

Electronic Supplementary Information

**Theoretical Modeling of Valence Tautomeric Dinuclear Cobalt Complexes. Adducts of Co^{II}
Diketonates with Cyclic Redox-Active Tetraone Ligands**

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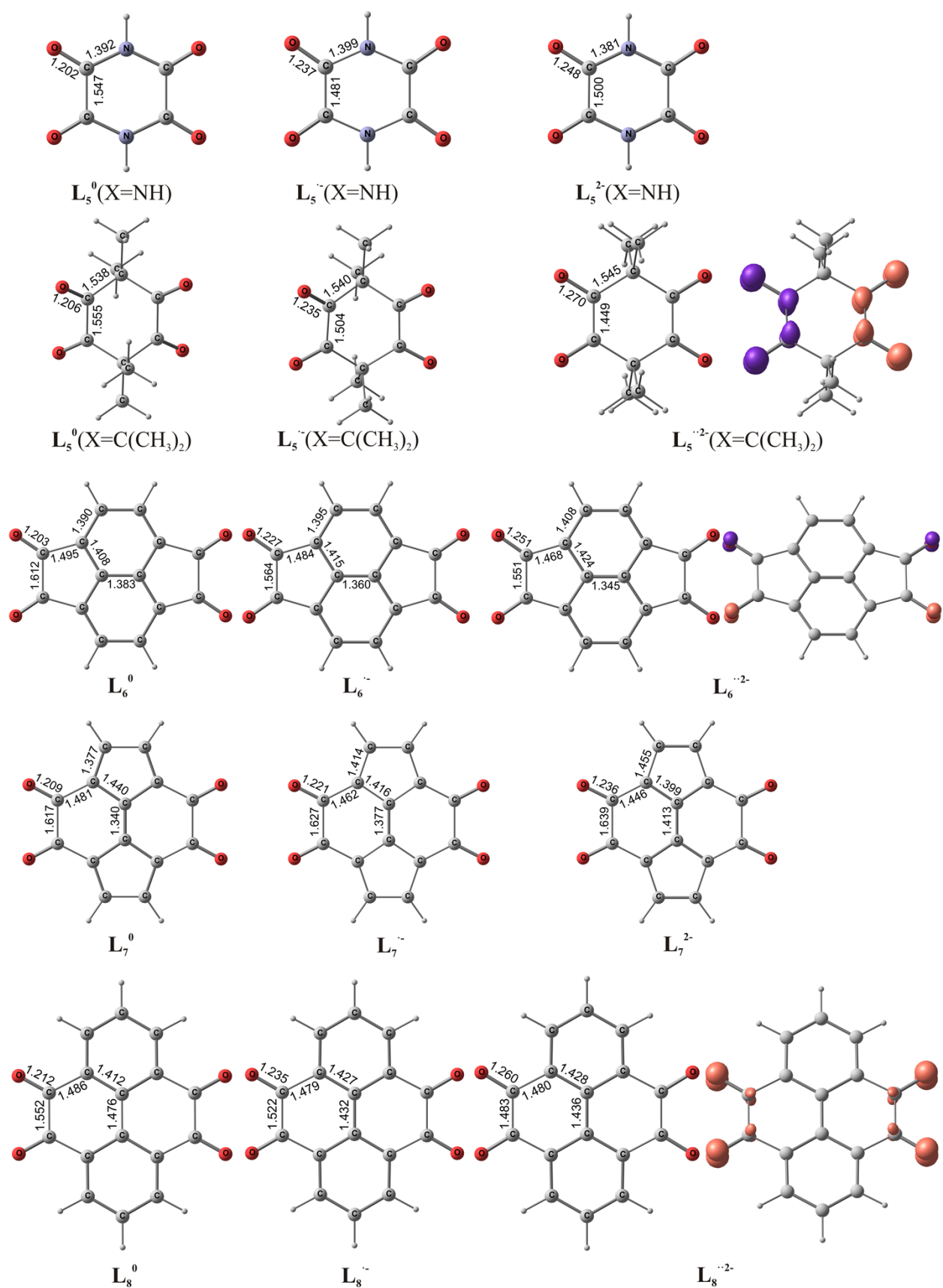


Figure S1. Optimized geometries of the ligands $L_5 - L_8$ calculated by the B3LYP*/6-311++G(d,p) method and distribution of spin density in the diradical-dianions (cutoff=0.020 a.u.). Hereafter bond lengths are given in Å.

Table S1. Spin states (S), total energies (E_{total} , given in a.u.), relative energies (ΔE , given in kcal mol⁻¹), exchange spin coupling constants (J, given in cm⁻¹) of the ligands **L**₅ – **L**₈ calculated by the B3LYP*/6-311++G(d,p) method.

Ligand	S	E_{total}	ΔE	J
<i>X=NH</i>				
L ₅ ⁰	0	-563.91886	50.0	–
L ₅ ^{•-}	1/2	-563.99856	0.0	
L ₅ ^{••2-}	2/2	-563.87013	80.6	
L ₅ ²⁻	0	-563.88887	68.8	
<i>X=C(CH₃)₂</i>				
L ₅ ⁰	0	-688.93505	43.0	-521
L ₅ ^{•-}	1/2	-689.00362	0.0	
L ₅ ^{••2-}	2/2	-688.91893	53.1	
BS L ₅ ^{••2-}		-688.92109	51.8	
L ₆ ⁰	0	-836.47932	63.0	-176
L ₆ ^{•-}	1/2	-836.57975	0.0	
L ₆ ^{••2-}	2/2	-836.52556	34.0	
BS L ₆ ^{••2-}		-836.52682	33.2	
L ₇ ⁰	0	-836.41008	83.6	–
L ₇ ^{•-}	1/2	-836.54337	0.0	
L ₇ ^{••2-}	2/2	-836.49041	33.2	
L ₇ ²⁻	0	-836.52539	11.3	
L ₈ ⁰	0	-913.89493	60.4	269
L ₈ ^{•-}	1/2	-913.99113	0.0	
L ₈ ^{••2-}	2/2	-913.95617	21.9	
BS L ₈ ^{••2-}		-913.95494	22.7	

