	4.068873000	3.594534000
6	-4.075392000	4.070413000	1.457924000
1	-4.462646000	5.048692000	1.214682000
6	-6.411011000	2.225201000	-2.146931000
1	-6.849302000	3.197857000	-2.315041000
6	-6.851769000	0.953554000	-2.502095000
1	-7.757727000	0.691314000	-3.026635000
6	-5.861526000	0.096079000	-2.018393000
1	-5.802877000	-0.981656000	-2.060530000
6	-5.861580000	-0.095517000	2.018170000
1	-5.802702000	0.982211000	2.060192000
6	-6.852025000	-0.952732000	2.501914000
1	-7.757951000	-0.690244000	3.026385000
6	-6.411515000	-2.224512000	2.146911000
1	-6.850017000	-3.197058000	2.315108000
6	-4.076122000	-4.070610000	-1.457638000

1	-4.463503000	-5.048810000	-1.214285000
6	-3.564784000	-3.562738000	-2.646247000
1	-3.467183000	-4.069360000	-3.594264000
6	-3.211156000	-2.245591000	-2.331503000
1	-2.789525000	-1.485548000	-2.973441000
8	3.117801000	0.524071000	-1.202027000
8	3.117771000	-0.524279000	1.202081000
6	2.009676000	0.303267000	-0.680333000
6	2.009658000	-0.303517000	0.680344000
6	0.680305000	1.178240000	-2.603440000
6	-0.559218000	1.434789000	-3.166776000
6	0.737033000	0.601863000	-1.327080000
6	-1.710220000	1.112890000	-2.441798000
6	-0.474307000	0.304069000	-0.665388000
7	-1.674450000	0.560071000	-1.223513000
6	0.736992000	-0.602141000	1.327040000
6	-0.474333000	-0.304403000	0.665290000
1	1.607186000	1.408254000	-3.119046000
1	-0.651541000	1.883276000	-4.149817000
1	-2.699952000	1.305768000	-2.841399000
6	0.680228000	-1.178484000	2.603411000
7	-1.674506000	-0.560417000	1.223356000
6	-1.710297000	-1.113195000	2.441665000
6	-0.559319000	-1.435040000	3.166699000
1	1.607091000	-1.408451000	3.119071000
1	-2.700035000	-1.306102000	2.841236000
1	-0.651674000	-1.883493000	4.149753000
27	4.799082000	-0.000043000	0.000050000
8	4.768796000	-1.771415000	-0.950412000
8	6.135015000	-0.788149000	1.267616000
8	6.134933000	0.788191000	-1.267519000
8	4.768614000	1.771344000	0.950497000
6	5.594143000	-2.734254000	-0.842430000
6	6.606200000	-2.818653000	0.130214000
6	6.807999000	-1.859859000	1.139581000
6	6.807755000	1.860012000	-1.139555000
6	6.605717000	2.818907000	-0.130333000
6	5.593662000	2.734412000	0.842308000
1	7.243254000	-3.694811000	0.126916000
1	7.242526000	3.695244000	-0.127189000
6	7.882428000	-2.084401000	2.180836000
1	7.423160000	-2.094827000	3.175126000
1	8.428280000	-3.017556000	2.025413000
1	8.585613000	-1.244928000	2.159732000
6	5.424198000	-3.855439000	-1.843451000
1	6.144602000	-4.663081000	-1.696322000

1	4.408547000	-4.258333000	-1.766613000
1	5.535370000	-3.451091000	-2.855360000
6	5.423360000	3.855771000	1.843077000
1	4.407561000	4.258279000	1.766177000
1	5.534714000	3.451713000	2.855083000
1	6.143474000	4.663631000	1.695729000
6	7.882453000	2.084420000	-2.180558000
1	8.587507000	1.246556000	-2.156781000
1	7.423981000	2.091328000	-3.175219000
1	8.426241000	3.019071000	-2.026905000

$\text{LSCo}^{\text{III}}\text{-SQ-LSFe}^{\text{II}}$, **5** ($\text{R}_1 = \text{CH}_3$, $\text{R}_2 = \text{CF}_3$)

$E = -5606.85491$ a.u., $E^{\text{ZPE}} = -5606.22205$ a.u.

26	3.869402000	-0.059033000	-0.053607000
7	3.905628000	-1.839971000	0.942403000
7	4.375563000	-3.009544000	0.429767000
7	5.546771000	-2.046546000	-1.594600000
7	5.239795000	-0.735368000	-1.378449000
7	5.411422000	0.569455000	1.099173000
7	5.796051000	1.867883000	1.260220000
7	4.422174000	2.869173000	-0.613591000
7	3.840549000	1.719754000	-1.052210000
5	4.683684000	-3.232577000	-1.079743000
1	3.643193000	-3.307670000	-1.694946000
1	5.330893000	-4.243962000	-1.186062000
5	4.923914000	3.085423000	0.843158000
1	3.972057000	3.205477000	1.582281000
1	5.619212000	4.069868000	0.860361000
6	3.625928000	-2.075860000	2.237633000
1	3.264805000	-1.286056000	2.876434000
6	3.908267000	-3.404091000	2.569622000
1	3.793948000	-3.885470000	3.528678000
6	4.384908000	-3.957752000	1.388628000
1	4.725068000	-4.956295000	1.158541000
6	6.638822000	-2.130531000	-2.383637000
1	7.030076000	-3.096756000	-2.665166000
6	7.065913000	-0.846490000	-2.694530000
1	7.913064000	-0.559230000	-3.298175000
6	6.162305000	-0.008517000	-2.033516000
1	6.141173000	1.068953000	-1.984743000
6	6.378729000	-0.190473000	1.643414000
1	6.310004000	-1.266446000	1.611027000
6	7.390457000	0.613611000	2.177377000
1	8.293857000	0.295397000	2.674539000
6	6.979936000	1.912104000	1.906768000

1	7.441308000	2.863366000	2.126132000
6	4.337561000	3.817686000	-1.568737000
1	4.742251000	4.802571000	-1.390127000
6	3.682094000	3.285229000	-2.670696000
1	3.453061000	3.772705000	-3.605758000
6	3.395228000	1.969154000	-2.297533000
1	2.915289000	1.198427000	-2.878390000
8	-2.377574000	0.454707000	1.559141000
8	-2.524847000	-0.760027000	-0.745198000
6	-1.266590000	0.211696000	0.953203000
6	-1.348754000	-0.451919000	-0.320815000
6	0.170725000	1.218237000	2.747096000
6	1.452345000	1.504183000	3.185255000
6	0.016488000	0.575021000	1.507703000
6	2.553227000	1.157584000	2.392086000
6	1.178142000	0.262745000	0.769038000
7	2.430387000	0.554608000	1.201174000
6	-0.150648000	-0.749980000	-1.070111000
6	1.095459000	-0.401326000	-0.506762000
1	-0.706730000	1.471158000	3.332360000
1	1.623703000	1.998541000	4.135252000
1	3.564156000	1.363240000	2.716961000
6	-0.160489000	-1.363205000	-2.333986000
7	2.279544000	-0.648142000	-1.120149000
6	2.245020000	-1.224902000	-2.329998000
6	1.051004000	-1.590082000	-2.963954000
1	-1.105839000	-1.635409000	-2.790948000
1	3.203619000	-1.392940000	-2.802599000
1	1.095847000	-2.055005000	-3.942720000
27	-3.852936000	-0.174367000	0.508304000
8	-3.687335000	-1.845571000	1.399480000
8	-5.271718000	-0.717194000	-0.621828000
8	-5.114477000	0.328068000	1.829173000
8	-3.862233000	1.498072000	-0.392628000
6	-4.408430000	-2.867730000	1.190852000
6	-5.453166000	-2.942552000	0.242197000
6	-5.789923000	-1.874494000	-0.574535000
6	-5.713004000	1.447786000	1.890870000
6	-5.514937000	2.523797000	1.000714000
6	-4.611600000	2.460482000	-0.050589000
1	-6.005700000	-3.865978000	0.146740000
1	-6.080969000	3.432286000	1.147065000
6	-6.941404000	-2.032767000	-1.587517000
9	-7.509685000	-3.257518000	-1.537517000
9	-7.910085000	-1.126927000	-1.342258000
9	-6.501098000	-1.839054000	-2.844097000

6	-4.421928000	3.693714000	-0.957465000
9	-4.628500000	3.375294000	-2.246958000
9	-5.266618000	4.700065000	-0.643053000
9	-3.164384000	4.168636000	-0.842372000
6	-4.085353000	-4.064758000	2.047986000
1	-4.699963000	-4.930017000	1.795018000
1	-3.027302000	-4.319059000	1.930211000
1	-4.241066000	-3.803264000	3.100055000
6	-6.706107000	1.577755000	3.017022000
1	-7.552541000	0.908935000	2.823795000
1	-6.240778000	1.254276000	3.952533000
1	-7.076589000	2.598776000	3.120679000

$LSCo^{III}-SQ-HSFe^{II}$, **5** ($R_1=CH_3$, $R_2=CF_3$)

$E=-5606.84901$ a.u., $E^{ZPE}=-5606.22032$ a.u.

26	4.022181000	-0.035440000	-0.067923000
7	4.026519000	-1.982901000	1.032823000
7	4.509193000	-3.143011000	0.511742000
7	5.638800000	-2.241925000	-1.595719000
7	5.324117000	-0.915894000	-1.534191000
7	5.567101000	0.702063000	1.241920000
7	6.007192000	1.994007000	1.260237000
7	4.675749000	3.012181000	-0.665769000
7	4.027632000	1.901327000	-1.111728000
5	4.720059000	-3.364256000	-1.018430000
1	3.646608000	-3.334765000	-1.576318000
1	5.284693000	-4.417931000	-1.169746000
5	5.119033000	3.196738000	0.820291000
1	4.134636000	3.252648000	1.523485000
1	5.785392000	4.198255000	0.889345000
6	3.812347000	-2.209263000	2.339947000
1	3.442574000	-1.419777000	2.978089000
6	4.151942000	-3.524761000	2.676193000
1	4.092722000	-4.000624000	3.643163000
6	4.590617000	-4.079501000	1.479403000
1	4.945625000	-5.072542000	1.247057000
6	6.762450000	-2.401244000	-2.319691000
1	7.164300000	-3.389659000	-2.486613000
6	7.207317000	-1.152983000	-2.746241000
1	8.079629000	-0.930866000	-3.341498000
6	6.275392000	-0.255392000	-2.222367000
1	6.240281000	0.821898000	-2.294368000
6	6.542125000	-0.047096000	1.792195000
1	6.421787000	-1.117559000	1.869388000
6	7.615047000	0.756916000	2.181770000

1	8.538261000	0.450311000	2.649067000
6	7.229289000	2.045184000	1.822300000
1	7.737006000	2.992022000	1.932674000
6	4.675236000	3.956158000	-1.627694000
1	5.132830000	4.917477000	-1.446750000
6	4.014228000	3.457671000	-2.745501000
1	3.840029000	3.955085000	-3.687319000
6	3.628670000	2.167778000	-2.368284000
1	3.098901000	1.421957000	-2.942775000
8	-2.636611000	-0.756923000	-0.742390000
8	-2.495330000	0.444293000	1.572671000
6	-1.460303000	-0.443760000	-0.311685000
6	-1.381540000	0.207030000	0.961281000
6	-0.287301000	-1.329674000	-2.328695000
6	0.908131000	-1.561283000	-2.984825000
6	-0.260618000	-0.723959000	-1.060691000
6	2.109132000	-1.193224000	-2.364189000
6	0.998517000	-0.374079000	-0.511249000
7	2.158180000	-0.614153000	-1.162266000
6	-0.099912000	0.568079000	1.513345000
6	1.078807000	0.271336000	0.783244000
1	-1.242876000	-1.597803000	-2.767295000
1	0.932615000	-2.026754000	-3.964078000
1	3.065886000	-1.371246000	-2.843290000
6	0.034311000	1.209546000	2.757833000
7	2.308488000	0.578235000	1.253688000
6	2.413124000	1.187179000	2.435695000
6	1.299548000	1.521794000	3.219464000
1	-0.857804000	1.446450000	3.328224000
1	3.421162000	1.420719000	2.761447000
1	1.445798000	2.022579000	4.170270000
27	-3.963263000	-0.177101000	0.510540000
8	-3.967186000	1.502254000	-0.379777000
8	-5.232955000	0.319418000	1.829421000
8	-5.379379000	-0.710857000	-0.631448000
8	-3.806459000	-1.855306000	1.391853000
6	-4.713039000	2.464717000	-0.031283000
6	-5.619681000	2.523570000	1.017553000
6	-5.827045000	1.440424000	1.897449000
6	-5.892165000	-1.870589000	-0.601766000
6	-5.556803000	-2.946677000	0.205366000
6	-4.521618000	-2.877317000	1.164998000
1	-6.182246000	3.433350000	1.169194000
1	-6.104185000	-3.871506000	0.094906000
6	-4.515112000	3.704956000	-0.926626000
9	-5.356595000	4.712778000	-0.607206000

9	-3.255854000	4.174319000	-0.802983000
9	-4.717695000	3.399435000	-2.220053000
6	-7.034513000	-2.023270000	-1.625836000
9	-8.007022000	-1.120606000	-1.383825000
9	-6.583420000	-1.820390000	-2.877558000
9	-7.602081000	-3.249207000	-1.590248000
6	-4.203286000	-4.082337000	2.013248000
1	-3.143681000	-4.333113000	1.901955000
1	-4.368588000	-3.831721000	3.066477000
1	-4.813626000	-4.946539000	1.746500000
6	-6.826529000	1.565608000	3.018857000
1	-6.366761000	1.236307000	3.955128000
1	-7.196388000	2.586499000	3.126408000
1	-7.672647000	0.898876000	2.817326000

${}^{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}{}_{\text{LS}}\text{Fe}^{\text{II}}$, **5** ($\text{R}_1 = \text{CH}_3$, $\text{R}_2 = \text{CF}_3$)

$E = -5606.84393$ a.u., $E^{\text{ZPE}} = -5606.21505$ a.u.