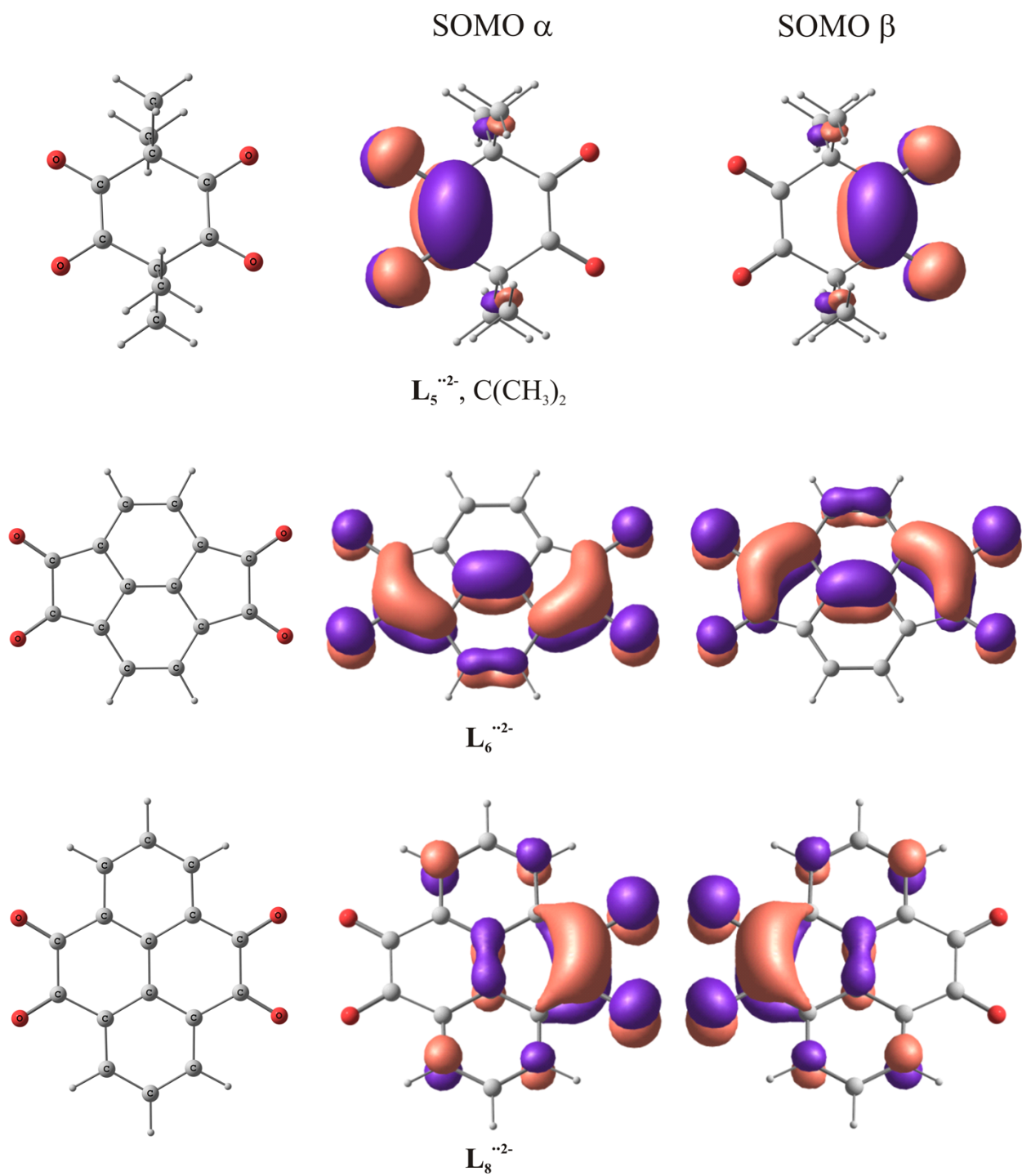


Figure S2. Nonbonding molecular orbitals of the diradicals $L_5^{\cdot\cdot-}$ ($C(CH_3)_2$), $L_6^{\cdot\cdot-}$ and $L_8^{\cdot\cdot-}$ calculated by the B3LYP*/6-311++G(d,p) method.

Table S2. Spin states (S), total energies (E_{total} , given in a.u.), stabilization energies, relative energies (E_{stab} , ΔE , given in kcal mol⁻¹), and exchange spin coupling constants (J, given in cm⁻¹) of the electromeric forms of the complexes **5–7** (X = NH, C(CH₃)₂; R = H, CF₃), calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure		S	E_{total}	E_{stab}^*	ΔE	J
Complexes 5 (X = NH)						
R = H	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	2/2	-4395.21963	-25.5	0.0	–
	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	0	-4395.25467	-3.5	-22.0	
	$\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$	4/2	-4395.25827	-1.3	-24.2	80
	BS $\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$		-4395.25717	-1.9	-23.6	
	$\text{HS Co}^{\text{II}}\text{-(Q)}_2\text{-HS Co}^{\text{II}}$	6/2	-4395.25681	-2.2	-23.3	
R = CF₃	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	2/2	-7091.18605	-3.5	0.0	-147
	BS $\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$		-7091.18672	-3.0	-0.4	
	$\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$	4/2	-7091.20126	6.1	-9.5	70
	BS $\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$		-7091.20030	5.5	-8.9	
	$\text{HS Co}^{\text{II}}\text{-(Q)}_2\text{-HS Co}^{\text{II}}$	6/2	-7091.21227	13.0	-16.5	
Complexes 5 (X = C(CH₃)₂)						
R = H	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	2/2	-4520.29532	11.8	0.0	-285
	BS $\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$		-4520.29669	12.7	-0.9	
	$\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$	4/2	-4520.28957	8.2	3.6	6
	BS $\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$		-4520.28949	8.2	3.7	
	$\text{HS Co}^{\text{II}}\text{-(Q)}_2\text{-HS Co}^{\text{II}}$	6/2	-4520.27702	0.4	11.5	
R = CF₃	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	2/2	-7216.22881	13.2	0.0	-216
	BS $\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$		-7216.22985	13.9	-0.7	
	$\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$	4/2	-7216.23639	18.0	-4.8	1
	BS $\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$		-7216.23637	18.0	-4.7	
	$\text{HS Co}^{\text{II}}\text{-(Q)}_2\text{-HS Co}^{\text{II}}$	6/2	-7216.23827	19.2	-5.9	
Complexes 6						
R = H	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	2/2	-4667.81905	-1.0	0.0	-1939
	BS $\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$		-4667.83580	9.5	-10.5	
	$\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$	4/2	-4667.82986	5.7	-6.8	67
	BS $\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$		-4667.82894	5.2	-6.2	
	$\text{HS Co}^{\text{II}}\text{-(Q)}_2\text{-HS Co}^{\text{II}}$	6/2	-4667.81890	-1.1	0.1	
R = CF₃	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	2/2	-7363.74822	-2.4	0.0	-2017
	BS $\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$		-7363.76623	8.9	-11.3	
	$\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$	4/2	-7363.77484	14.3	-16.7	44
	BS $\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$		-7363.77424	13.9	-16.3	
	$\text{HS Co}^{\text{II}}\text{-(Q)}_2\text{-HS Co}^{\text{II}}$	6/2	-7363.77913	17.0	-19.4	
Complexes 7						
R = H	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	2/2	-4667.81419	39.3	0.0	–
	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	0	-4667.82161	44.0	-4.7	
	$\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$	4/2	-4667.79746	28.9	10.5	-32
	BS $\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$		-4667.79789	29.1	10.2	
	$\text{HS Co}^{\text{II}}\text{-(Q)}_2\text{-HS Co}^{\text{II}}$	6/2	-4667.77290	13.4	25.9	
R = CF₃	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	2/2	-7363.74436	38.6	0.0	–
	$\text{LS Co}^{\text{III}}\text{-(SQ)}_2\text{-LS Co}^{\text{III}}$	0	-7363.74639	39.9	-1.3	
	$\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$	4/2	-7363.74107	36.6	2.1	-7
	BS $\text{LS Co}^{\text{III}}\text{-(SQ-Q)}\text{-HS Co}^{\text{II}}$		-7363.74117	36.6	2.0	
	$\text{HS Co}^{\text{II}}\text{-(Q)}_2\text{-HS Co}^{\text{II}}$	6/2	-7363.72560	26.9	11.8	

* Stabilization energies were calculated relative to the isolated molecules of cobalt diketonates and corresponding redox-active ligand (see Tables S1, S3)

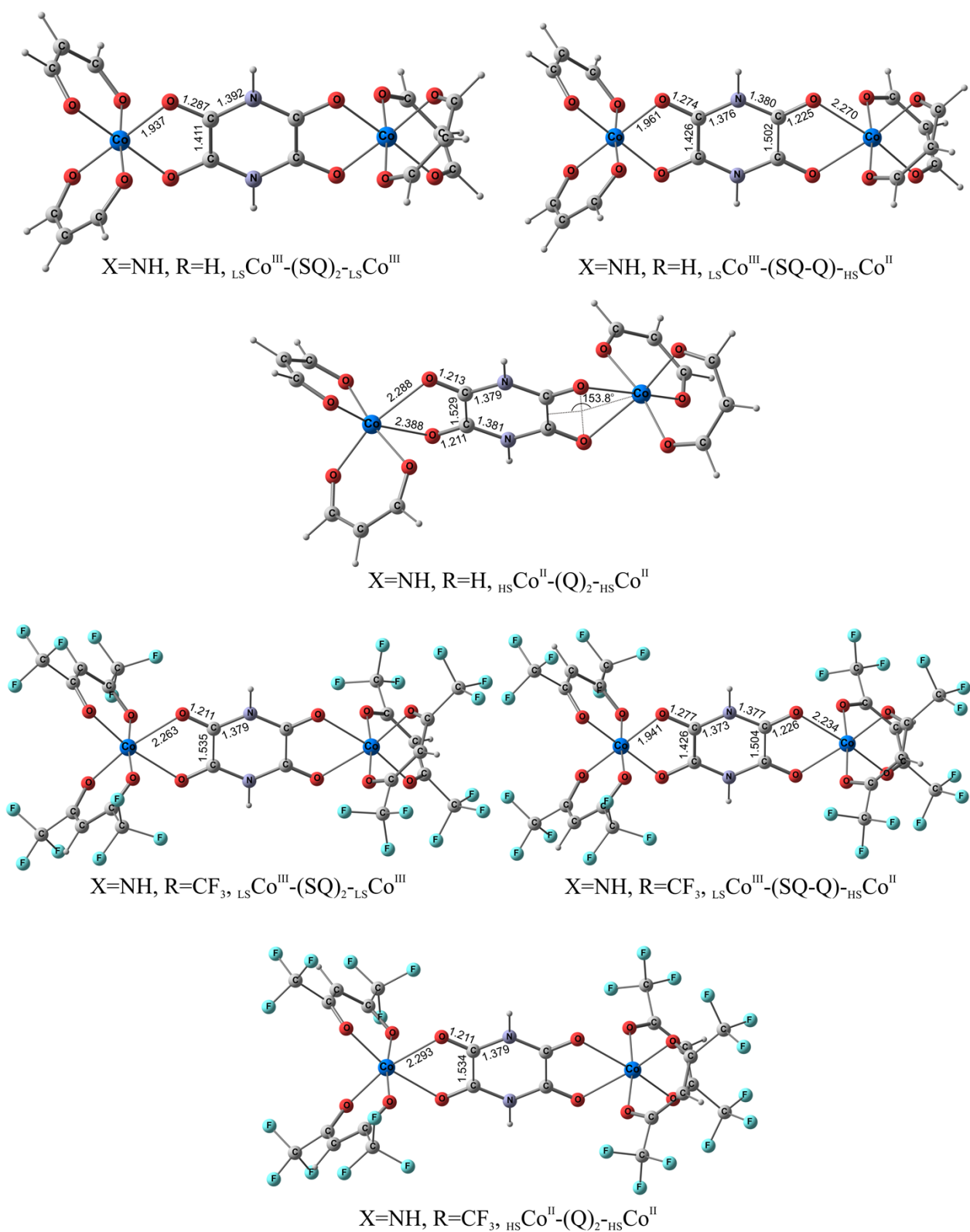


Figure S3. Optimized geometries of the electromeric forms of the complexes **5** ($X=NH$; $R=H$, CF_3) calculated by the B3LYP*/6-311++G(d,p) method. Angle is in degrees.

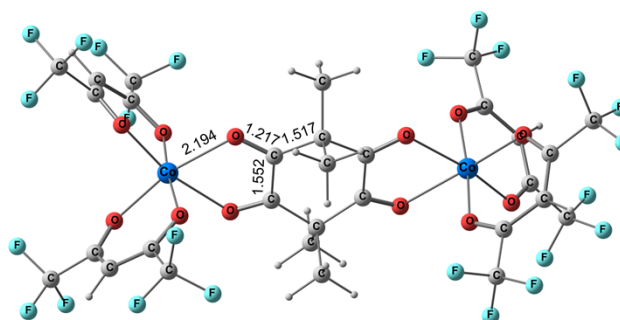
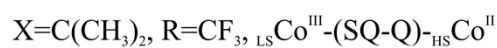
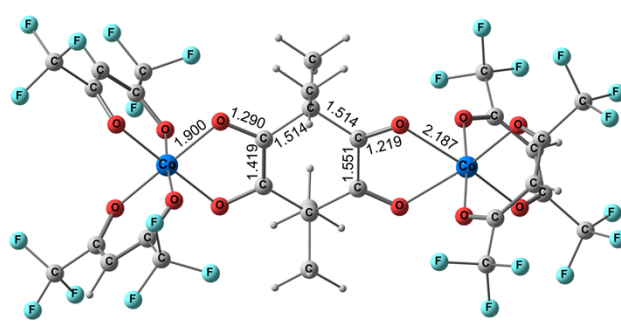
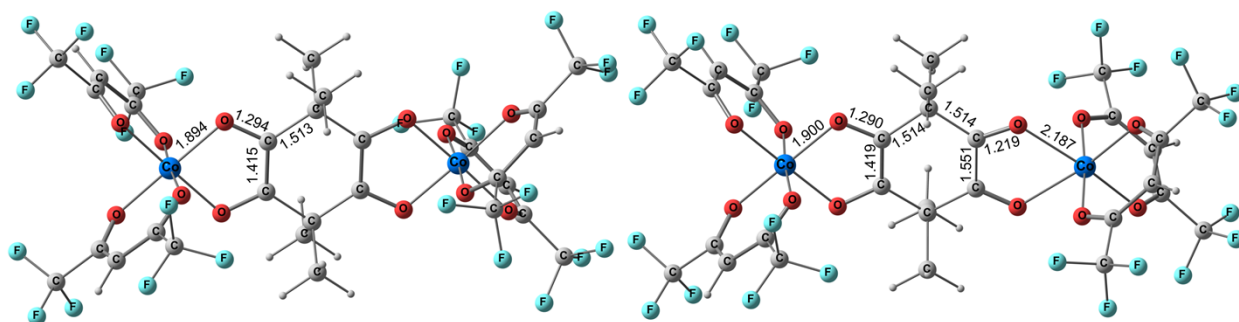
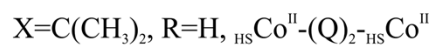
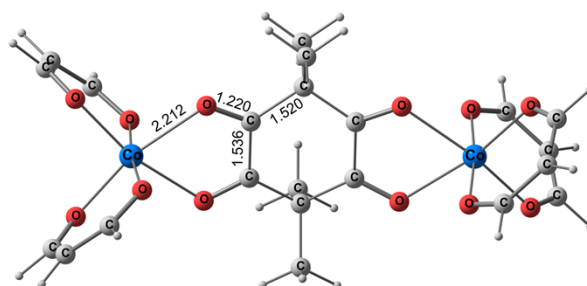
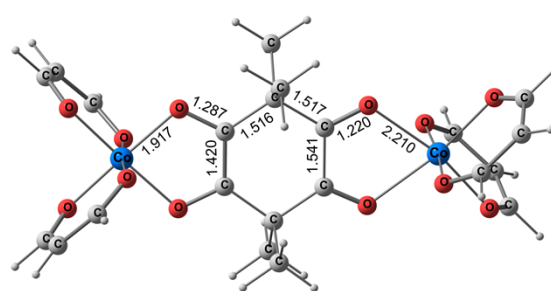
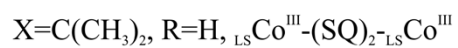
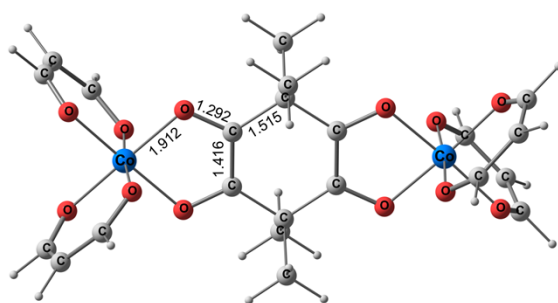


Figure S4. Optimized geometries of the electromeric forms of the complexes **5** ($X=C(CH_3)_2$; $R=H$, CF_3) calculated by the B3LYP*/6-311++G(d,p) method.