26	-4.004260000	-0.088718000	0.051248000
7	-4.102286000	-1.948817000	-0.775417000
7	-4.573176000	-3.056378000	-0.139791000
7	-5.676743000	-1.885738000	1.807874000
7	-5.362801000	-0.606066000	1.453552000
7	-5.540040000	0.473892000	-1.134111000
7	-5.863261000	1.763309000	-1.441295000
7	-4.449858000	2.893471000	0.320619000
7	-3.921988000	1.770432000	0.880473000
5	-4.836366000	-3.124726000	1.391838000
1	-3.775596000	-3.143141000	1.978485000
1	-5.480231000	-4.115870000	1.622602000
5	-4.934293000	2.975881000	-1.154411000
1	-3.972666000	2.966836000	-1.893038000
1	-5.576775000	3.985482000	-1.288306000
6	-3.867252000	-2.312294000	-2.050422000
1	-3.513143000	-1.596765000	-2.774909000
6	-4.179654000	-3.660083000	-2.245191000
1	-4.100843000	-4.232843000	-3.156281000
6	-4.626941000	-4.090610000	-1.002986000
1	-4.973199000	-5.057133000	-0.668871000
6	-6.756888000	-1.877449000	2.617248000
1	-7.151620000	-2.805692000	3.002597000
6	-7.169037000	-0.564229000	2.799917000
1	-8.003846000	-0.208481000	3.383814000
6	-6.269780000	0.193090000	2.043435000
1	-6.240465000	1.259870000	1.886063000
6	-6.549740000	-0.295353000	-1.579539000

1	-6.531864000	-1.362786000	-1.424612000
6	-7.527776000	0.491131000	-2.195314000
1	-8.451557000	0.162868000	-2.646155000
6	-7.051741000	1.790417000	-2.080129000
1	-7.470598000	2.731500000	-2.403845000
6	-4.345333000	3.925451000	1.182024000
1	-4.707795000	4.903185000	0.902150000
6	-3.731499000	3.477891000	2.344275000
1	-3.498994000	4.045438000	3.232002000
6	-3.489965000	2.122723000	2.106159000
1	-3.052649000	1.395218000	2.770694000
8	2.199687000	0.225327000	-1.672512000
8	2.369959000	-0.703123000	0.782570000
6	1.139752000	0.073784000	-1.061154000
6	1.237513000	-0.471487000	0.353658000
6	-0.346875000	0.874411000	-2.912676000
6	-1.637955000	1.103750000	-3.365333000
6	-0.177329000	0.371743000	-1.617350000
6	-2.719334000	0.841235000	-2.522164000
6	-1.318969000	0.132083000	-0.829988000
7	-2.576748000	0.371624000	-1.268619000
6	0.013158000	-0.698648000	1.115195000
6	-1.225529000	-0.407934000	0.514264000
1	0.524452000	1.064528000	-3.530716000
1	-1.825683000	1.487872000	-4.361726000
1	-3.737291000	0.996368000	-2.853075000
6	0.027386000	-1.190175000	2.425688000
7	-2.408434000	-0.597336000	1.143395000
6	-2.373901000	-1.062178000	2.406372000
6	-1.186151000	-1.364992000	3.074826000
1	0.975901000	-1.413408000	2.903162000
1	-3.334224000	-1.179719000	2.889904000
1	-1.231634000	-1.737424000	4.092073000
27	4.002862000	-0.201380000	-0.528831000
8	3.889585000	1.642893000	0.309828000
8	5.292600000	0.568972000	-1.882396000
8	5.429140000	-0.871654000	0.737154000
8	4.002122000	-2.030673000	-1.403522000
6	4.680503000	2.603347000	0.079564000
6	5.676849000	2.691277000	-0.886216000
6	5.920200000	1.666500000	-1.836117000
6	6.105076000	-1.927836000	0.583643000
6	5.932938000	-2.939025000	-0.358469000
6	4.872404000	-2.944283000	-1.297700000
1	6.265000000	3.596674000	-0.941300000
1	6.611894000	-3.780055000	-0.341340000

6	4.431028000	3.818274000	0.998325000
9	3.183071000	4.308247000	0.802695000
9	4.528590000	3.470057000	2.296721000
9	5.296101000	4.836887000	0.787369000
6	7.245849000	-2.067753000	1.615728000
9	8.105197000	-1.030438000	1.519176000
9	6.754948000	-2.075362000	2.872964000
9	7.969866000	-3.202232000	1.461465000
6	4.728744000	-4.116657000	-2.240591000
1	5.472406000	-4.895581000	-2.061168000
1	3.724529000	-4.541276000	-2.139247000
1	4.824697000	-3.756890000	-3.271000000
6	6.986845000	1.873076000	-2.886282000
1	7.417398000	2.875882000	-2.856694000
1	7.783822000	1.136994000	-2.731361000
1	6.560421000	1.684182000	-3.876486000

$\text{HS-Co}^{\text{II}}\text{-BQ-HS-Fe}^{\text{II}}$, **5** ($\text{R}_1 = \text{CH}_3$, $\text{R}_2 = \text{CF}_3$)

$E = -5606.83786$ a.u., $E^{\text{ZPE}} = -5606.21299$ a.u.

26	-4.171928000	-0.064429000	0.065605000
7	-4.200540000	-2.082290000	-0.866941000
7	-4.665558000	-3.196031000	-0.237816000
7	-5.763091000	-2.116023000	1.798012000
7	-5.452029000	-0.800136000	1.611358000
7	-5.696186000	0.587047000	-1.292273000
7	-6.095538000	1.884384000	-1.439900000
7	-4.751279000	3.031430000	0.398637000
7	-4.139061000	1.945958000	0.947474000
5	-4.848986000	-3.282492000	1.309039000
1	-3.765181000	-3.196919000	1.841950000
1	-5.401494000	-4.320849000	1.565387000
5	-5.173897000	3.095135000	-1.102494000
1	-4.179672000	3.052009000	-1.792915000
1	-5.804371000	4.106072000	-1.273785000
6	-4.005487000	-2.421671000	-2.153367000
1	-3.653859000	-1.690051000	-2.866161000
6	-4.339166000	-3.762903000	-2.366451000
1	-4.290452000	-4.321792000	-3.288391000
6	-4.753830000	-4.213586000	-1.118133000
1	-5.095693000	-5.185354000	-0.794221000
6	-6.877247000	-2.208702000	2.546812000
1	-7.275117000	-3.177761000	2.809389000
6	-7.319948000	-0.926673000	2.862092000
1	-8.185394000	-0.652082000	3.445219000
6	-6.397280000	-0.079722000	2.247661000

1	-6.363956000	0.999580000	2.220461000
6	-6.692044000	-0.183296000	-1.774377000
1	-6.605073000	-1.259379000	-1.746551000
6	-7.736466000	0.611440000	-2.248089000
1	-8.666362000	0.289070000	-2.690684000
6	-7.312272000	1.916704000	-2.013528000
1	-7.790220000	2.862865000	-2.220402000
6	-4.736034000	4.053764000	1.276147000
1	-5.164846000	5.007926000	1.007993000
6	-4.102341000	3.635898000	2.441950000
1	-3.924816000	4.208276000	3.339406000
6	-3.748207000	2.309300000	2.182990000
1	-3.247305000	1.603128000	2.828912000
8	2.476016000	-0.699456000	0.781307000
8	2.312652000	0.248229000	-1.678380000
6	1.346487000	-0.451905000	0.342376000
6	1.253963000	0.095653000	-1.056966000
6	0.148447000	-1.162726000	2.410684000
6	-1.049011000	-1.346604000	3.084066000
6	0.117791000	-0.667192000	1.101094000
6	-2.244292000	-1.035518000	2.430859000
6	-1.133217000	-0.369205000	0.518370000
7	-2.292438000	-0.555723000	1.181247000
6	-0.063200000	0.404296000	-1.607544000
6	-1.223044000	0.167288000	-0.838102000
1	1.107219000	-1.387740000	2.867190000
1	-1.074346000	-1.729923000	4.097986000
1	-3.202767000	-1.173480000	2.919103000
6	-0.209893000	0.929035000	-2.898566000
7	-2.457935000	0.423776000	-1.314891000
6	-2.580173000	0.924684000	-2.549524000
6	-1.483787000	1.193687000	-3.374432000
1	0.677886000	1.115211000	-3.494724000
1	-3.594371000	1.118753000	-2.881099000
1	-1.644154000	1.605119000	-4.364701000
27	4.112623000	-0.195359000	-0.528761000
8	4.004356000	1.649674000	0.316148000
8	5.413566000	0.574772000	-1.876796000
8	5.538684000	-0.873663000	0.739345000
8	4.108995000	-2.024067000	-1.409518000
6	4.793357000	2.610437000	0.083737000
6	5.790490000	2.699129000	-0.881555000
6	6.038403000	1.673161000	-1.829309000
6	6.203592000	-1.936791000	0.590023000
6	6.025393000	-2.948279000	-0.350992000
6	4.970087000	-2.944713000	-1.296368000

1	6.377302000	3.605413000	-0.936734000
1	6.696211000	-3.795735000	-0.329414000
6	4.541829000	3.827070000	0.999963000
9	3.293098000	4.315663000	0.802789000
9	4.638560000	3.482431000	2.299545000
9	5.405314000	4.847351000	0.788206000
6	7.339008000	-2.087308000	1.626764000
9	8.210137000	-1.059414000	1.532882000
9	6.843559000	-2.088122000	2.882568000
9	8.052327000	-3.229689000	1.477704000
6	4.822106000	-4.117915000	-2.238404000
1	5.559485000	-4.901906000	-2.054807000
1	3.814511000	-4.535278000	-2.140243000
1	4.924605000	-3.760454000	-3.268963000
6	7.109130000	1.880869000	-2.875793000
1	7.906925000	1.146544000	-2.716813000
1	6.686938000	1.689901000	-3.867423000
1	7.537687000	2.884585000	-2.845833000

MECP₂₋₄, **5** (R₁= CH₃, R₂=CF₃)

E= -5606.83712 a.u.

26	3.959028000	-0.086556000	-0.050370000
7	4.062828000	-1.952025000	0.757745000
7	4.535363000	-3.054571000	0.113651000
7	5.640956000	-1.870909000	-1.822744000
7	5.325848000	-0.594536000	-1.457772000
7	5.503398000	0.466151000	1.139924000
7	5.830194000	1.752061000	1.457664000
7	4.417984000	2.896040000	-0.293849000
7	3.886712000	1.778231000	-0.862149000
5	4.801768000	-3.114395000	-1.418179000
1	3.744137000	-3.131621000	-2.007576000
1	5.451021000	-4.102273000	-1.651271000
5	4.905107000	2.969867000	1.181258000
1	3.946547000	2.960681000	1.921500000
1	5.554073000	3.975876000	1.316809000
6	3.829296000	-2.324871000	2.030616000
1	3.473534000	-1.614772000	2.759072000
6	4.143066000	-3.673662000	2.214759000
1	4.063625000	-4.254387000	3.120772000
6	4.590268000	-4.094603000	0.969111000
1	4.936237000	-5.058665000	0.627421000
6	6.722060000	-1.856378000	-2.630251000
1	7.116725000	-2.781582000	-3.023516000
6	7.135028000	-0.541876000	-2.801264000
1	7.970195000	-0.182008000	-3.382411000

6	6.234871000	0.209182000	-2.039334000
1	6.207735000	1.274497000	-1.873236000
6	6.513065000	-0.308365000	1.577673000
1	6.495284000	-1.374262000	1.413758000
6	7.493068000	0.471169000	2.199510000
1	8.416289000	0.138107000	2.648360000
6	7.019021000	1.772087000	2.095486000
1	7.439487000	2.709834000	2.427427000
6	4.317082000	3.933829000	-1.147971000
1	4.681076000	4.908845000	-0.860401000
6	3.703263000	3.496181000	-2.314165000
1	3.472055000	4.071839000	-3.197040000
6	3.457626000	2.140126000	-2.086449000
1	3.017965000	1.418157000	-2.754899000
8	-2.283940000	0.269905000	1.650107000
8	-2.443181000	-0.756926000	-0.759763000
6	-1.197438000	0.081630000	1.031139000
6	-1.288174000	-0.482306000	-0.325682000
6	0.279800000	0.850933000	2.912629000
6	1.570104000	1.072237000	3.366280000
6	0.106332000	0.361376000	1.608370000
6	2.657105000	0.816755000	2.524193000
6	1.258863000	0.123962000	0.827904000
7	2.518727000	0.358794000	1.272185000
6	-0.079843000	-0.687253000	-1.104163000
6	1.166889000	-0.396650000	-0.510435000
1	-0.586913000	1.044273000	3.536364000
1	1.756499000	1.449034000	4.365327000
1	3.673345000	0.971044000	2.856915000
6	-0.091298000	-1.163516000	-2.424309000
7	2.351468000	-0.579994000	-1.144619000
6	2.314079000	-1.033503000	-2.405430000
6	1.121441000	-1.329668000	-3.073397000
1	-1.036347000	-1.388209000	-2.908014000
1	3.272759000	-1.149885000	-2.889949000
1	1.165620000	-1.693900000	-4.093346000
27	-3.922055000	-0.204896000	0.520542000
8	-3.838523000	1.568224000	-0.338582000
8	-5.246110000	0.460126000	1.832544000
8	-5.375015000	-0.775326000	-0.701851000
8	-3.933517000	-1.970925000	1.412312000
6	-4.614610000	2.536361000	-0.077967000
6	-5.598472000	2.617434000	0.895819000
6	-5.850368000	1.574333000	1.816349000
6	-6.030329000	-1.849005000	-0.577588000
6	-5.849172000	-2.880524000	0.337398000

6	-4.796286000	-2.890840000	1.280898000
1	-6.176025000	3.529184000	0.979539000
1	-6.517785000	-3.729006000	0.293951000
6	-4.361428000	3.764359000	-0.974548000
9	-3.116229000	4.248385000	-0.764817000
9	-4.461252000	3.435832000	-2.275777000
9	-5.229642000	4.776473000	-0.743648000
6	-7.160342000	-1.992483000	-1.616607000
9	-8.030465000	-0.965416000	-1.525517000
9	-6.658615000	-1.995135000	-2.868051000
9	-7.868291000	-3.136228000	-1.461607000
6	-4.656555000	-4.077692000	2.200469000
1	-5.407009000	-4.847204000	1.996829000
1	-3.652924000	-4.501329000	2.089633000
1	-4.754259000	-3.734841000	3.236849000
6	-6.903525000	1.781768000	2.876430000
1	-7.311378000	2.793871000	2.841983000
1	-7.713690000	1.058572000	2.728677000
1	-6.470036000	1.591726000	3.863589000

MECP₆₋₈, **5** (R₁= CH₃, R₂=CF₃)

E= -5606.83123 a.u.

26	4.106374000	-0.059275000	-0.066911000
7	4.137082000	-2.089326000	0.859039000
7	4.601506000	-3.199608000	0.224420000
7	5.703742000	-2.107895000	-1.806221000
7	5.393771000	-0.792975000	-1.614142000
7	5.635382000	0.585165000	1.296560000
7	6.035135000	1.881459000	1.449330000
7	4.688444000	3.038932000	-0.384052000
7	4.075189000	1.956707000	-0.937349000
5	4.788453000	-3.277214000	-1.322833000
1	3.706086000	-3.191071000	-1.858056000
1	5.343822000	-4.314132000	-1.582771000
5	5.113339000	3.094177000	1.117415000
1	4.119726000	3.050214000	1.808577000
1	5.745699000	4.104301000	1.292054000
6	3.943012000	-2.434741000	2.143385000
1	3.590716000	-1.706088000	2.859169000
6	4.276449000	-3.777529000	2.350078000
1	4.228722000	-4.340564000	3.269410000
6	4.690554000	-4.222104000	1.099553000
1	5.034151000	-5.191711000	0.771566000
6	6.817271000	-2.198206000	-2.556903000
1	7.214616000	-3.166277000	-2.823435000
6	7.260130000	-0.915137000	-2.867764000

1	8.125853000	-0.638278000	-3.449368000
6	6.338072000	-0.070514000	-2.248192000
1	6.304908000	1.008861000	-2.215759000
6	6.629969000	-0.186985000	1.776448000
1	6.541914000	-1.263048000	1.744014000
6	7.674964000	0.605260000	2.254570000
1	8.605081000	0.280557000	2.694909000
6	7.251594000	1.911512000	2.024619000
1	7.729763000	2.856466000	2.235674000
6	4.673912000	4.065366000	-1.256858000
1	5.104359000	5.017638000	-0.985354000
6	4.040417000	3.652792000	-2.424757000
1	3.864648000	4.228837000	-3.320052000
6	3.684885000	2.325280000	-2.171086000
1	3.181931000	1.622084000	-2.818950000
8	-2.547126000	-0.746586000	-0.751640000
8	-2.391937000	0.282948000	1.655065000
6	-1.395573000	-0.465623000	-0.317262000
6	-1.307614000	0.099227000	1.033175000
6	-0.218933000	-1.156520000	-2.407082000
6	0.974625000	-1.330489000	-3.087775000
6	-0.184470000	-0.670957000	-1.090672000
6	2.175610000	-1.021684000	-2.439140000
6	1.072317000	-0.368139000	-0.517457000
7	2.228917000	-0.548858000	-1.189259000
6	-0.005564000	0.401194000	1.598923000
6	1.161537000	0.163502000	0.836191000
1	-1.178664000	-1.378066000	-2.862436000
1	0.996255000	-1.704264000	-4.106046000
1	3.131845000	-1.158494000	-2.932773000
6	0.138532000	0.918371000	2.896131000
7	2.394569000	0.418874000	1.322146000
6	2.512249000	0.913106000	2.557528000
6	1.409702000	1.177092000	3.379568000
1	-0.750630000	1.101841000	3.490536000
1	3.525215000	1.105987000	2.894924000
1	1.566271000	1.580138000	4.374132000
27	-4.022127000	-0.196886000	0.526609000
8	-3.939989000	1.579389000	-0.335941000
8	-5.341047000	0.483540000	1.837590000
8	-5.455504000	-0.790517000	-0.703191000
8	-4.019093000	-1.962395000	1.417813000
6	-4.707805000	2.551785000	-0.080967000
6	-5.691696000	2.638837000	0.895318000
6	-5.946775000	1.596354000	1.817727000
6	-6.101069000	-1.872706000	-0.582930000

6	-5.910919000	-2.900629000	0.332285000
6	-4.864307000	-2.895561000	1.284178000
1	-6.262748000	3.552754000	0.974482000
1	-6.564800000	-3.760187000	0.288728000
6	-4.439596000	3.773792000	-0.985912000
9	-3.191176000	4.250593000	-0.775790000
9	-4.534898000	3.440368000	-2.286789000
9	-5.300017000	4.793057000	-0.764088000
6	-7.220861000	-2.017578000	-1.634854000
9	-8.094908000	-0.993810000	-1.545422000
9	-6.701287000	-2.010117000	-2.878917000
9	-7.929060000	-3.162928000	-1.499479000
6	-4.698266000	-4.072722000	2.214683000
1	-5.430129000	-4.860226000	2.027935000
1	-3.688531000	-4.482784000	2.108421000
1	-4.799252000	-3.726088000	3.248835000
6	-7.001142000	1.794510000	2.879220000
1	-7.802750000	1.063450000	2.727586000
1	-6.560583000	1.595868000	3.860897000
1	-7.424488000	2.800762000	2.861183000

MECP₄₋₆, **5** (R₁= CH₃, R₂=CF₃)

E= -5606.83539 a.u.

26	4.018125000	-0.044861000	-0.050030000
7	4.034194000	-1.746122000	1.008963000
7	4.480300000	-2.955902000	0.566137000
7	5.656203000	-2.214997000	-1.547780000
7	5.331939000	-0.892480000	-1.503676000
7	5.560710000	0.669546000	1.183914000
7	5.983420000	1.964500000	1.201934000
7	4.596477000	2.826484000	-0.726634000
7	4.015053000	1.654592000	-1.107802000
5	4.739512000	-3.306394000	-0.934150000
1	3.682289000	-3.348341000	-1.519737000
1	5.319925000	-4.361732000	-0.969948000
5	5.081117000	3.134422000	0.723986000
1	4.122055000	3.248476000	1.452292000
1	5.744301000	4.139605000	0.688969000
6	3.796804000	-1.882234000	2.328271000
1	3.459075000	-1.043432000	2.914403000
6	4.085851000	-3.181882000	2.747451000
1	4.000979000	-3.589729000	3.742875000
6	4.518248000	-3.825982000	1.594235000
1	4.846667000	-4.840911000	1.429553000
6	6.791070000	-2.382695000	-2.253106000
1	7.200848000	-3.371102000	-2.399896000

6	7.235689000	-1.137397000	-2.686466000
1	8.118260000	-0.917104000	-3.267124000
6	6.290693000	-0.238036000	-2.186325000
1	6.260496000	0.837928000	-2.270903000
6	6.542111000	-0.064986000	1.743712000
1	6.444463000	-1.136959000	1.821804000
6	7.599878000	0.755431000	2.139094000
1	8.524843000	0.461302000	2.610793000
6	7.199896000	2.037062000	1.772851000
1	7.694765000	2.990942000	1.880828000
6	4.542356000	3.708867000	-1.743605000
1	4.954269000	4.699005000	-1.620059000
6	3.908420000	3.111551000	-2.826104000
1	3.704802000	3.541366000	-3.794932000
6	3.599873000	1.825757000	-2.378272000
1	3.122610000	1.022150000	-2.914594000
8	-2.624576000	-0.782522000	-0.709615000
8	-2.493567000	0.502053000	1.559946000
6	-1.449077000	-0.451614000	-0.286370000
6	-1.376158000	0.246042000	0.961011000
6	-0.266559000	-1.420856000	-2.260816000
6	0.933810000	-1.684610000	-2.894068000
6	-0.247150000	-0.763377000	-1.017890000
6	2.132111000	-1.302187000	-2.274463000
6	1.009225000	-0.393453000	-0.475204000
7	2.173883000	-0.674207000	-1.098092000
6	-0.098046000	0.635258000	1.501683000
6	1.083774000	0.319486000	0.783336000
1	-1.219593000	-1.700309000	-2.698176000
1	0.966122000	-2.186613000	-3.854920000
1	3.091509000	-1.503585000	-2.737742000
6	0.032885000	1.320144000	2.722482000
7	2.311648000	0.659339000	1.227886000
6	2.411600000	1.311566000	2.387063000
6	1.298295000	1.658584000	3.166334000
1	-0.858794000	1.566517000	3.290032000
1	3.417130000	1.567086000	2.702670000
1	1.444572000	2.188859000	4.101182000
27	-3.955326000	-0.160339000	0.516637000
8	-3.959453000	1.485931000	-0.434792000
8	-5.231113000	0.383428000	1.813495000
8	-5.368091000	-0.740267000	-0.610357000
8	-3.797978000	-1.805396000	1.459246000
6	-4.701704000	2.462247000	-0.119374000
6	-5.608273000	2.560330000	0.926542000
6	-5.820805000	1.508232000	1.842406000

6	-5.871898000	-1.902252000	-0.544925000
6	-5.531912000	-2.949056000	0.298287000
6	-4.503313000	-2.840028000	1.261136000
1	-6.167364000	3.476877000	1.046757000
1	-6.071464000	-3.881303000	0.215491000
6	-4.499557000	3.671270000	-1.055776000
9	-5.341162000	4.690454000	-0.773963000
9	-3.240275000	4.144058000	-0.943513000
9	-4.697626000	3.322951000	-2.339045000
6	-7.008167000	-2.098994000	-1.568286000
9	-7.987123000	-1.193843000	-1.365051000
9	-6.551643000	-1.940058000	-2.824509000
9	-7.569356000	-3.326250000	-1.490651000
6	-4.180179000	-4.015159000	2.149071000
1	-3.119738000	-4.265718000	2.044572000
1	-4.345232000	-3.730766000	3.193669000
1	-4.787341000	-4.890087000	1.911435000
6	-6.821834000	1.676305000	2.957024000
1	-6.364280000	1.379090000	3.905027000
1	-7.188709000	2.701515000	3.027757000
1	-7.669698000	1.005451000	2.777956000

MECP₂₋₈, **5** (R₁= CH₃, R₂=CF₃)

E= -5606.82627 a.u.

26	4.028112000	-0.067798000	-0.051434000
7	4.075173000	-2.033258000	0.818653000
7	4.563705000	-3.135723000	0.188436000
7	5.671558000	-2.014170000	-1.808508000
7	5.367969000	-0.710615000	-1.544883000
7	5.594289000	0.518888000	1.231188000
7	5.985547000	1.808365000	1.443030000
7	4.627139000	2.977160000	-0.359382000
7	4.006543000	1.896343000	-0.906547000
5	4.781122000	-3.209729000	-1.353899000
1	3.706245000	-3.163276000	-1.909109000
1	5.371453000	-4.229964000	-1.601181000
5	5.079323000	3.035966000	1.131329000
1	4.100541000	3.021389000	1.843742000
1	5.735240000	4.033933000	1.286279000
6	3.861556000	-2.385764000	2.099246000
1	3.492328000	-1.664072000	2.812042000
6	4.208089000	-3.724256000	2.306290000
1	4.152204000	-4.290279000	3.223484000
6	4.649878000	-4.159108000	1.061417000
1	5.010863000	-5.122251000	0.733036000
6	6.765319000	-2.069830000	-2.592961000

1	7.152099000	-3.025364000	-2.914886000
6	7.200422000	-0.774092000	-2.852514000
1	8.050263000	-0.468760000	-3.443514000
6	6.295717000	0.040171000	-2.167740000
1	6.268222000	1.115966000	-2.081268000
6	6.582004000	-0.268760000	1.697713000
1	6.503126000	-1.342374000	1.616972000
6	7.614453000	0.507324000	2.228422000
1	8.536288000	0.167100000	2.674573000
6	7.191579000	1.819780000	2.042367000
1	7.660336000	2.758602000	2.297701000
6	4.608794000	4.002943000	-1.233444000
1	5.048348000	4.951953000	-0.964240000
6	3.960913000	3.592563000	-2.393196000
1	3.777190000	4.168394000	-3.287426000
6	3.604558000	2.265809000	-2.136359000
1	3.098725000	1.563644000	-2.781591000
8	-2.509855000	-0.760519000	-0.752491000
8	-2.357293000	0.280216000	1.656489000
6	-1.359424000	-0.475425000	-0.313647000
6	-1.272822000	0.089603000	1.034682000
6	-0.177681000	-1.162765000	-2.404777000
6	1.018962000	-1.324370000	-3.082363000
6	-0.149018000	-0.678649000	-1.088075000
6	2.218196000	-1.012725000	-2.432620000
6	1.103505000	-0.372291000	-0.511335000
7	2.266535000	-0.548849000	-1.178785000
6	0.028649000	0.390614000	1.603392000
6	1.192788000	0.158266000	0.836151000
1	-1.133961000	-1.392515000	-2.863154000
1	1.044527000	-1.692658000	-4.101946000
1	3.174013000	-1.136070000	-2.927729000
6	0.178247000	0.903589000	2.901196000
7	2.432494000	0.415512000	1.312195000
6	2.553548000	0.900113000	2.552384000
6	1.453189000	1.156807000	3.377989000
1	-0.706750000	1.087110000	3.501588000
1	3.566162000	1.088686000	2.889337000
1	1.614801000	1.552934000	4.374578000
27	-3.983566000	-0.204467000	0.524619000
8	-3.902389000	1.574356000	-0.332974000
8	-5.299691000	0.455399000	1.835563000
8	-5.419062000	-0.775653000	-0.701018000
8	-3.981115000	-1.976072000	1.403752000
6	-4.673895000	2.540654000	-0.064833000
6	-5.655627000	2.619052000	0.915050000

6	-5.907041000	1.567664000	1.828211000
6	-6.066823000	-1.857108000	-0.594199000
6	-5.877566000	-2.898514000	0.306804000
6	-4.828742000	-2.905668000	1.256956000
1	-6.230958000	3.529686000	1.002241000
1	-6.537153000	-3.753212000	0.254874000
6	-4.412663000	3.768916000	-0.961100000
9	-3.161534000	4.239511000	-0.756759000
9	-4.519607000	3.444142000	-2.262938000
9	-5.269519000	4.787509000	-0.723601000
6	-7.192549000	-1.977007000	-1.643560000
9	-8.061986000	-0.951598000	-1.527214000
9	-6.685188000	-1.945490000	-2.892107000
9	-7.902356000	-3.122887000	-1.524595000
6	-4.661887000	-4.094083000	2.172456000
1	-5.389930000	-4.881937000	1.970861000
1	-3.648503000	-4.493519000	2.062542000
1	-4.766170000	-3.758141000	3.209895000
6	-6.960667000	1.745332000	2.894238000
1	-7.761571000	1.016275000	2.728166000
1	-6.523164000	1.529483000	3.874006000
1	-7.385138000	2.750648000	2.894685000

${}_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}{}_{\text{LS}}\text{Fe}^{\text{II}}$, **5** ($\text{R}_1 = \text{CF}_3$, $\text{R}_2 = \text{CF}_3$)

$E = -6202.22208$ a.u., $E^{\text{ZPE}} = -6201.63560$ a.u.