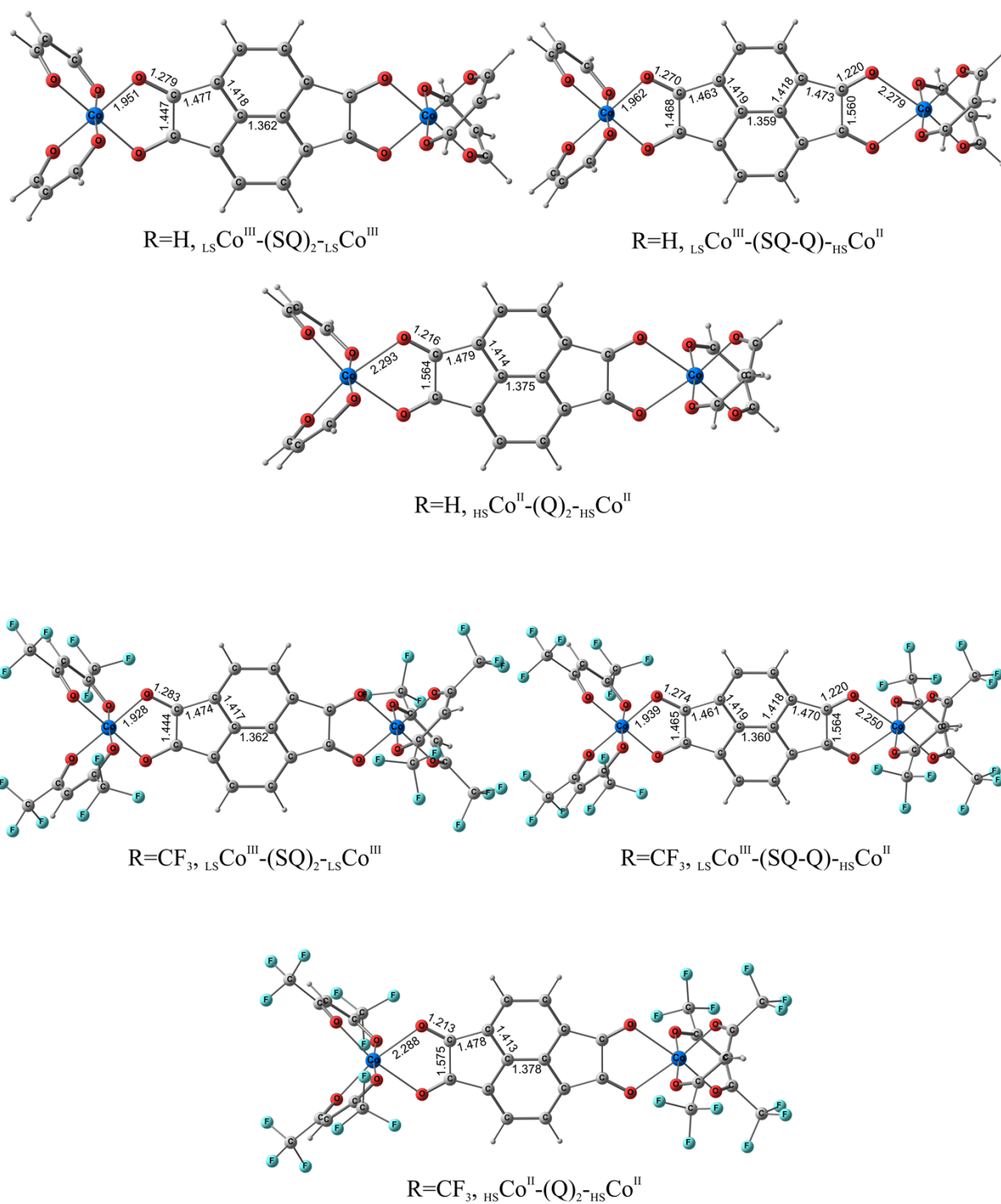


Figure S5. Optimized geometries of the electromeric forms of the complexes **6** ($R=\text{H}$, CF_3) calculated by the B3LYP*/6-311++G(d,p) method.

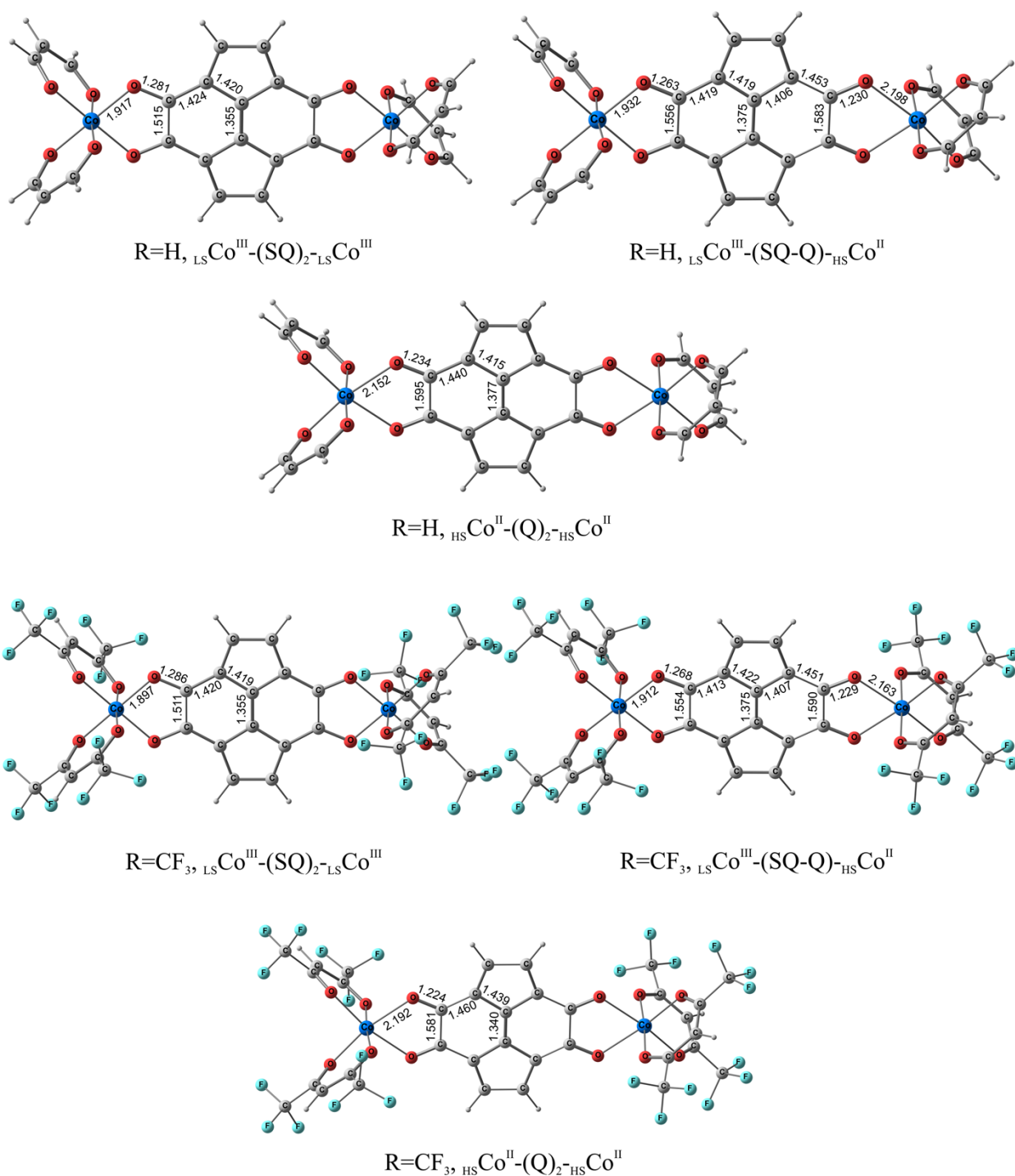


Figure S6. Optimized geometries of the electromeric forms of the complexes **7** (R=H, CF₃) calculated by the B3LYP*/6-311++G(d,p) method.

Table S3. Total energies without (E) and with account (E^{ZPE}) taken for energies of zero harmonic vibrations (all energy values are given in a.u.) of the structures of Co^{II} diketonates calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure	E	E ^{ZPE}
<i>bis</i> -(malonate)Co ^{II}	-1915.67070	-1915.55690
<i>bis</i> -(acetylacetonate)Co ^{II}	-2072.89123	-2072.66825
<i>bis</i> -(hexafluoroacetylacetonate)Co ^{II}	-3263.63635	-3263.50515
<i>bis</i> -(trifluoroacetylacetonate)Co ^{II}	-2668.26938	-2668.09245

Table S4. Spin states (S), total energies without (E) and with account (E^{ZPE}) taken for energies of zero harmonic vibrations (all energy values are given in a.u.), square of spin density (S^2) of the electromeric forms of the adducts **8** ($R_1, R_2 = H, CH_3, CF_3$) calculated by the DFT B3LYP*/6-311++G(d,p) method.

Structure		S	E	E^{ZPE}	S^2
$R_1=H$ $R_2=H$	$LSCo^{III}-(SQ)_2-LSCo^{III}$	2/2	-4745.28388	-4744.87182	2.01
	BS $LSCo^{III}-(SQ)_2-LSCo^{III}$		-4745.28277		0.97
	$LSCo^{III}-(SQ-Q)-HSCo^{II}$	4/2	-4745.27001	-4744.86217	6.13
	BS $LSCo^{III}-(SQ-Q)-HSCo^{II}$		-4745.27016		3.15
	MECP _{T-Q}		-4745.26464		
	$HSCo^{II}-(Q)_2-HSCo^{II}$	6/2	-4745.25254	-4744.84899	12.47
$R_1=CH_3$ $R_2=CH_3$	$LSCo^{III}-(SQ)_2-LSCo^{III}$	2/2	-5059.72511	-5059.09607	2.01
	BS $LSCo^{III}-(SQ)_2-LSCo^{III}$		-5059.72385		0.98
	$LSCo^{III}-(SQ-Q)-HSCo^{II}$	4/2	-5059.70861	-5059.08338	6.20
	BS $LSCo^{III}-(SQ-Q)-HSCo^{II}$		-5059.70888		3.22
	MECP _{T-Q}		-5059.70475		
	$HSCo^{II}-(Q)_2-HSCo^{II}$	6/2	-5059.68977	-5059.06840	12.65
$R_1=CF_3$ $R_2=CF_3$	$LSCo^{III}-(SQ)_2-LSCo^{III}$	2/2	-7441.21543	-7440.76948	2.02
	BS $LSCo^{III}-(SQ)_2-LSCo^{III}$		-7441.21479		0.94
	$LSCo^{III}-(SQ-Q)-HSCo^{II}$	4/2	-7441.21715	-7440.77453	6.05
	BS $LSCo^{III}-(SQ-Q)-HSCo^{II}$		-7441.21712		3.05
	MECP _{T-Q}		-7441.18890		
	$HSCo^{II}-(Q)_2-HSCo^{II}$	6/2	-7441.21314	-7440.77397	12.15
$R_1=CH_3$ $R_2=CF_3$	MECP _{Q-S}		-7441.20287		
	$LSCo^{III}-(SQ)_2-LSCo^{III}$	2/2	-6250.48040	-6249.94295	2.02
	BS $LSCo^{III}-(SQ)_2-LSCo^{III}$		-6250.47943		0.97
	$LSCo^{III}-(SQ-Q)-HSCo^{II}$	4/2	-6250.47272	-6249.93896	6.08
	BS $LSCo^{III}-(SQ-Q)-HSCo^{II}$		-6250.47277		3.09
	MECP _{T-Q}		-6250.45946		
	$HSCo^{II}-(Q)_2-HSCo^{II}$	6/2	-6250.46048	6249.93043	12.30
	MECP _{Q-S}		-6250.44872		

Total energies and optimized geometries of the electromeric forms of the complexes **8 ($R_1, R_2 = H, CH_3, CF_3$) calculated by DFT B3LYP*/6-311++G(d,p)**

$LSCo^{III}-(SQ)_2-LSCo^{III}$ ($R_1, R_2=H$)

$E = -4745.28388$ a.u., $E^{ZPE} = -4744.87182$ a.u.

8	-3.614497000	1.302530000	-0.019094000
8	-3.614354000	-1.302914000	0.017628000
6	-0.000063000	0.723898000	-0.001134000
6	-1.221134000	1.451021000	-0.004900000
6	-0.000287000	3.549138000	-0.001206000
6	1.220944000	1.451170000	0.002675000
6	-2.465665000	0.717818000	-0.007070000
6	-2.465562000	-0.718107000	0.005176000
6	-1.207784000	2.856101000	-0.004317000
6	1.207304000	2.856260000	0.002001000
1	-2.156496000	3.382030000	-0.004571000
1	2.155891000	3.382419000	0.002282000
6	0.000063000	-0.723898000	-0.001134000
6	1.221134000	-1.451021000	-0.004899000
6	2.465665000	-0.717818000	-0.007070000
8	3.614497000	-1.302530000	-0.019094000
6	2.465562000	0.718107000	0.005175000
8	3.614354000	1.302914000	0.017628000
6	1.207784000	-2.856101000	-0.004317000
6	0.000287000	-3.549138000	-0.001205000
6	-1.207304000	-2.856260000	0.002001000
6	-1.220944000	-1.451170000	0.002675000
1	-2.155891000	-3.382419000	0.002282000
1	2.156496000	-3.382030000	-0.004571000
1	-0.000340000	4.634933000	-0.001254000
1	0.000340000	-4.634933000	-0.001254000
27	-5.022657000	-0.000220000	0.000131000
8	-4.936906000	0.052732000	1.906574000
8	-6.367782000	-1.336186000	-0.105556000
8	-6.367392000	1.335991000	0.107645000
8	-4.939563000	-0.053222000	-1.906414000
6	-5.664721000	-0.666650000	2.651769000
6	-6.620534000	-1.606991000	2.256376000
6	-6.896944000	-1.873302000	0.914715000
6	-6.897732000	1.873332000	-0.911902000
6	-6.623093000	1.607082000	-2.253935000
6	-5.668038000	0.666502000	-2.650619000
1	-7.163631000	-2.151558000	3.019339000
1	-7.166937000	2.151932000	-3.016164000

1	-7.656469000	2.632568000	-0.681367000
1	-5.509435000	0.517072000	-3.726864000
1	-7.656205000	-2.632333000	0.685229000
1	-5.504740000	-0.517129000	3.727796000
27	5.022657000	0.000220000	0.000131000
8	4.936906000	-0.052732000	1.906574000
8	6.367782000	1.336186000	-0.105557000
8	6.367391000	-1.335991000	0.107645000
8	4.939563000	0.053221000	-1.906414000
6	5.664721000	0.666650000	2.651769000
6	6.620534000	1.606991000	2.256376000
6	6.896944000	1.873302000	0.914715000
6	6.897732000	-1.873332000	-0.911902000
6	6.623093000	-1.607082000	-2.253935000
6	5.668038000	-0.666502000	-2.650619000
1	7.163631000	2.151558000	3.019339000
1	7.166937000	-2.151931000	-3.016164000
1	7.656469000	-2.632567000	-0.681367000
1	5.509435000	-0.517072000	-3.726864000
1	7.656205000	2.632333000	0.685229000
1	5.504740000	0.517129000	3.727796000

$\text{LsCo}^{\text{III}}\text{-(SQ-Q)}\text{-HsCo}^{\text{II}}$ ($\text{R}_1, \text{R}_2=\text{H}$)

$E = -4745.27001 \text{ a.u.}$, $E^{\text{ZPE}} = -4744.86217 \text{ a.u.}$

6	-0.100583000	-0.726772000	-0.021430000
6	-1.324446000	-1.445716000	-0.039387000
6	-0.119558000	-3.556239000	-0.107183000
6	1.109346000	-1.467045000	-0.045733000
6	-2.573024000	-0.717803000	-0.014486000
6	-2.573003000	0.717940000	0.013913000
6	-1.316209000	-2.852968000	-0.083357000
6	1.092401000	-2.865131000	-0.086950000
1	-2.269868000	-3.370308000	-0.099857000
1	2.041239000	-3.391627000	-0.101926000
6	-0.100563000	0.726808000	0.021651000
6	1.109385000	1.467042000	0.046292000
6	2.385843000	0.757360000	0.021899000
8	3.488430000	1.310995000	0.030992000
6	2.385824000	-0.757403000	-0.021044000
8	3.488393000	-1.311074000	-0.029912000
6	1.092474000	2.865131000	0.087481000
6	-0.119466000	3.556282000	0.107348000
6	-1.316133000	2.853050000	0.083170000
6	-1.324403000	1.445799000	0.039225000
1	-2.269781000	3.370421000	0.099362000
1	2.041326000	3.391593000	0.102708000