26	-4.377901000	0.000220000	0.000105000
7	-4.366707000	-1.791489000	-0.922030000
7	-4.872958000	-2.943561000	-0.397980000
7	-6.158986000	-1.905550000	1.510840000
7	-5.822906000	-0.607913000	1.263374000
7	-5.822844000	0.606324000	-1.264813000
7	-6.161979000	1.903292000	-1.511283000
7	-4.879299000	2.942951000	0.398849000
7	-4.370554000	1.791769000	0.922461000
5	-5.283748000	-3.121068000	1.093183000
1	-4.290028000	-3.191844000	1.778110000
1	-5.955230000	-4.116490000	1.181413000
5	-5.289623000	3.120416000	-1.092447000
1	-4.295619000	3.193630000	-1.776733000
1	-5.963140000	4.114478000	-1.180507000
6	-4.001890000	-2.073131000	-2.189757000
1	-3.588391000	-1.310690000	-2.828584000
6	-4.266499000	-3.408503000	-2.489541000
1	-4.084411000	-3.925567000	-3.418823000

6	-4.822438000	-3.920338000	-1.322499000
1	-5.178573000	-4.910791000	-1.081815000
6	-7.299597000	-1.944033000	2.229226000
1	-7.720363000	-2.893540000	2.524529000
6	-7.729494000	-0.643421000	2.459478000
1	-8.608447000	-0.322811000	2.996942000
6	-6.776955000	0.157406000	1.825366000
1	-6.739965000	1.231581000	1.735220000
6	-6.774460000	-0.160831000	-1.828401000
1	-6.734915000	-1.234990000	-1.739202000
6	-7.728491000	0.638235000	-2.462568000
1	-8.606177000	0.315930000	-3.001088000
6	-7.302032000	1.939662000	-2.230730000
1	-7.724756000	2.888411000	-2.525672000
6	-4.830903000	3.919482000	1.323728000
1	-5.189062000	4.909282000	1.083363000
6	-4.273889000	3.408409000	2.490597000
1	-4.092928000	3.925511000	3.420077000
6	-4.006347000	2.073748000	2.190298000
1	-3.591111000	1.312032000	2.828848000
8	1.981601000	0.564677000	-1.176930000
8	1.981854000	-0.565362000	1.175617000
6	0.818370000	0.304141000	-0.642114000
6	0.818503000	-0.304588000	0.641156000
6	-0.494923000	1.192308000	-2.581407000
6	-1.739448000	1.434676000	-3.132008000
6	-0.418107000	0.608932000	-1.302609000
6	-2.897632000	1.109161000	-2.409043000
6	-1.637098000	0.306088000	-0.642869000
7	-2.856378000	0.564391000	-1.189984000
6	-0.417829000	-0.608537000	1.302265000
6	-1.636951000	-0.305075000	0.643057000
1	0.420511000	1.433037000	-3.111854000
1	-1.841675000	1.879113000	-4.115818000
1	-3.881454000	1.283615000	-2.823452000
6	-0.494396000	-1.191123000	2.581473000
7	-2.856117000	-0.562177000	1.190973000
6	-2.897115000	-1.105990000	2.410428000
6	-1.738770000	-1.432057000	3.132953000
1	0.421145000	-1.432268000	3.111544000
1	-3.880841000	-1.279435000	2.825510000
1	-1.840809000	-1.875834000	4.117079000
27	3.351866000	0.000074000	-0.000627000
8	3.289652000	-1.714252000	-0.830420000
8	4.712890000	-0.481855000	1.253276000
8	4.712722000	0.482867000	-1.254393000

8	3.288528000	1.714221000	0.829307000
6	3.991450000	-2.696665000	-0.468946000
6	4.942562000	-2.755589000	0.552243000
6	5.224411000	-1.631518000	1.331175000
6	5.224910000	1.632323000	-1.330861000
6	4.942934000	2.755918000	-0.551273000
6	3.990806000	2.696709000	0.468933000
1	5.468878000	-3.679380000	0.737512000
1	5.469795000	3.679619000	-0.735435000
6	3.700926000	-3.966687000	-1.298965000
9	4.486549000	-5.002976000	-0.939947000
9	2.418999000	-4.346252000	-1.129975000
9	3.898769000	-3.733301000	-2.607033000
6	6.280437000	-1.737829000	2.452929000
9	6.886698000	-2.942664000	2.472349000
9	7.231724000	-0.800813000	2.293308000
9	5.703808000	-1.548878000	3.654857000
6	6.281782000	1.739156000	-2.451780000
9	7.232451000	0.801532000	-2.292476000
9	5.705812000	1.551694000	-3.654308000
9	6.888646000	2.943713000	-2.469626000
6	3.699514000	3.966455000	1.299094000
9	3.895632000	3.732553000	2.607309000
9	4.485791000	5.002718000	0.941461000
9	2.417850000	4.346336000	1.128605000

LSCo^{III}-SQ-HSFe^{II}, **5** (R₁= CF₃, R₂=CF₃)

E= -6202.21702 a.u., E^{ZPE}= -6201.63381 a.u.

26	-4.529903000	-0.001016000	-0.000107000
7	-4.529729000	1.977992000	0.964287000
7	-5.094853000	3.091546000	0.421469000
7	-6.333206000	2.032777000	-1.541425000
7	-5.957859000	0.726362000	-1.419404000
7	-5.960494000	-0.723901000	1.419029000
7	-6.339819000	-2.029211000	1.540913000
7	-5.102231000	-3.092230000	-0.420003000
7	-4.534170000	-1.980184000	-0.962870000
5	-5.425050000	3.221176000	-1.098833000
1	-4.393203000	3.198672000	-1.730048000
1	-6.041328000	4.242447000	-1.262904000
5	-5.434145000	-3.220064000	1.100116000
1	-4.402875000	-3.199189000	1.732315000
1	-6.052816000	-4.239856000	1.264347000
6	-4.210316000	2.287918000	2.234161000
1	-3.757988000	1.550184000	2.880383000

6	-4.564201000	3.608747000	2.522044000
1	-4.435533000	4.143717000	3.450420000
6	-5.121830000	4.079290000	1.337613000
1	-5.523591000	5.048289000	1.081100000
6	-7.508664000	2.101010000	-2.192445000
1	-7.962908000	3.060148000	-2.392640000
6	-7.927607000	0.810918000	-2.507567000
1	-8.827974000	0.517087000	-3.024742000
6	-6.925379000	-0.014022000	-1.996703000
1	-6.850159000	-1.091330000	-2.004123000
6	-6.926608000	0.019354000	1.994999000
1	-6.848307000	1.096435000	2.002326000
6	-7.931844000	-0.802563000	2.504827000
1	-8.831999000	-0.506012000	3.020820000
6	-7.516192000	-2.093940000	2.190616000
1	-7.973393000	-3.051725000	2.390579000
6	-5.130606000	-4.080312000	-1.335683000
1	-5.534654000	-5.048330000	-1.079048000
6	-4.570994000	-3.611549000	-2.519917000
1	-4.442822000	-4.147244000	-3.447944000
6	-4.214329000	-2.291428000	-2.232342000
1	-3.759689000	-1.555018000	-2.878450000
8	2.069548000	0.539922000	-1.185826000
8	2.069592000	-0.541522000	1.186329000
6	0.909937000	0.289624000	-0.648833000
6	0.909954000	-0.291735000	0.649154000
6	-0.384906000	1.133821000	-2.608374000
6	-1.618445000	1.375579000	-3.182896000
6	-0.328882000	0.575608000	-1.317748000
6	-2.780721000	1.061083000	-2.463942000
6	-1.554279000	0.286176000	-0.661418000
7	-2.753145000	0.530852000	-1.239986000
6	-0.328853000	-0.578471000	1.317757000
6	-1.554255000	-0.289446000	0.661259000
1	0.540747000	1.360389000	-3.127287000
1	-1.703726000	1.806959000	-4.174177000
1	-3.764969000	1.243978000	-2.881012000
6	-0.384891000	-1.137269000	2.608157000
7	-2.753107000	-0.534962000	1.239530000
6	-2.780723000	-1.065859000	2.463155000
6	-1.618407000	-1.380092000	3.182229000
1	0.540775000	-1.363541000	3.127178000
1	-3.764965000	-1.249814000	2.879760000
1	-1.703673000	-1.812067000	4.173251000
27	3.445754000	-0.000359000	0.000441000
8	3.382476000	-1.728404000	-0.797164000

8	4.804575000	-0.456980000	1.260666000
8	4.804397000	0.457288000	-1.259616000
8	3.381067000	1.727712000	0.797951000
6	4.095828000	-2.700363000	-0.428745000
6	5.054105000	-2.736991000	0.586702000
6	5.327995000	-1.601192000	1.350624000
6	5.326018000	1.602251000	-1.350456000
6	5.050552000	2.738111000	-0.587192000
6	4.092774000	2.700558000	0.428697000
1	5.590085000	-3.653440000	0.780755000
1	5.584998000	3.655293000	-0.782016000
6	3.810980000	-3.983156000	-1.241172000
9	4.603840000	-5.008694000	-0.869149000
9	2.531961000	-4.367084000	-1.064557000
9	4.005775000	-3.764840000	-2.552100000
6	6.389536000	-1.681710000	2.469325000
9	6.999416000	-2.883604000	2.508856000
9	7.336246000	-0.744603000	2.285065000
9	5.817836000	-1.470375000	3.669375000
6	6.387094000	1.683712000	-2.469527000
9	7.334606000	0.747354000	-2.285755000
9	5.815070000	1.472048000	-3.669390000
9	6.995986000	2.886109000	-2.509191000
6	3.806426000	3.983299000	1.240678000
9	4.002816000	3.766038000	2.551551000
9	4.597142000	5.010032000	0.867366000
9	2.526588000	4.364877000	1.065028000

$\text{HS-Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$, **5** ($\text{R}_1 = \text{CF}_3$, $\text{R}_2 = \text{CF}_3$)

$E = -6202.22567$ a.u., $E^{\text{ZPE}} = -6201.64213$ a.u.

26	4.570369000	-0.000096000	0.000011000
7	4.501102000	-1.916844000	0.620265000
7	5.121230000	-2.960374000	0.004452000
7	6.427561000	-1.610716000	-1.687563000
7	5.987921000	-0.370932000	-1.321914000
7	5.987860000	0.369899000	1.322273000
7	6.428278000	1.609364000	1.687994000
7	5.123169000	2.959745000	-0.004330000
7	4.502461000	1.916575000	-0.620183000
5	5.631219000	-2.933202000	-1.465298000
1	4.692554000	-2.988138000	-2.221366000
1	6.391212000	-3.851466000	-1.619963000
5	5.632824000	2.932307000	1.465559000
1	4.693986000	2.987827000	2.221366000
1	6.393314000	3.850140000	1.620354000

6	3.999671000	-2.386764000	1.781483000
1	3.480889000	-1.738465000	2.467761000
6	4.289111000	-3.743346000	1.916771000
1	4.018217000	-4.395507000	2.732248000
6	5.000820000	-4.063745000	0.767747000
1	5.415586000	-5.001433000	0.429152000
6	7.568040000	-1.483642000	-2.384780000
1	8.063234000	-2.361574000	-2.772323000
6	7.897812000	-0.132879000	-2.481437000
1	8.751628000	0.304564000	-2.974827000
6	6.887361000	0.525411000	-1.792275000
1	6.766432000	1.579119000	-1.599618000
6	6.886615000	-0.527056000	1.792779000
1	6.765008000	-1.580684000	1.600120000
6	7.897452000	0.130558000	2.482026000
1	8.750916000	-0.307470000	2.975509000
6	7.568572000	1.481532000	2.385398000
1	8.064261000	2.359139000	2.773043000
6	5.003336000	4.063208000	-0.767564000
1	5.418597000	5.000668000	-0.428940000
6	4.291376000	3.743274000	-1.916564000
1	4.020821000	4.395644000	-2.731988000
6	4.001176000	2.386854000	-1.781340000
1	3.482022000	1.738855000	-2.467616000
8	-1.766343000	0.428956000	1.259522000
8	-1.766195000	-0.429071000	-1.260370000
6	-0.655792000	0.237999000	0.688658000
6	-0.655697000	-0.237936000	-0.689426000
6	0.693738000	0.915802000	2.693138000
6	1.938065000	1.097647000	3.267443000
6	0.611366000	0.470634000	1.361129000
6	3.096354000	0.847000000	2.516120000
6	1.822456000	0.235940000	0.674432000
7	3.039751000	0.431881000	1.247918000
6	0.611526000	-0.470365000	-1.361813000
6	1.822533000	-0.235667000	-0.674987000
1	-0.226016000	1.098810000	3.239667000
1	2.041603000	1.434999000	4.292743000
1	4.081144000	0.977012000	2.943016000
6	0.694043000	-0.915364000	-2.693884000
7	3.039909000	-0.431529000	-1.248370000
6	3.096638000	-0.846439000	-2.516613000
6	1.938420000	-1.097031000	-3.268098000
1	-0.225662000	-1.098356000	-3.240501000
1	4.081461000	-0.976342000	-2.943464000
1	2.042089000	-1.434216000	-4.293440000

27	-3.407715000	-0.000149000	-0.000609000
8	-3.423119000	1.913490000	-0.783885000
8	-4.829382000	0.644843000	1.340111000
8	-4.829373000	-0.644962000	-1.341190000
8	-3.423622000	-1.913599000	0.783091000
6	-4.225241000	2.833880000	-0.495885000
6	-5.231604000	2.840173000	0.479422000
6	-5.434782000	1.743110000	1.329128000
6	-5.435770000	-1.742691000	-1.329393000
6	-5.233378000	-2.839388000	-0.479050000
6	-4.226716000	-2.833407000	0.495963000
1	-5.842195000	3.721828000	0.602138000
1	-5.844818000	-3.720557000	-0.601024000
6	-4.009362000	4.118901000	-1.330069000
9	-2.777812000	4.631264000	-1.093083000
9	-4.091039000	3.856713000	-2.648934000
9	-4.905920000	5.093452000	-1.054601000
6	-6.512957000	1.864013000	2.432520000
9	-7.205155000	3.025897000	2.374482000
9	-7.405228000	0.858638000	2.341554000
9	-5.944222000	1.798195000	3.656651000
6	-4.011785000	-4.118099000	1.330906000
9	-4.092862000	-3.854983000	2.649617000
9	-4.909321000	-5.091997000	1.056300000
9	-2.780781000	-4.631752000	1.093910000
6	-6.514320000	-1.863277000	-2.432439000
9	-7.405960000	-0.857331000	-2.341517000
9	-5.945905000	-1.798173000	-3.656750000
9	-7.207204000	-3.024723000	-2.373838000

$\text{HS-Co}^{\text{II}}\text{-BQ-HS-Fe}^{\text{II}}$, **5** ($\text{R}_1 = \text{CF}_3$, $\text{R}_2 = \text{CF}_3$)

$E = -6202.21727$ a.u., $E^{\text{ZPE}} = -6201.63780$ a.u.