1	-0.125938000	-4.640964000	-0.141000000
1	-0.125820000	4.641008000	0.141141000
27	5.212294000	-0.000016000	0.000067000
8	5.150933000	-0.218819000	2.027418000
8	6.568337000	1.490325000	0.227239000
8	6.568184000	-1.490334000	-0.228211000
8	5.149280000	0.218723000	-2.027275000
6	5.986308000	0.271946000	2.841296000
6	7.003144000	1.193380000	2.556982000
6	7.205745000	1.752822000	1.287231000
6	7.204843000	-1.752730000	-1.288676000
6	7.001243000	-1.193269000	-2.558262000
6	5.984105000	-0.271931000	-2.841788000
1	7.634898000	1.528754000	3.372678000
1	7.632416000	-1.528563000	-3.374441000
1	5.881812000	0.049776000	-3.891516000
1	7.993950000	-2.517916000	-1.201076000
1	5.884850000	-0.049765000	3.891104000
1	7.994723000	2.518070000	1.199020000
8	-3.717640000	1.304991000	0.016338000
8	-3.717686000	-1.304820000	-0.017482000
27	-5.132949000	0.000102000	-0.000116000
8	-5.045256000	0.004008000	1.905490000
8	-6.473821000	-1.330174000	-0.140481000
8	-6.473723000	1.330384000	0.141313000
8	-5.046738000	-0.003787000	-1.905787000
6	-5.786510000	-0.720222000	2.633738000
6	-6.750639000	-1.640960000	2.214280000
6	-7.017084000	-1.880968000	0.866159000
6	-7.018313000	1.880627000	-0.864918000
6	-6.753210000	1.640309000	-2.213244000
6	-5.789029000	0.719961000	-2.633448000
1	-7.305616000	-2.193470000	2.962680000
1	-7.309183000	2.192385000	-2.961225000
1	-7.780172000	2.629280000	-0.612924000
1	-5.633070000	0.593112000	-3.712648000
1	-7.778946000	-2.629814000	0.614748000
1	-5.629624000	-0.593438000	3.712810000

MECP_{T-Q} (R₁, R₂=H)

E= -4745.26464 a.u.

6	-0.059807000	0.724648000	0.032926000
6	-1.282311000	1.447838000	0.056346000
6	-0.068256000	3.549754000	0.150773000
6	1.156477000	1.457125000	0.075097000
6	-2.528969000	0.718366000	0.022062000

6	-2.528622000	-0.717135000	-0.021092000
6	-1.271012000	2.852716000	0.115274000
6	1.140874000	2.857674000	0.132067000
1	-2.221525000	3.375331000	0.133432000
1	2.089805000	3.383477000	0.156910000
6	-0.059628000	-0.722322000	-0.033017000
6	1.156741000	-1.454468000	-0.075813000
6	2.416412000	-0.733395000	-0.051285000
8	3.540960000	-1.298420000	-0.101616000
6	2.416456000	0.736284000	0.049722000
8	3.541181000	1.301044000	0.099062000
6	1.141795000	-2.854977000	-0.132644000
6	-0.067015000	-3.547558000	-0.150771000
6	-1.269974000	-2.850890000	-0.114798000
6	-1.281770000	-1.446056000	-0.055849000
1	-2.220309000	-3.373815000	-0.132626000
1	2.090981000	-3.380323000	-0.157845000
1	-0.071136000	4.634314000	0.192183000
1	-0.069472000	-4.632088000	-0.192149000
27	5.109100000	0.000516000	-0.000500000
8	5.068637000	0.286139000	-1.974195000
8	6.479862000	-1.419612000	-0.198271000
8	6.480561000	1.419230000	0.200145000
8	5.065451000	-0.286671000	1.972947000
6	5.870305000	-0.229858000	-2.805662000
6	6.869086000	-1.174348000	-2.542760000
6	7.088989000	-1.711242000	-1.269247000
6	7.089190000	1.708783000	1.272284000
6	6.867703000	1.170274000	2.544692000
6	5.867698000	0.226792000	2.805849000
1	7.475902000	-1.530064000	-3.367653000
1	7.474449000	1.524149000	3.370581000
1	5.743081000	-0.103633000	3.848405000
1	7.868269000	2.480095000	1.178503000
1	5.746649000	0.098788000	-3.848948000
1	7.867312000	-2.483220000	-1.173980000
8	-3.675349000	-1.303428000	-0.029044000
8	-3.676042000	1.303946000	0.030398000
27	-5.086637000	-0.000287000	0.000220000
8	-5.000007000	0.014888000	-1.905993000
8	-6.430293000	1.329364000	0.153843000
8	-6.428892000	-1.331221000	-0.154590000
8	-5.001642000	-0.015449000	1.906509000
6	-5.738683000	0.748978000	-2.626132000
6	-6.702224000	1.666460000	-2.197584000
6	-6.970904000	1.891756000	-0.847062000

6	-6.969690000	-1.894341000	0.845839000
6	-6.702386000	-1.668832000	2.196578000
6	-5.740162000	-0.750351000	2.625976000
1	-7.255152000	2.228114000	-2.940683000
1	-7.255354000	-2.231105000	2.939187000
1	-7.730519000	-2.642255000	0.587698000
1	-5.583226000	-0.636239000	3.706640000
1	-7.732832000	2.638799000	-0.589638000
1	-5.580714000	0.634958000	-3.706652000

$\text{HSCo}^{\text{II}}\text{-(Q)}_2\text{-HSCo}^{\text{II}}$ ($R_1, R_2=\text{H}$)

$E = -4745.25254$ a.u., $E^{\text{ZPE}} = -4744.84899$ a.u.

8	-3.591508000	-1.308661000	-0.001435000
8	-3.591513000	1.308691000	0.001734000
6	0.000014000	-0.733620000	0.000068000
6	-1.212275000	-1.464241000	0.002735000
6	-0.000005000	-3.567506000	0.000148000
6	1.212294000	-1.464258000	-0.002567000
6	-2.486723000	-0.751657000	0.001234000
6	-2.486727000	0.751694000	-0.001021000
6	-1.202212000	-2.867368000	0.001233000
6	1.202212000	-2.867387000	-0.000980000
1	-2.155771000	-3.385680000	-0.000028000
1	2.155766000	-3.385708000	0.000294000
6	0.000024000	0.733627000	0.000022000
6	1.212317000	1.464247000	0.002569000
6	2.486775000	0.751662000	0.001036000
8	3.591568000	1.308645000	-0.001809000
6	2.486749000	-0.751693000	-0.001149000
8	3.591531000	-1.308712000	0.001475000
6	1.202249000	2.867374000	0.000984000
6	0.000043000	3.567511000	-0.000097000
6	-1.202176000	2.867390000	-0.001119000
6	-1.212260000	1.464264000	-0.002585000
1	-2.155727000	3.385714000	0.000182000
1	2.155808000	3.385684000	-0.000358000
1	-0.000018000	-4.652534000	0.000187000
1	0.000052000	4.652541000	-0.000146000
27	-5.294792000	-0.000186000	0.000045000
8	-5.241623000	-0.182141000	-2.022932000
8	-6.644690000	1.486198000	-0.203974000
8	-6.644879000	-1.486478000	0.203627000
8	-5.242129000	0.181771000	2.022977000
6	-6.072608000	0.322995000	-2.833845000
6	-7.087192000	1.241767000	-2.536270000
6	-7.286847000	1.774422000	-1.255598000

6	-7.287800000	-1.774077000	1.254952000
6	-7.088748000	-1.241050000	2.535569000
6	-6.073897000	-0.322703000	2.833517000
1	-7.718260000	1.593241000	-3.345289000
1	-7.720495000	-1.591999000	3.344287000
1	-5.968170000	-0.015731000	3.886385000
1	-8.074918000	-2.536982000	1.143989000
1	-5.966387000	0.016268000	-3.886737000
1	-8.073780000	2.537541000	-1.144832000
27	5.294828000	-0.000191000	-0.000047000
8	5.241643000	-0.182040000	2.022931000
8	6.644775000	1.486166000	0.203898000
8	6.644800000	-1.486559000	-0.203655000
8	5.242164000	0.181818000	-2.022993000
6	6.072576000	0.323182000	2.833847000
6	7.087152000	1.241953000	2.536243000
6	7.286856000	1.774506000	1.255532000
6	7.287619000	-1.774277000	-1.255011000
6	7.088546000	-1.241291000	-2.535641000
6	6.073814000	-0.322800000	-2.833560000
1	7.718172000	1.593525000	3.345258000
1	7.720207000	-1.592350000	-3.344377000
1	5.968078000	-0.015842000	-3.886433000
1	8.074664000	-2.537259000	-1.144063000
1	5.966298000	0.016551000	3.886760000
1	8.073786000	2.537622000	1.144745000

$\text{LiCo}^{\text{III}}\text{-(SQ)}_2\text{-LiCo}^{\text{III}}$ ($\text{R}_1, \text{R}_2=\text{CH}_3$)