26	-4.737997000	-0.000240000	-0.000176000
7	-4.729071000	-2.079717000	-0.681745000
7	-5.282090000	-3.113896000	0.011638000
7	-6.516696000	-1.800160000	1.813774000
7	-6.143868000	-0.521384000	1.512547000
7	-6.143347000	0.524419000	-1.511919000
7	-6.513117000	1.804074000	-1.813115000
7	-5.275160000	3.114933000	-0.011200000
7	-4.724589000	2.079482000	0.682223000
5	-5.607852000	-3.036474000	1.535895000
1	-4.573522000	-2.925646000	2.155247000
1	-6.218989000	-4.026404000	1.841723000
5	-5.601281000	3.038269000	-1.535390000

1	-4.567338000	2.925025000	-2.154955000
1	-6.210176000	4.029589000	-1.841181000
6	-4.410144000	-2.559400000	-1.899175000
1	-3.967614000	-1.915218000	-2.644460000
6	-4.752036000	-3.909271000	-2.000680000
1	-4.620297000	-4.565950000	-2.846744000
6	-5.301816000	-4.217503000	-0.760021000
1	-5.693770000	-5.145786000	-0.371643000
6	-7.687642000	-1.779322000	2.474831000
1	-8.139474000	-2.702306000	2.806957000
6	-8.107093000	-0.458400000	2.613574000
1	-9.004830000	-0.097919000	3.091518000
6	-7.110271000	0.290508000	1.990150000
1	-7.037730000	1.359099000	1.852315000
6	-7.111792000	-0.285210000	-1.989213000
1	-7.041801000	-1.353961000	-1.851261000
6	-8.106929000	0.466067000	-2.612470000
1	-9.005641000	0.107722000	-3.090184000
6	-7.684251000	1.785985000	-2.473921000
1	-8.133934000	2.710033000	-2.806005000
6	-5.292772000	4.218507000	0.760596000
1	-5.682694000	5.147655000	0.372243000
6	-4.743965000	3.908954000	2.001339000
1	-4.611034000	4.565249000	2.847515000
6	-4.404990000	2.558329000	1.899780000
1	-3.964196000	1.913080000	2.645172000
8	1.840624000	-0.397456000	1.263166000
8	1.840294000	0.397276000	-1.264675000
6	0.741958000	-0.221511000	0.718016000
6	0.741775000	0.220723000	-0.719428000
6	-0.595336000	-0.802477000	2.741944000
6	-1.834962000	-0.962628000	3.339358000
6	-0.535086000	-0.414743000	1.396323000
6	-2.985146000	-0.733502000	2.578273000
6	-1.745318000	-0.203434000	0.699489000
7	-2.947025000	-0.363250000	1.292344000
6	-0.535468000	0.413216000	-1.397611000
6	-1.745538000	0.201589000	-0.700561000
1	0.330553000	-0.964708000	3.284910000
1	-1.928210000	-1.263762000	4.376696000
1	-3.974309000	-0.850554000	3.006954000
6	-0.596073000	0.800545000	-2.743304000
7	-2.947428000	0.360821000	-1.293203000
6	-2.985834000	0.730643000	-2.579280000
6	-1.835876000	0.959942000	-3.340606000
1	0.329662000	0.963027000	-3.286459000

1	-3.975090000	0.847093000	-3.007921000
1	-1.929398000	1.260687000	-4.378031000
27	3.555294000	0.000155000	-0.000863000
8	3.517892000	1.896630000	0.765708000
8	4.943137000	0.654600000	-1.346478000
8	4.943465000	-0.654348000	1.344660000
8	3.517188000	-1.896700000	-0.766738000
6	4.334278000	2.818588000	0.511900000
6	5.357185000	2.830442000	-0.444025000
6	5.560191000	1.748062000	-1.312092000
6	5.559008000	-1.748679000	1.311621000
6	5.354736000	-2.831753000	0.444693000
6	4.332221000	-2.819496000	-0.511635000
1	5.976921000	3.708788000	-0.543280000
1	5.973242000	-3.710836000	0.545088000
6	4.109697000	4.088125000	1.365395000
9	2.883100000	4.604450000	1.119879000
9	4.173941000	3.798007000	2.678740000
9	5.013034000	5.061297000	1.117633000
6	6.646988000	1.877333000	-2.405390000
9	7.343740000	3.032953000	-2.322305000
9	7.529680000	0.863974000	-2.319663000
9	6.084798000	1.832366000	-3.632269000
6	4.106314000	-4.089587000	-1.363955000
9	4.171854000	-3.800918000	-2.677570000
9	5.008036000	-5.063845000	-1.114600000
9	2.878787000	-4.603846000	-1.118738000
6	6.645345000	-1.878284000	2.405350000
9	7.529006000	-0.865808000	2.319330000
9	6.082772000	-1.832062000	3.632020000
9	7.341044000	-3.034605000	2.323211000

${}_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}{}_{\text{LS}}\text{Fe}^{\text{II}}$, **6** (R=Ph)

E= -5583.55901 a.u., E^{ZPE}= -5582.71262 a.u.

26	-4.038710000	0.000000000	-0.000002000
7	-4.043754000	2.017474000	0.316210000
7	-4.580112000	2.938038000	-0.530320000
7	-5.861490000	1.336656000	-2.012705000
7	-5.501280000	0.177260000	-1.391746000
7	-5.501278000	-0.177256000	1.391745000
7	-5.861489000	-1.336651000	2.012704000
7	-4.580112000	-2.938036000	0.530324000
7	-4.043761000	-2.017474000	-0.316212000
5	-4.998393000	2.628947000	-1.997813000
1	-4.006306000	2.492354000	-2.678511000

1	-5.680330000	3.541460000	-2.392795000
5	-4.998391000	-2.628940000	1.997817000
1	-4.006303000	-2.492343000	2.678514000
1	-5.680327000	-3.541453000	2.392803000
6	-3.673081000	2.687250000	1.422864000
1	-3.243346000	2.168213000	2.264213000
6	-3.962774000	4.049235000	1.296276000
1	-3.791028000	4.832636000	2.018446000
6	-4.541437000	4.160146000	0.038768000
1	-4.923303000	5.017592000	-0.494866000
6	-7.007108000	1.144716000	-2.700323000
1	-7.444218000	1.957392000	-3.261058000
6	-7.416140000	-0.171004000	-2.529223000
1	-8.293844000	-0.649170000	-2.936149000
6	-6.444406000	-0.732403000	-1.694836000
1	-6.388631000	-1.730127000	-1.288770000
6	-6.444399000	0.732411000	1.694840000
1	-6.388621000	1.730135000	1.288776000
6	-7.416136000	0.171012000	2.529223000
1	-8.293840000	0.649179000	2.936149000
6	-7.007108000	-1.144710000	2.700320000
1	-7.444220000	-1.957386000	3.261053000
6	-4.541440000	-4.160145000	-0.038761000
1	-4.923306000	-5.017590000	0.494875000
6	-3.962778000	-4.049238000	-1.296270000
1	-3.791032000	-4.832641000	-2.018438000
6	-3.673086000	-2.687253000	-1.422863000
1	-3.243353000	-2.168218000	-2.264214000
8	2.300687000	-0.125882000	1.298680000
8	2.300687000	0.125883000	-1.298683000
6	1.156483000	-0.076646000	0.716021000
6	1.156484000	0.076647000	-0.716024000
6	-0.165780000	-0.309901000	2.836935000
6	-1.416265000	-0.370554000	3.427708000
6	-0.091748000	-0.161078000	1.442100000
6	-2.566658000	-0.291635000	2.632999000
6	-1.298787000	-0.086730000	0.715335000
7	-2.520827000	-0.158805000	1.300351000
6	-0.091747000	0.161077000	-1.442104000
6	-1.298787000	0.086729000	-0.715339000
1	0.748755000	-0.367617000	3.417153000
1	-1.525432000	-0.483259000	4.500962000
1	-3.554753000	-0.332493000	3.071825000
6	-0.165780000	0.309896000	-2.836940000
7	-2.520827000	0.158800000	-1.300356000
6	-2.566657000	0.291626000	-2.633005000

6	-1.416264000	0.370545000	-3.427713000
1	0.748756000	0.367611000	-3.417158000
1	-3.554752000	0.332480000	-3.071831000
1	-1.525430000	0.483245000	-4.500967000
27	3.756710000	0.000000000	-0.000001000
7	3.751991000	1.974788000	0.041477000
8	5.061462000	-0.116218000	-1.350195000
8	5.061460000	0.116216000	1.350195000
7	3.751985000	-1.974789000	-0.041480000
6	5.644616000	0.855500000	-1.988810000
6	5.384457000	2.242299000	-1.764317000
6	4.470268000	2.695346000	-0.765800000
1	4.389567000	3.780448000	-0.658894000
6	2.912450000	2.678965000	0.966044000
6	3.134744000	2.553292000	2.341539000
6	2.330969000	3.257619000	3.234190000
1	2.514280000	3.170390000	4.301398000
6	1.297119000	4.074112000	2.767761000
6	1.070098000	4.187207000	1.397191000
1	0.262227000	4.810411000	1.025493000
6	1.875740000	3.490854000	0.494308000
1	1.696083000	3.563848000	-0.574357000
6	5.644600000	-0.855504000	1.988822000
6	5.384433000	-2.242302000	1.764332000
6	4.470252000	-2.695347000	0.765806000
1	4.389549000	-3.780449000	0.658901000
6	2.912452000	-2.678963000	-0.966055000
6	3.134754000	-2.553284000	-2.341548000
1	3.934158000	-1.906143000	-2.683303000
6	2.330986000	-3.257608000	-3.234207000
1	2.514304000	-3.170374000	-4.301413000
6	1.297134000	-4.074104000	-2.767787000
6	1.070105000	-4.187205000	-1.397220000
1	0.262232000	-4.810411000	-1.025529000
6	1.875740000	-3.490855000	-0.494329000
1	1.696076000	-3.563853000	0.574335000
1	3.934147000	1.906154000	2.683302000
6	6.071112000	3.218520000	-2.529240000
6	6.989057000	2.865967000	-3.494740000
6	6.605051000	-0.519441000	2.982719000
6	7.250496000	-1.497433000	3.711738000
6	6.071073000	-3.218525000	2.529266000
6	6.989010000	-2.865974000	3.494774000
6	6.605076000	0.519435000	-2.982700000
6	7.250536000	1.497425000	-3.711707000
1	6.813133000	0.533538000	3.143324000

1	7.977672000	-1.203687000	4.464529000
1	7.505560000	-3.624339000	4.073155000
1	5.858158000	-4.267665000	2.336351000
1	6.813152000	-0.533545000	-3.143307000
1	7.977717000	1.203678000	-4.464492000
1	7.505618000	3.624331000	-4.073112000
1	5.858203000	4.267661000	-2.336323000
1	0.671470000	4.616790000	3.470140000
1	0.671490000	-4.616780000	-3.470173000

${}_{\text{LS}}\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$, **6** (R=Ph)

E= -5583.55286 a.u., E^{ZPE} = -5582.71079 a.u.