$E = -5059.72511 \text{ a.u.}, E^{\text{ZPE}} = -5059.09607 \text{ a.u.}$

8	3.615152000	-1.201276000	-0.508113000
8	3.615116000	1.201248000	0.508059000
6	0.000176000	-0.669967000	-0.273908000
6	1.221896000	-1.341380000	-0.551774000
6	0.000227000	-3.284667000	-1.342325000
6	-1.221525000	-1.343610000	-0.546401000
6	2.468409000	-0.663012000	-0.276915000
6	2.468390000	0.662963000	0.276824000
6	1.207958000	-2.642206000	-1.082809000
6	-1.207530000	-2.644039000	-1.078420000
1	2.156935000	-3.128693000	-1.281667000
1	-2.156492000	-3.130380000	-1.277717000
6	0.000159000	0.669884000	0.273749000
6	-1.221558000	1.343510000	0.546212000
6	-2.468085000	0.666578000	0.267856000
8	-3.614830000	1.211987000	0.481740000
6	-2.468069000	-0.666701000	-0.268066000
8	-3.614797000	-1.212126000	-0.481982000
6	-1.207595000	2.643941000	1.078227000
6	0.000147000	3.284591000	1.342152000
6	1.207894000	2.642147000	1.082665000
6	1.221862000	1.341317000	0.551640000
1	2.156859000	3.128652000	1.281536000
1	-2.156567000	3.130269000	1.277504000
1	0.000250000	-4.290036000	-1.752877000
1	0.000145000	4.289964000	1.752696000
27	5.030799000	-0.000013000	0.000024000
8	4.950426000	-0.757808000	1.741961000
8	6.366209000	1.272883000	0.415187000
8	6.366235000	-1.272919000	-0.415039000
8	4.950569000	0.757793000	-1.741906000
6	5.674850000	-0.394705000	2.722656000
6	6.632815000	0.630945000	2.693855000
6	6.915720000	1.401935000	1.558679000
6	6.915772000	-1.402023000	-1.558507000
6	6.632914000	-0.631064000	-2.693722000
6	5.675037000	0.394660000	-2.722564000
1	7.178945000	0.844097000	3.603909000
1	7.179068000	-0.844259000	-3.603753000
27	-5.030427000	-0.000099000	-0.000089000
8	-4.950528000	-0.684883000	1.771924000
8	-6.365755000	-1.197414000	-0.599261000
8	-6.365771000	1.197151000	0.599159000

8	-4.950637000	0.684740000	-1.772092000
6	-5.675652000	-1.631878000	2.214486000
6	-6.633149000	-2.341625000	1.472886000
6	-6.915352000	-2.092917000	0.123323000
6	-6.915325000	2.092759000	-0.123333000
6	-6.633184000	2.341529000	-1.472890000
6	-5.675724000	1.631805000	-2.214562000
1	-7.179554000	-3.132729000	1.970408000
1	-7.179541000	3.132719000	-1.970326000
6	5.434509000	-1.167247000	3.998491000
1	6.074914000	-0.826572000	4.814342000
1	4.384882000	-1.061954000	4.292114000
1	5.614517000	-2.231249000	3.813458000
6	7.949743000	2.501181000	1.630408000
1	8.731245000	2.313282000	0.886790000
1	7.478804000	3.455335000	1.371990000
1	8.402100000	2.577015000	2.621028000
6	7.949405000	-2.501627000	-1.630315000
1	8.402971000	-2.576429000	-2.620459000
1	8.729967000	-2.315137000	-0.885383000
1	7.477646000	-3.455919000	-1.373833000
6	5.435575000	1.167931000	-3.998117000
1	4.384940000	1.067394000	-4.289645000
1	5.620798000	2.231178000	-3.813634000
1	6.073046000	0.824415000	-4.815072000
6	-5.437826000	-1.977408000	3.665818000
1	-4.385807000	-2.246712000	3.805549000
1	-5.630893000	-1.093073000	4.282007000
1	-6.070898000	-2.800303000	4.003213000
6	-7.948997000	-2.925701000	-0.598336000
1	-8.400130000	-3.676861000	0.052730000
1	-8.731544000	-2.269881000	-0.994025000
1	-7.478212000	-3.421469000	-1.453621000
6	-7.947599000	2.926721000	0.598930000
1	-8.727674000	2.271370000	1.000059000
1	-7.474244000	3.426458000	1.450556000
1	-8.401868000	3.675093000	-0.053170000
6	-5.437739000	1.977611000	-3.665801000
1	-6.071351000	2.800037000	-4.003328000
1	-4.385898000	2.247844000	-3.805126000
1	-5.629810000	1.093175000	-4.282145000

$\text{LsCo}^{\text{III}}\text{-(SQ-Q)}\text{-HsCo}^{\text{II}}$ ($\text{R}_1, \text{R}_2=\text{CH}_3$)

$E = -5059.70861$ a.u., $E^{\text{ZPE}} = -5059.08338$ a.u.

6	0.119523000	-0.117789000	0.716812000
6	1.343922000	-0.232303000	1.427076000

6	0.136632000	-0.575381000	3.509198000
6	-1.092055000	-0.242228000	1.445444000
6	2.594295000	-0.116082000	0.709055000
6	2.594286000	0.115866000	-0.709146000
6	1.334418000	-0.457927000	2.816370000
6	-1.075084000	-0.470287000	2.825739000
1	2.287879000	-0.536912000	3.328338000
1	-2.024179000	-0.562256000	3.343884000
6	0.119515000	0.117466000	-0.716892000
6	-1.092072000	0.241861000	-1.445518000
6	-2.367047000	0.135647000	-0.741591000
8	-3.472629000	0.255353000	-1.284342000
6	-2.367039000	-0.136053000	0.741525000
8	-3.472614000	-0.255799000	1.284280000
6	-1.075116000	0.469924000	-2.825812000
6	0.136591000	0.575062000	-3.509278000
6	1.334386000	0.457654000	-2.816456000
6	1.343905000	0.232030000	-1.427163000
1	2.287841000	0.536676000	-3.328429000
1	-2.024218000	0.561863000	-3.343951000
1	0.142494000	-0.749762000	4.580524000
1	0.142442000	0.749446000	-4.580604000
27	-5.182367000	-0.000025000	-0.000018000
8	-5.138665000	-2.009414000	-0.258616000
8	-6.527512000	0.099398000	-1.498730000
8	-6.527575000	-0.099108000	1.498671000
8	-5.138058000	2.009328000	0.258701000
6	-5.981417000	-2.719930000	-0.891414000
6	-7.003350000	-2.219900000	-1.719745000
6	-7.204630000	-0.853837000	-1.995173000
6	-7.204315000	0.854309000	1.995271000
6	-7.002553000	2.220334000	1.719993000
6	-5.980517000	2.720083000	0.891627000
1	-7.649828000	-2.935834000	-2.213454000
1	-7.648757000	2.936446000	2.213806000
8	3.737118000	0.213966000	-1.288882000
8	3.737135000	-0.214127000	1.288785000
27	5.159367000	-0.000008000	-0.000046000
8	5.075912000	-1.870178000	-0.328142000
8	6.491750000	-0.102899000	1.332047000
8	6.491748000	0.103027000	-1.332133000
8	5.075713000	1.870151000	0.328045000
6	5.817296000	-2.736200000	0.238316000
6	6.785856000	-2.464494000	1.217183000
6	7.059176000	-1.182030000	1.709311000
6	7.059229000	1.182191000	-1.709223000

6	6.785871000	2.464606000	-1.216988000
6	5.817139000	2.736231000	-0.238269000
1	7.346363000	-3.296414000	1.623944000
1	7.346446000	3.296560000	-1.623587000
6	5.585510000	-4.156288000	-0.220419000
1	6.225475000	-4.868455000	0.303680000
1	4.535973000	-4.422840000	-0.058843000
1	5.774821000	-4.221363000	-1.296985000
6	8.102646000	-0.990432000	2.784354000
1	7.641218000	-0.510449000	3.653466000
1	8.556466000	-1.934950000	3.089858000
1	8.882196000	-0.315078000	2.416475000
6	8.102744000	0.990705000	-2.784243000
1	8.556885000	1.935206000	-3.089321000
1	8.882031000	0.314930000	-2.416590000
1	7.641227000	0.511252000	-3.653605000
6	5.585119000	4.156306000	0.220387000
1	4.535860000	4.423138000	0.057410000
1	5.772972000	4.221190000	1.297210000
1	6.225917000	4.868396000	-0.302796000
6	-5.826191000	-4.218166000	-0.729603000
1	-4.819007000	-4.513500000	-1.043366000
1	-5.922310000	-4.474766000	0.331037000
1	-6.563183000	-4.782701000	-1.305480000
6	-8.291474000	-0.445596000	-2.968525000
1	-8.846845000	-1.299983000	-3.362305000
1	-8.985114000	0.237830000	-2.467013000
1	-7.840312000	0.106771000	-3.800015000
6	-8.291294000	0.446345000	2.968588000
1	-8.985387000	-0.236485000	2.466889000
1	-7.840375000	-0.106599000	3.799825000
1	-8.846136000	1.300910000	3.362728000
6	-5.824907000	4.218272000	0.729769000
1	-6.561354000	4.783030000	1.306124000
1	-4.817421000	4.513269000	1.042864000
1	-5.921652000	4.474936000	-0.330804000

MECP_{T-Q} (R₁, R₂=CH₃)

E= -5059.70475 a.u.