26	4.202180000	0.012603000	-0.004148000
7	4.266210000	2.201607000	-0.434791000
7	4.849495000	3.119703000	0.381650000
7	6.028898000	1.564962000	2.027811000
7	5.629922000	0.336678000	1.587090000
7	5.621447000	-0.381572000	-1.582892000
7	5.962229000	-1.627142000	-2.023450000
7	4.704822000	-3.130709000	-0.386868000
7	4.174042000	-2.187186000	0.435950000
5	5.146521000	2.842955000	1.889610000
1	4.100026000	2.680232000	2.476443000
1	5.773368000	3.776691000	2.323473000
5	5.018483000	-2.862259000	-1.892465000
1	3.983854000	-2.646222000	-2.482431000
1	5.601537000	-3.822649000	-2.329177000
6	3.996606000	2.832217000	-1.590142000
1	3.541326000	2.297153000	-2.411012000
6	4.402612000	4.170633000	-1.529912000
1	4.325227000	4.925002000	-2.298107000
6	4.938322000	4.306158000	-0.253988000
1	5.366187000	5.161737000	0.247239000
6	7.208579000	1.451961000	2.667235000
1	7.679835000	2.324467000	3.095116000
6	7.606360000	0.118412000	2.648319000
1	8.504081000	-0.308964000	3.068115000
6	6.585879000	-0.537059000	1.955447000
1	6.491026000	-1.580985000	1.695049000
6	6.619152000	0.446409000	-1.946572000
1	6.573407000	1.493540000	-1.685332000
6	7.609055000	-0.256387000	-2.636994000
1	8.527503000	0.128033000	-3.053418000
6	7.148114000	-1.569492000	-2.658615000
1	7.578640000	-2.463014000	-3.085996000

6	4.735869000	-4.323243000	0.243689000
1	5.118665000	-5.197003000	-0.262556000
6	4.213498000	-4.165643000	1.522261000
1	4.101508000	-4.917984000	2.288212000
6	3.878641000	-2.807588000	1.590125000
1	3.457235000	-2.253275000	2.416323000
8	-2.399597000	0.174088000	1.292964000
8	-2.400704000	-0.134519000	-1.299583000
6	-1.255976000	0.118828000	0.707621000
6	-1.256503000	-0.064449000	-0.717125000
6	0.048289000	0.414368000	2.817325000
6	1.283940000	0.507166000	3.432390000
6	-0.006463000	0.223940000	1.426186000
6	2.442549000	0.406494000	2.651363000
6	1.213459000	0.132411000	0.713099000
7	2.412081000	0.221265000	1.329875000
6	-0.007171000	-0.157425000	-1.438222000
6	1.213400000	-0.065281000	-0.726210000
1	-0.878498000	0.484291000	3.376981000
1	1.371613000	0.660721000	4.502546000
1	3.429371000	0.483930000	3.095296000
6	0.046371000	-0.339803000	-2.830300000
7	2.412287000	-0.151577000	-1.342999000
6	2.440865000	-0.329236000	-2.665796000
6	1.282005000	-0.425062000	-3.446769000
1	-0.880728000	-0.409098000	-3.389508000
1	3.426982000	-0.404818000	-3.111627000
1	1.369297000	-0.571098000	-4.518020000
27	-3.854807000	0.002217000	-0.000236000
7	-3.825469000	-1.971052000	0.085146000
8	-5.164767000	0.071638000	-1.349088000
8	-5.155505000	-0.099813000	1.355189000
7	-3.872765000	1.975248000	-0.085781000
6	-5.744461000	-0.921204000	-1.957359000
6	-5.469779000	-2.299513000	-1.699610000
6	-4.541867000	-2.718602000	-0.698839000
1	-4.446843000	-3.799956000	-0.568104000
6	-2.968348000	-2.643507000	1.017149000
6	-3.186041000	-2.498375000	2.391414000
6	-2.363328000	-3.170621000	3.291624000
1	-2.542930000	-3.068656000	4.358184000
6	-1.315129000	-3.973510000	2.833626000
6	-1.093028000	-4.106000000	1.463998000
1	-0.274139000	-4.718735000	1.098950000
6	-1.918125000	-3.442642000	0.553752000
1	-1.743482000	-3.531445000	-0.514535000

6	-5.740099000	0.879187000	1.980838000
6	-5.493140000	2.263645000	1.727701000
6	-4.591826000	2.705153000	0.712388000
1	-4.523482000	3.788597000	0.582398000
6	-3.047811000	2.667963000	-1.031637000
6	-3.275059000	2.505740000	-2.402518000
1	-4.066834000	1.839173000	-2.724041000
6	-2.486324000	3.199912000	-3.316271000
1	-2.674038000	3.084290000	-4.380030000
6	-1.462159000	4.042510000	-2.875503000
6	-1.229868000	4.191930000	-1.509303000
1	-0.429433000	4.835808000	-1.157150000
6	-2.020594000	3.506016000	-0.585483000
1	-1.836627000	3.607580000	0.480121000
1	-3.996364000	-1.861336000	2.726510000
6	-6.153709000	-3.301150000	-2.433508000
6	-7.082793000	-2.981815000	-3.399912000
6	-6.689465000	0.554691000	2.989273000
6	-7.336893000	1.541197000	3.704835000
6	-6.181762000	3.248715000	2.479483000
6	-7.088573000	2.907421000	3.459424000
6	-6.715712000	-0.619548000	-2.951883000
6	-7.358271000	-1.621676000	-3.649974000
1	-6.887452000	-0.496685000	3.171718000
1	-8.055277000	1.256097000	4.469308000
1	-7.606589000	3.672580000	4.027459000
1	-5.979556000	4.295681000	2.264428000
1	-6.934370000	0.427088000	-3.137954000
1	-8.094154000	-1.353886000	-4.403988000
1	-7.597217000	-3.759431000	-3.954130000
1	-5.929622000	-4.343061000	-2.215590000
1	-0.674460000	-4.490663000	3.541618000
1	-0.848046000	4.577076000	-3.594022000

$\text{HS}^{\text{Co}^{\text{II}}}\text{-BQ-}_{\text{LS}}\text{Fe}^{\text{II}}$, **6** (R=Ph)

E= -5583.53789 a.u., E^{ZPE} = -5582.69540 a.u.

26	4.103642000	-0.045808000	-0.009066000
7	4.065373000	1.933138000	-0.512228000
7	4.586496000	2.938359000	0.242724000
7	5.919204000	1.506615000	1.845995000
7	5.582531000	0.288510000	1.333154000
7	5.545759000	-0.327578000	-1.403492000
7	5.910070000	-1.533443000	-1.926240000
7	4.694155000	-3.008903000	-0.270547000
7	4.154857000	-2.022821000	0.496621000

5	5.023226000	2.770779000	1.727416000
1	4.039602000	2.669221000	2.426790000
1	5.683741000	3.730930000	2.035228000
5	5.070052000	-2.831894000	-1.770501000
1	4.058307000	-2.773819000	-2.433768000
1	5.756976000	-3.766421000	-2.098728000
6	3.676110000	2.491032000	-1.673545000
1	3.252560000	1.889674000	-2.461578000
6	3.938624000	3.864093000	-1.674335000
1	3.746772000	4.574248000	-2.463948000
6	4.520370000	4.101749000	-0.436030000
1	4.886835000	5.012136000	0.014190000
6	7.079368000	1.404869000	2.528379000
1	7.502373000	2.274173000	3.009351000
6	7.522264000	0.090520000	2.464073000
1	8.418716000	-0.327208000	2.895850000
6	6.554897000	-0.566385000	1.697257000
1	6.521369000	-1.596563000	1.379055000
6	6.469579000	0.563199000	-1.806219000
1	6.408033000	1.592474000	-1.489478000
6	7.432169000	-0.058329000	-2.607675000
1	8.294531000	0.392519000	-3.074177000
6	7.038724000	-1.389082000	-2.652354000
1	7.477229000	-2.243112000	-3.146632000
6	4.698205000	-4.170741000	0.414257000
1	5.087526000	-5.067360000	-0.044283000
6	4.145701000	-3.951638000	1.669141000
1	4.006233000	-4.665618000	2.466207000
6	3.825380000	-2.591037000	1.671296000
1	3.400585000	-2.004690000	2.469871000
8	-2.207773000	0.214947000	1.341261000
8	-2.241930000	-0.300574000	-1.193770000
6	-1.091276000	0.095849000	0.785769000
6	-1.105500000	-0.202620000	-0.657506000
6	0.277610000	0.505198000	2.849597000
6	1.538495000	0.611064000	3.414604000
6	0.182638000	0.233716000	1.477326000
6	2.672496000	0.460288000	2.610134000
6	1.373444000	0.086225000	0.739303000
7	2.604569000	0.209576000	1.293119000
6	0.142550000	-0.362627000	-1.380218000
6	1.354384000	-0.219904000	-0.674448000
1	-0.629307000	0.619269000	3.433882000
1	1.666046000	0.817052000	4.471742000
1	3.668334000	0.537525000	3.025934000
6	0.200775000	-0.638431000	-2.754768000

7	2.569612000	-0.343511000	-1.261297000
6	2.601932000	-0.600321000	-2.578598000
6	1.445869000	-0.753713000	-3.351022000
1	-0.721077000	-0.745437000	-3.316287000
1	3.585798000	-0.677601000	-3.021540000
1	1.544584000	-0.964042000	-4.410410000
27	-3.908445000	0.015213000	-0.021122000
7	-4.081122000	-2.096903000	0.303168000
8	-5.118032000	-0.151299000	-1.535470000
8	-5.102300000	0.381799000	1.444869000
7	-3.764227000	2.162733000	-0.323652000
6	-5.738298000	-1.166310000	-2.057368000
6	-5.595982000	-2.514384000	-1.585868000
6	-4.782716000	-2.879339000	-0.460940000
1	-4.789521000	-3.948903000	-0.220811000
6	-3.333704000	-2.719048000	1.346253000
6	-3.478016000	-2.259845000	2.661980000
6	-2.763323000	-2.868985000	3.690100000
1	-2.894663000	-2.520447000	4.710726000
6	-1.883044000	-3.919777000	3.419307000
6	-1.721953000	-4.361982000	2.106817000
1	-1.029346000	-5.168134000	1.882733000
6	-2.444494000	-3.767134000	1.071877000
1	-2.304733000	-4.097428000	0.046527000
6	-5.437085000	1.461185000	2.087953000
6	-5.023484000	2.775158000	1.690817000
6	-4.238766000	3.032018000	0.514514000
1	-4.058585000	4.093504000	0.307701000
6	-2.997933000	2.667346000	-1.415131000
6	-3.303994000	2.248580000	-2.716824000
1	-4.118236000	1.546141000	-2.856370000
6	-2.566468000	2.737364000	-3.792052000
1	-2.821199000	2.423100000	-4.800447000
6	-1.505736000	3.623107000	-3.584370000
6	-1.184552000	4.020056000	-2.286779000
1	-0.349130000	4.691481000	-2.110783000
6	-1.927559000	3.547975000	-1.204183000
1	-1.664012000	3.842026000	-0.192165000
1	-4.156482000	-1.436318000	2.853817000
6	-6.302823000	-3.554228000	-2.236014000
6	-7.132263000	-3.310137000	-3.312540000
6	-6.264704000	1.347822000	3.237612000
6	-6.643690000	2.461242000	3.962493000
6	-5.437427000	3.890583000	2.454996000
6	-6.228921000	3.750464000	3.578865000
6	-6.607313000	-0.945193000	-3.161844000

6	-7.280614000	-1.986372000	-3.769564000
1	-6.588604000	0.351680000	3.522424000
1	-7.274467000	2.338261000	4.839115000
1	-6.532946000	4.619990000	4.152052000
1	-5.118623000	4.880875000	2.136850000
1	-6.722433000	0.077769000	-3.506392000
1	-7.935694000	-1.779153000	-4.611920000
1	-7.664639000	-4.122729000	-3.795541000
1	-6.182099000	-4.569680000	-1.864714000
1	-1.323742000	-4.386185000	4.224858000
1	-0.930017000	3.994406000	-4.427023000

${}_{\text{HS}}\text{Co}^{\text{II}}\text{-BQ-}{}_{\text{HS}}\text{Fe}^{\text{II}}$, **6** (R=Ph)

E= -5583.53140 a.u., E^{ZPE}= -5582.69340 a.u.

26	-4.280200000	0.000027000	0.000152000
7	-4.298124000	2.165548000	0.568050000
7	-4.857757000	3.144597000	-0.191527000
7	-6.073551000	1.715406000	-1.923593000
7	-5.699021000	0.453353000	-1.563589000
7	-5.699145000	-0.453137000	1.563724000
7	-6.073868000	-1.715114000	1.923765000
7	-4.858226000	-3.144546000	0.191773000
7	-4.298500000	-2.165592000	-0.567839000
5	-5.163942000	2.964322000	-1.711556000
1	-4.122768000	2.814676000	-2.311705000
1	-5.771392000	3.934703000	-2.088407000
5	-5.164410000	-2.964161000	1.711781000
1	-4.123240000	-2.814555000	2.311930000
1	-5.771986000	-3.934440000	2.088686000
6	-4.014430000	2.719271000	1.758738000
1	-3.574225000	2.125572000	2.546972000
6	-4.386467000	4.068871000	1.778591000
1	-4.289881000	4.774001000	2.590109000
6	-4.917655000	4.293352000	0.513730000
1	-5.324503000	5.187322000	0.064789000
6	-7.255709000	1.667056000	-2.566339000
1	-7.709884000	2.574486000	-2.936056000
6	-7.680055000	0.343247000	-2.632635000
1	-8.586372000	-0.038271000	-3.077345000
6	-6.672702000	-0.375864000	-1.985590000
1	-6.598839000	-1.436340000	-1.794230000
6	-6.672662000	0.376275000	1.985726000
1	-6.598625000	1.436729000	1.794314000
6	-7.680111000	-0.342648000	2.632824000
1	-8.586349000	0.039035000	3.077554000

6	-7.255998000	-1.666534000	2.566539000
1	-7.710316000	-2.573877000	2.936292000
6	-4.918380000	-4.293298000	-0.513480000
1	-5.325330000	-5.187204000	-0.064508000
6	-4.387197000	-4.068913000	-1.778356000
1	-4.290751000	-4.774074000	-2.589864000
6	-4.014955000	-2.719366000	-1.758536000
1	-3.574706000	-2.125737000	-2.546798000
8	2.314643000	0.258782000	-1.265212000
8	2.314731000	-0.258582000	1.264968000
6	1.187614000	0.149779000	-0.719203000
6	1.187656000	-0.149713000	0.719011000
6	-0.129953000	0.576805000	-2.798467000
6	-1.368861000	0.700398000	-3.404465000
6	-0.073835000	0.297260000	-1.424516000
6	-2.521883000	0.544028000	-2.628017000
6	-1.287224000	0.149447000	-0.715572000
7	-2.486902000	0.273402000	-1.318498000
6	-0.073723000	-0.297481000	1.424376000
6	-1.287177000	-0.149718000	0.715527000
1	0.796837000	0.686990000	-3.351821000
1	-1.460961000	0.920909000	-4.462396000
1	-3.511073000	0.644850000	-3.061597000
6	-0.129711000	-0.577188000	2.798298000
7	-2.486825000	-0.273723000	1.318523000
6	-2.521663000	-0.544448000	2.628032000
6	-1.368575000	-0.700917000	3.404362000
1	0.797123000	-0.687357000	3.351579000
1	-3.510795000	-0.645238000	3.061746000
1	-1.460596000	-0.921605000	4.462263000
27	3.994934000	-0.000054000	-0.000071000
7	4.021539000	2.132801000	0.319502000
8	5.201904000	0.264260000	-1.492199000
8	5.202438000	-0.264193000	1.491541000
7	4.021560000	-2.132877000	-0.319405000
6	5.710551000	1.319539000	-2.054318000
6	5.449973000	2.657634000	-1.607891000
6	4.634902000	2.965015000	-0.466311000
1	4.558653000	4.033638000	-0.234031000
6	3.253081000	2.696951000	1.380197000
6	3.458409000	2.245512000	2.690597000
6	2.722582000	2.798180000	3.735626000
1	2.900671000	2.457722000	4.751935000
6	1.762180000	3.782544000	3.487785000
6	1.540300000	4.214237000	2.180636000
1	0.784012000	4.965880000	1.973768000

6	2.282888000	3.676786000	1.128575000
1	2.096799000	3.998451000	0.107812000
6	5.711700000	-1.319325000	2.053419000
6	5.451105000	-2.657480000	1.607218000
6	4.635387000	-2.965008000	0.466152000
1	4.558987000	-4.033651000	0.234029000
6	3.252546000	-2.697196000	-1.379627000
6	3.457380000	-2.246130000	-2.690233000
1	4.197151000	-1.472427000	-2.862778000
6	2.721022000	-2.798958000	-3.734796000
1	2.898724000	-2.458793000	-4.751271000
6	1.760581000	-3.783121000	-3.486286000
6	1.539207000	-4.214446000	-2.178935000
1	0.782915000	-4.965942000	-1.971545000
6	2.282326000	-3.676821000	-1.127330000
1	2.096655000	-3.998213000	-0.106403000
1	4.198150000	1.471669000	2.862628000
6	6.042485000	3.744095000	-2.293453000
6	6.868292000	3.554224000	-3.384176000
6	6.575766000	-1.153755000	3.170612000
6	7.134455000	-2.239975000	3.815211000
6	6.044202000	-3.743808000	2.292492000
6	6.870645000	-3.553715000	3.382690000
6	6.573971000	1.154209000	-3.172063000
6	7.132068000	2.240555000	-3.816947000
1	6.780373000	-0.138386000	3.495423000
1	7.789104000	-2.076333000	4.667383000
1	7.314536000	-4.401382000	3.893982000
1	5.837248000	-4.751504000	1.938619000
1	6.778564000	0.138893000	-3.497048000
1	7.786222000	2.077074000	-4.669530000
1	7.311713000	4.402009000	-3.895676000
1	5.835583000	4.751734000	-1.939386000
1	1.185120000	-4.204970000	-4.304892000
1	1.187131000	4.204265000	4.306747000

$LSCo^{III}\text{-}SQ\text{-}LSFe^{II}$, **6** (R=Ph-*p*-NO₂)

E= -5992.49433 a.u., E^{ZPE}= -5991.64349 a.u.

26	4.053285000	-0.000070000	0.000012000
7	4.055848000	-1.846734000	-0.865359000
7	4.565591000	-2.131269000	-2.094699000
7	5.847611000	0.023233000	-2.431736000
7	5.509438000	0.625561000	-1.255639000
7	5.509391000	-0.625786000	1.255655000
7	5.847615000	-0.023461000	2.431738000

7	4.565636000	2.131082000	2.094763000
7	4.056020000	1.846582000	0.865366000
5	4.970521000	-1.048932000	-3.136767000
1	3.971302000	-0.548451000	-3.604462000
1	5.635811000	-1.578012000	-3.991266000
5	4.970586000	1.048729000	3.136808000
1	3.971376000	0.548273000	3.604554000
1	5.635926000	1.577787000	3.991281000
6	3.692994000	-3.023620000	-0.321508000
1	3.289494000	-3.070478000	0.676974000
6	3.958274000	-4.077651000	-1.200266000
1	3.777280000	-5.129871000	-1.042909000
6	4.515734000	-3.461604000	-2.312889000
1	4.876377000	-3.870552000	-3.244857000
6	6.988591000	0.567259000	-2.905429000
1	7.410521000	0.216150000	-3.835313000
6	7.416993000	1.548759000	-2.021721000
1	8.296664000	2.169110000	-2.098145000
6	6.461593000	1.540557000	-1.000853000
1	6.422892000	2.129765000	-0.098069000
6	6.461472000	-1.540861000	1.000882000
1	6.422719000	-2.130082000	0.098108000
6	7.416866000	-1.549130000	2.021755000
1	8.296482000	-2.169557000	2.098193000
6	6.988565000	-0.567556000	2.905428000
1	7.410533000	-0.216452000	3.835296000
6	4.515746000	3.461410000	2.312989000
1	4.876292000	3.870334000	3.245004000
6	3.958432000	4.077491000	1.200311000
1	3.777479000	5.129719000	1.042958000
6	3.693232000	3.023484000	0.321503000
1	3.289840000	3.070363000	-0.677022000
8	-2.286128000	-0.604710000	1.154643000
8	-2.286101000	0.604668000	-1.154735000
6	-1.137324000	-0.328968000	0.639913000
6	-1.137307000	0.328880000	-0.640002000
6	0.182947000	-1.321445000	2.530504000
6	1.433565000	-1.613123000	3.047381000
6	0.108148000	-0.664759000	1.290300000
6	2.583211000	-1.238452000	2.341009000
6	1.315481000	-0.326793000	0.641475000
7	2.537561000	-0.597369000	1.164544000
6	0.108180000	0.664652000	-1.290370000
6	1.315497000	0.326688000	-0.641511000
1	-0.729596000	-1.591734000	3.050758000
1	1.543377000	-2.125757000	3.996740000

1	3.570826000	-1.461950000	2.721289000
6	0.183015000	1.321363000	-2.530557000
7	2.537590000	0.597299000	-1.164528000
6	2.583272000	1.238405000	-2.340978000
6	1.433646000	1.613071000	-3.047385000
1	-0.729512000	1.591649000	-3.050841000
1	3.570898000	1.461927000	-2.721217000
1	1.543481000	2.125725000	-3.996730000
27	-3.734650000	0.000117000	-0.000001000
7	-3.726722000	-1.680605000	-1.042159000
8	-5.041985000	0.828847000	-1.069604000
8	-5.042089000	-0.828362000	1.069688000
7	-3.726360000	1.680835000	1.042165000
6	-5.609317000	0.368510000	-2.145464000
6	-5.336955000	-0.912712000	-2.719391000
6	-4.431290000	-1.836991000	-2.126561000
1	-4.346325000	-2.802215000	-2.632717000
6	-2.898309000	-2.771554000	-0.644256000
6	-3.081265000	-3.359516000	0.615250000
6	-2.284562000	-4.427878000	1.002660000
1	-2.413744000	-4.907983000	1.965193000
6	-1.300456000	-4.892415000	0.129843000
6	-1.096866000	-4.319589000	-1.121292000
1	-0.314436000	-4.700373000	-1.766604000
6	-1.901515000	-3.250932000	-1.505136000
1	-1.744952000	-2.772551000	-2.466761000
6	-5.609218000	-0.367960000	2.145617000
6	-5.336532000	0.913189000	2.719572000
6	-4.430758000	1.837309000	2.126667000
1	-4.345546000	2.802500000	2.632844000
6	-2.897786000	2.771629000	0.644198000
6	-3.080766000	3.359663000	-0.615272000
1	-3.850211000	2.965270000	-1.267709000
6	-2.283874000	4.427855000	-1.002759000
1	-2.413048000	4.907987000	-1.965280000
6	-1.299577000	4.892179000	-0.130042000
6	-1.095972000	4.319296000	1.121063000
1	-0.313403000	4.699914000	1.766305000
6	-1.900789000	3.250786000	1.504971000
1	-1.744202000	2.772345000	2.466562000
1	-3.850550000	-2.964944000	1.267768000
6	-6.009914000	-1.309151000	-3.905039000
6	-6.921982000	-0.485955000	-4.525491000
6	-6.565379000	-1.192108000	2.800757000
6	-7.194458000	-0.774703000	3.955181000
6	-6.009278000	1.309720000	3.905307000

6	-6.921449000	0.486688000	4.525828000
6	-6.565374000	1.192837000	-2.800531000
6	-7.194668000	0.775519000	-3.954867000
1	-6.783795000	-2.158134000	2.357176000
1	-7.918543000	-1.431409000	4.430429000
1	-7.426400000	0.801338000	5.432546000
1	-5.788325000	2.290470000	4.320243000
1	-6.783538000	2.158924000	-2.356957000
1	-7.918671000	1.432352000	-4.430063000
1	-7.427094000	-0.800535000	-5.432144000
1	-5.789206000	-2.289963000	-4.319960000
7	-0.441946000	6.019776000	-0.549404000
8	0.374877000	6.448744000	0.261384000
8	-0.593603000	6.458705000	-1.687189000
7	-0.443027000	-6.020202000	0.549118000
8	-0.594952000	-6.459370000	1.686774000
8	0.373898000	-6.449082000	-0.261614000

$LS\text{Co}^{\text{III}}\text{-SQ-}_{\text{HS}}\text{Fe}^{\text{II}}$, **6** (R=Ph-*p*-NO₂)

E= -5992.48834 a.u., E^{ZPE}= -5991.64169 a.u.

26	4.227818000	0.038566000	0.002400000
7	4.267326000	2.044927000	0.922434000
7	4.859892000	2.326835000	2.114955000
7	6.069049000	0.116240000	2.531729000
7	5.661718000	-0.619507000	1.456747000
7	5.635162000	0.647474000	-1.499845000
7	5.984695000	-0.103630000	-2.584582000
7	4.715105000	-2.273967000	-2.132126000
7	4.178263000	-1.974442000	-0.917829000
5	5.192035000	1.232419000	3.177345000
1	4.158890000	0.749503000	3.584468000
1	5.832664000	1.747253000	4.058095000
5	5.052600000	-1.190313000	-3.203350000
1	4.025341000	-0.673014000	-3.582838000
1	5.650770000	-1.725504000	-4.101726000
6	3.951897000	3.225985000	0.361188000
1	3.481346000	3.262113000	-0.610440000
6	4.335223000	4.284663000	1.190344000
1	4.214933000	5.342647000	1.014365000
6	4.907326000	3.662379000	2.294657000
1	5.333722000	4.074644000	3.197139000
6	7.240195000	-0.366539000	2.986477000
1	7.716838000	0.084279000	3.844372000
6	7.623515000	-1.445022000	2.193898000
1	8.511795000	-2.050550000	2.288080000

6	6.604517000	-1.559311000	1.247173000
1	6.501123000	-2.255629000	0.428014000
6	6.614673000	1.555773000	-1.321895000
1	6.560580000	2.256690000	-0.501866000
6	7.599710000	1.405923000	-2.299171000
1	8.504259000	1.981473000	-2.422029000
6	7.156728000	0.339229000	-3.076257000
1	7.591599000	-0.129132000	-3.946801000
6	4.702257000	-3.609858000	-2.318016000
1	5.079962000	-4.034436000	-3.236372000
6	4.145693000	-4.214136000	-1.196112000
1	3.987034000	-5.266893000	-1.018990000
6	3.836377000	-3.144737000	-0.349712000
1	3.403181000	-3.167386000	0.639497000
8	-2.370170000	-0.589297000	1.177197000
8	-2.380695000	0.595735000	-1.149882000
6	-1.221058000	-0.299385000	0.656648000
6	-1.226591000	0.339483000	-0.622672000
6	0.089057000	-1.239945000	2.563690000
6	1.325390000	-1.514897000	3.118174000
6	0.026809000	-0.609683000	1.307480000
6	2.483471000	-1.158256000	2.412770000
6	1.248098000	-0.280638000	0.664871000
7	2.449448000	-0.558880000	1.221426000
6	0.016294000	0.678682000	-1.269203000
6	1.242832000	0.368597000	-0.626932000
1	-0.834417000	-1.498509000	3.071275000
1	1.415765000	-1.998012000	4.084905000
1	3.470196000	-1.355444000	2.817368000
6	0.068684000	1.313362000	-2.523617000
7	2.439747000	0.663555000	-1.184234000
6	2.464123000	1.266736000	-2.373962000
6	1.300627000	1.610309000	-3.076697000
1	-0.858636000	1.558172000	-3.031094000
1	3.447963000	1.476049000	-2.779696000
1	1.383306000	2.097936000	-4.041851000
27	-3.815008000	-0.036928000	0.001755000
7	-3.750117000	-1.730510000	-1.020819000
8	-5.142165000	0.738037000	-1.090399000
8	-5.110158000	-0.891493000	1.072019000
7	-3.867194000	1.656235000	1.022549000
6	-5.671786000	0.256019000	-2.174509000
6	-5.349656000	-1.020494000	-2.734264000
6	-4.430748000	-1.914631000	-2.116220000
1	-4.312417000	-2.881932000	-2.611758000
6	-2.900118000	-2.794851000	-0.600357000

6	-3.074923000	-3.364555000	0.668913000
6	-2.256081000	-4.407409000	1.078636000
1	-2.378785000	-4.872785000	2.049212000
6	-1.257379000	-4.865269000	0.218616000
6	-1.061795000	-4.310582000	-1.042153000
1	-0.268303000	-4.685043000	-1.677598000
6	-1.888461000	-3.267414000	-1.448034000
1	-1.737283000	-2.801858000	-2.416740000
6	-5.680113000	-0.444881000	2.150671000
6	-5.442715000	0.848031000	2.715224000
6	-4.573008000	1.797499000	2.108588000
1	-4.522330000	2.770497000	2.604347000
6	-3.083369000	2.773751000	0.611654000
6	-3.271507000	3.324352000	-0.664154000
1	-4.008350000	2.877977000	-1.320402000
6	-2.525493000	4.425450000	-1.060164000
1	-2.662863000	4.878323000	-2.034665000
6	-1.584483000	4.960930000	-0.180316000
6	-1.375305000	4.425682000	1.086693000
1	-0.628457000	4.862535000	1.738587000
6	-2.128663000	3.323618000	1.478737000
1	-1.964960000	2.874715000	2.453250000
1	-3.855714000	-2.975482000	1.310774000
6	-5.986423000	-1.444429000	-3.930382000
6	-6.909587000	-0.653095000	-4.575434000
6	-6.605593000	-1.293996000	2.819272000
6	-7.238222000	-0.889109000	3.975942000
6	-6.118902000	1.230935000	3.903505000
6	-7.000000000	0.383992000	4.536664000
6	-6.639116000	1.046674000	-2.855402000
6	-7.231667000	0.603386000	-4.019258000
1	-6.797807000	-2.268895000	2.382906000
1	-7.937944000	-1.564811000	4.461067000
1	-7.507424000	0.688699000	5.445436000
1	-5.925858000	2.220997000	4.310330000
1	-6.895297000	2.008469000	-2.422863000
1	-7.965134000	1.235062000	-4.513763000
1	-7.386387000	-0.988640000	-5.489903000
1	-5.728491000	-2.421041000	-4.333764000
7	-0.783630000	6.125929000	-0.606781000
8	0.001403000	6.608643000	0.205655000
8	-0.946319000	6.542058000	-1.751857000
7	-0.376191000	-5.964167000	0.661804000
8	-0.522362000	-6.386499000	1.806893000
8	0.455096000	-6.388657000	-0.137084000

$\text{HS-Co}^{\text{II}}\text{-SQ-}_{\text{LS}}\text{Fe}^{\text{III}}$, **6** (R=Ph-*p*-NO₂)

E= -5992.47886 a.u., E^{ZPE}= -5991.63174 a.u.

26	4.142806000	0.000042000	-0.000196000
7	4.064734000	1.900266000	0.666284000
7	4.683630000	2.366324000	1.785526000
7	6.015986000	0.274986000	2.301287000
7	5.560388000	-0.503947000	1.277189000
7	5.560239000	0.503936000	-1.277768000
7	6.015570000	-0.274975000	-2.302001000
7	4.683220000	-2.366262000	-1.786000000
7	4.064520000	-1.900186000	-0.666658000
5	5.222890000	1.461702000	2.930148000
1	4.298378000	1.040783000	3.582867000
1	5.989767000	2.106066000	3.595489000
5	5.222303000	-1.461657000	-2.930718000
1	4.297686000	-1.040697000	-3.583262000
1	5.989028000	-2.106047000	-3.596208000
6	3.516317000	2.967174000	0.047267000
1	2.992389000	2.862702000	-0.887949000
6	3.770294000	4.130276000	0.771684000
1	3.445285000	5.130989000	0.531386000
6	4.513987000	3.701741000	1.863585000
1	4.921288000	4.247223000	2.701841000
6	7.155479000	-0.251455000	2.778695000
1	7.661403000	0.221043000	3.607526000
6	7.467773000	-1.400727000	2.054844000
1	8.315708000	-2.054374000	2.187354000
6	6.447553000	-1.514016000	1.118498000
1	6.309291000	-2.250137000	0.343169000
6	6.447502000	1.513939000	-1.119209000
1	6.309441000	2.250030000	-0.343816000
6	7.467522000	1.400627000	-2.055769000
1	8.315475000	2.054222000	-2.188419000
6	7.155004000	0.251410000	-2.779611000
1	7.660733000	-0.221086000	-3.608562000
6	4.513545000	-3.701677000	-1.864020000
1	4.920694000	-4.247173000	-2.702341000
6	3.770032000	-4.130193000	-0.771988000
1	3.445046000	-5.130899000	-0.531627000
6	3.516196000	-2.967081000	-0.047537000
1	2.992430000	-2.862590000	0.887768000
8	-2.199461000	-0.461328000	1.226692000
8	-2.199608000	0.461339000	-1.226375000
6	-1.073365000	-0.240753000	0.682852000
6	-1.073445000	0.240816000	-0.682648000

6	0.271978000	-0.917327000	2.693622000
6	1.515823000	-1.114220000	3.262074000
6	0.185906000	-0.459758000	1.364745000
6	2.674499000	-0.851454000	2.513734000
6	1.398964000	-0.222079000	0.678109000
7	2.615999000	-0.411431000	1.255335000
6	0.185747000	0.459871000	-1.364670000
6	1.398885000	0.222203000	-0.678171000
1	-0.645907000	-1.111397000	3.239145000
1	1.620414000	-1.472408000	4.280140000
1	3.659532000	-1.005666000	2.931585000
6	0.271664000	0.917476000	-2.693545000
7	2.615854000	0.411579000	-1.255528000
6	2.674206000	0.851648000	-2.513919000
6	1.515443000	1.114416000	-3.262124000
1	-0.646283000	1.111538000	-3.238965000
1	3.659190000	1.005892000	-2.931873000
1	1.619915000	1.472635000	-4.280191000
27	-3.885029000	-0.000046000	0.000218000
7	-3.959762000	-1.971327000	-0.926806000
8	-5.103033000	0.632681000	-1.422947000
8	-5.102915000	-0.632834000	1.423431000
7	-3.959842000	1.971205000	0.927240000
6	-5.772714000	0.012418000	-2.337277000
6	-5.613807000	-1.387262000	-2.643656000
6	-4.703149000	-2.251296000	-1.959340000
1	-4.660544000	-3.274098000	-2.355125000
6	-3.059244000	-2.949026000	-0.470506000
6	-3.029698000	-3.271205000	0.899655000
6	-2.092049000	-4.167213000	1.386764000
1	-2.056329000	-4.428570000	2.437550000
6	-1.160277000	-4.728303000	0.507076000
6	-1.179514000	-4.438726000	-0.856727000
1	-0.441912000	-4.888924000	-1.509999000
6	-2.133681000	-3.553913000	-1.341514000
1	-2.139862000	-3.287565000	-2.393705000
6	-5.772611000	-0.012621000	2.337788000
6	-5.613779000	1.387067000	2.644161000
6	-4.703212000	2.251154000	1.959788000
1	-4.660686000	3.273978000	2.355527000
6	-3.059441000	2.948969000	0.470848000
6	-3.029984000	3.271065000	-0.899335000
1	-3.743098000	2.785851000	-1.556879000
6	-2.092456000	4.167147000	-1.386537000
1	-2.056810000	4.428447000	-2.437340000
6	-1.160709000	4.728394000	-0.506923000

6	-1.179858000	4.438898000	0.856899000
1	-0.442279000	4.889218000	1.510113000
6	-2.133910000	3.554013000	1.341781000
1	-2.140018000	3.287731000	2.393989000
1	-3.742838000	-2.786111000	1.557259000
6	-6.382955000	-1.964419000	-3.687824000
6	-7.290756000	-1.230399000	-4.419316000
6	-6.721391000	-0.740587000	3.116909000
6	-7.452966000	-0.139233000	4.118555000
6	-6.382925000	1.964176000	3.688356000
6	-7.290655000	1.230097000	4.419878000
6	-6.721553000	0.740327000	-3.116384000
6	-7.453129000	0.138926000	-4.118000000
1	-6.847044000	-1.793103000	2.881747000
1	-8.167984000	-0.730921000	4.685284000
1	-7.871037000	1.693557000	5.210744000
1	-6.243011000	3.021834000	3.903681000
1	-6.847252000	1.792839000	-2.881229000
1	-8.168193000	0.730573000	-4.684713000
1	-7.871143000	-1.693899000	-5.210154000
1	-6.242988000	-3.022071000	-3.903146000
7	-0.113528000	5.607634000	-1.034650000
8	0.731035000	6.042993000	-0.246245000
8	-0.115118000	5.852823000	-2.241722000
7	-0.112973000	-5.607458000	1.034702000
8	-0.114458000	-5.852687000	2.241766000
8	0.731585000	-6.042700000	0.246228000

$\text{HS-Co}^{\text{II}}\text{-BQ-HS-Fe}^{\text{II}}$, **6** (R=Ph-*p*-NO₂)

E= -5992.47081 a.u., E^{ZPE}= -5991.62821 a.u.

26	-4.362715000	-0.133578000	0.009315000
7	-4.281777000	1.822992000	-1.004061000
7	-4.783201000	2.059043000	-2.247969000
7	-6.050581000	-0.126631000	-2.615705000
7	-5.733033000	-0.817723000	-1.481755000
7	-5.805043000	0.605310000	1.399966000
7	-6.220862000	-0.061761000	2.516241000
7	-5.023871000	-2.297063000	2.226991000
7	-4.418701000	-2.082601000	1.026093000
5	-5.096552000	0.920832000	-3.267901000
1	-4.061305000	0.379495000	-3.588097000
1	-5.665572000	1.407018000	-4.210810000
5	-5.354084000	-1.145593000	3.227797000
1	-4.318711000	-0.647740000	3.611037000
1	-6.000892000	-1.606770000	4.132193000

6	-3.949554000	3.021859000	-0.490174000
1	-3.544844000	3.099453000	0.508086000
6	-4.228889000	4.044266000	-1.400853000
1	-4.067528000	5.103880000	-1.274898000
6	-4.757541000	3.382606000	-2.504092000
1	-5.107332000	3.759118000	-3.453936000
6	-7.213226000	-0.589683000	-3.109723000
1	-7.623656000	-0.169237000	-4.015889000
6	-7.683325000	-1.607775000	-2.284252000
1	-8.588831000	-2.183784000	-2.396932000
6	-6.724307000	-1.708617000	-1.276417000
1	-6.696228000	-2.362045000	-0.416934000
6	-6.741590000	1.536885000	1.129413000
1	-6.630436000	2.181295000	0.269910000
6	-7.763687000	1.486170000	2.077119000
1	-8.648056000	2.102100000	2.131350000
6	-7.389935000	0.455454000	2.935714000
1	-7.872479000	0.060869000	3.817697000
6	-5.086411000	-3.620430000	2.473973000
1	-5.523653000	-3.982050000	3.392811000
6	-4.512035000	-4.304421000	1.407556000
1	-4.402037000	-5.371233000	1.287500000
6	-4.110941000	-3.294705000	0.528745000
1	-3.631703000	-3.386929000	-0.434844000
8	2.243813000	-0.669407000	-1.068074000
8	2.200076000	0.615039000	1.206585000
6	1.122312000	-0.434823000	-0.575118000
6	1.097857000	0.289729000	0.722902000
6	-0.174181000	-1.524925000	-2.410550000
6	-1.402580000	-1.866858000	-2.950879000
6	-0.136516000	-0.821778000	-1.197346000
6	-2.566746000	-1.491749000	-2.272142000
6	-1.360260000	-0.490508000	-0.572774000
7	-2.551100000	-0.822973000	-1.113863000
6	-0.183571000	0.606415000	1.338433000
6	-1.383811000	0.229602000	0.695158000
1	0.760215000	-1.787422000	-2.896284000
1	-1.477840000	-2.411132000	-3.885630000
1	-3.548745000	-1.729275000	-2.666571000
6	-0.265989000	1.299224000	2.555292000
7	-2.594353000	0.522777000	1.215027000
6	-2.653144000	1.186388000	2.374908000
6	-1.514360000	1.592538000	3.078240000
1	0.650206000	1.593032000	3.057192000
1	-3.649090000	1.396127000	2.749134000
1	-1.624227000	2.128514000	4.014337000

27	3.974240000	0.170124000	0.006025000
7	3.752721000	1.977921000	-1.136773000
8	5.192464000	-0.504338000	-1.377512000
8	5.069782000	1.063506000	1.360450000
7	4.249066000	-1.681290000	1.126150000
6	5.663248000	0.027698000	-2.461366000
6	5.278335000	1.325375000	-2.949331000
6	4.357912000	2.184386000	-2.274622000
1	4.175280000	3.141231000	-2.777993000
6	2.850373000	2.971303000	-0.692890000
6	2.961785000	3.456860000	0.621842000
6	2.062264000	4.399187000	1.096434000
1	2.137558000	4.792860000	2.103029000
6	1.035921000	4.844685000	0.259863000
6	0.904560000	4.380479000	-1.046590000
1	0.091618000	4.741855000	-1.664975000
6	1.815481000	3.442446000	-1.519769000
1	1.709469000	3.047023000	-2.525193000
6	5.724430000	0.643450000	2.396632000
6	5.684616000	-0.714829000	2.868959000
6	4.952118000	-1.759693000	2.219098000
1	5.034365000	-2.740531000	2.703009000
6	3.581993000	-2.851628000	0.699510000
6	3.708031000	-3.259673000	-0.639924000
1	4.336757000	-2.671696000	-1.299437000
6	3.041314000	-4.389026000	-1.091216000
1	3.136527000	-4.727216000	-2.116085000
6	2.230177000	-5.101738000	-0.206191000
6	2.084423000	-4.715124000	1.124333000
1	1.439580000	-5.287051000	1.780806000
6	2.762207000	-3.587944000	1.573474000
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1	3.757536000	3.069058000	1.248627000
6	5.840833000	1.809027000	-4.160212000
6	6.750680000	1.072671000	-4.886181000
6	6.527579000	1.565409000	3.127102000
6	7.229624000	1.179821000	4.250435000
6	6.421457000	-1.069555000	4.026685000
6	7.181824000	-0.149533000	4.717745000
6	6.612367000	-0.702812000	-3.232968000
6	7.134947000	-0.196576000	-4.404495000
1	6.566908000	2.586740000	2.761255000
1	7.831340000	1.913206000	4.781292000
1	7.738255000	-0.443086000	5.601489000
1	6.380096000	-2.102217000	4.366784000
1	6.911901000	-1.676374000	-2.857334000

1	7.857081000	-0.785715000	-4.964251000
1	7.168658000	1.461385000	-5.808662000
1	5.536887000	2.793069000	-4.511276000
7	1.498181000	-6.282241000	-0.693544000
8	0.824868000	-6.916973000	0.117117000
8	1.594501000	-6.564522000	-1.887418000
7	0.053780000	5.810162000	0.778477000
8	0.148262000	6.147351000	1.958307000
8	-0.814650000	6.218537000	0.008259000