6	-0.081642000	0.176206000	0.702622000
6	-1.305100000	0.358383000	1.402984000
6	-0.089016000	0.880976000	3.440064000
6	1.136031000	0.354537000	1.413368000
6	-2.554234000	0.178944000	0.696096000
6	-2.554060000	-0.180523000	-0.695342000
6	-1.292401000	0.708501000	2.764630000

6	1.120204000	0.704694000	2.770276000
1	-2.243064000	0.839372000	3.271324000
1	2.070051000	0.836894000	3.278442000
6	-0.081569000	-0.179640000	-0.700964000
6	1.136090000	-0.358294000	-1.411623000
6	2.397921000	-0.179608000	-0.713569000
8	3.522393000	-0.320086000	-1.262574000
6	2.397945000	0.178156000	0.714766000
8	3.522550000	0.321509000	1.262781000
6	1.120469000	-0.710140000	-2.767948000
6	-0.088599000	-0.887051000	-3.437889000
6	-1.292147000	-0.713137000	-2.762811000
6	-1.304884000	-0.361827000	-1.401584000
1	-2.242634000	-0.843660000	-3.269806000
1	2.070350000	-0.843232000	-3.275857000
1	-0.091134000	1.154957000	4.490562000
1	-0.090638000	-1.162322000	-4.487907000
27	5.104927000	0.000946000	-0.000370000
8	5.083293000	1.948578000	-0.387475000
8	6.466326000	-0.260184000	-1.413054000
8	6.466324000	0.260958000	1.412476000
8	5.081862000	-1.946763000	0.386218000
6	5.915184000	2.597416000	-1.097116000
6	6.931691000	2.024148000	-1.880602000
6	7.133752000	0.639991000	-2.014958000
6	7.132525000	-0.639708000	2.014891000
6	6.929523000	-2.023718000	1.880338000
6	5.912978000	-2.596231000	1.096280000
1	7.570611000	2.688597000	-2.449690000
1	7.567571000	-2.688670000	2.449799000
8	-3.699285000	-0.329238000	-1.262630000
8	-3.699562000	0.329441000	1.262602000
27	-5.119283000	0.000672000	-0.000270000
8	-5.039508000	1.835139000	-0.493515000
8	-6.454255000	0.222472000	1.318456000
8	-6.453706000	-0.220759000	-1.319748000
8	-5.040636000	-1.833535000	0.493422000
6	-5.788418000	2.745244000	-0.013090000
6	-6.760478000	2.560692000	0.982384000
6	-7.028638000	1.328764000	1.592008000
6	-7.028062000	-1.326662000	-1.593531000
6	-6.760943000	-2.558736000	-0.983584000
6	-5.789639000	-2.743460000	0.012794000
1	-7.326343000	3.424344000	1.308247000
1	-7.326923000	-3.422147000	-1.309512000
6	-5.563078000	4.118732000	-0.600111000

1	-6.207206000	4.872414000	-0.143088000
1	-4.515131000	4.404257000	-0.463385000
1	-5.752205000	4.083755000	-1.678126000
6	-8.075851000	1.233467000	2.676569000
1	-7.617748000	0.833345000	3.586841000
1	-8.531133000	2.201422000	2.894435000
1	-8.854307000	0.527908000	2.367660000
6	-8.074612000	-1.231575000	-2.678899000
1	-8.529575000	-2.199548000	-2.897194000
1	-8.853677000	-0.526537000	-2.370314000
1	-7.616121000	-0.831017000	-3.588781000
6	-5.565417000	-4.116641000	0.600614000
1	-4.517678000	-4.403138000	0.463875000
1	-5.754201000	-4.080648000	1.678620000
1	-6.210695000	-4.870054000	0.144820000
6	5.743212000	4.100284000	-1.077757000
1	4.733064000	4.352247000	-1.417889000
1	5.836992000	4.457625000	-0.046754000
1	6.474300000	4.611726000	-1.707117000
6	8.205593000	0.128548000	-2.953005000
1	8.760239000	0.937824000	-3.432454000
1	8.900958000	-0.508071000	-2.396005000
1	7.740966000	-0.496097000	-3.723508000
6	8.203789000	-0.128911000	2.953973000
1	8.899418000	0.508115000	2.397746000
1	7.738417000	0.494988000	3.724692000
1	8.758035000	-0.938654000	3.433077000
6	5.739759000	-4.098903000	1.076588000
1	6.470321000	-4.611149000	1.705916000
1	4.729203000	-4.350101000	1.416132000
1	5.833890000	-4.456194000	0.045630000

$\text{HS-Co}^{\text{II}}(\text{Q})_2\text{-HS-Co}^{\text{II}}(\text{R}_1, \text{R}_2=\text{CH}_3)$

$E = -5059.68977 \text{ a.u.}, E^{\text{ZPE}} = -5059.06840 \text{ a.u.}$

8	-3.595311000	0.008855000	-1.306571000
8	-3.595313000	-0.008797000	1.306569000
6	-0.000013000	-0.000087000	-0.732084000
6	-1.214046000	-0.001390000	-1.461836000
6	-0.000013000	-0.000442000	-3.564114000
6	1.214020000	0.001036000	-1.461836000
6	-2.486358000	0.001352000	-0.747431000
6	-2.486360000	-0.001306000	0.747432000
6	-1.203040000	-0.000027000	-2.864934000
6	1.203014000	-0.000680000	-2.864934000
1	-2.156349000	0.002064000	-3.383594000
1	2.156322000	-0.002903000	-3.383593000

6	-0.000014000	0.000096000	0.732086000
6	1.214018000	-0.001044000	1.461839000
6	2.486333000	0.001492000	0.747434000
8	3.595285000	0.009100000	1.306571000
6	2.486333000	-0.001522000	-0.747430000
8	3.595286000	-0.009146000	-1.306566000
6	1.203012000	0.000675000	2.864937000
6	-0.000016000	0.000455000	3.564117000
6	-1.203043000	0.000056000	2.864936000
6	-1.214047000	0.001417000	1.461837000
1	-2.156352000	-0.002022000	3.383595000
1	2.156320000	0.002884000	3.383597000
1	-0.000013000	-0.000580000	-4.649342000
1	-0.000017000	0.000593000	4.649344000
27	-5.282819000	0.000016000	-0.000017000
8	-5.254277000	2.010831000	-0.165252000
8	-6.617670000	0.216046000	1.483593000
8	-6.617599000	-0.216107000	-1.483662000
8	-5.254205000	-2.010808000	0.165279000
6	-6.091520000	2.842484000	0.309581000
6	-7.106376000	2.526907000	1.231128000
6	-7.298994000	1.247029000	1.782815000
6	-7.298939000	-1.247104000	-1.782813000
6	-7.106292000	-2.526959000	-1.231091000
6	-6.091409000	-2.842495000	-0.309555000
1	-7.752460000	3.328047000	1.569686000
1	-7.752363000	-3.328122000	-1.569621000
27	5.282792000	-0.000019000	0.000003000
8	5.254243000	-2.010864000	-0.164788000
8	6.617671000	-0.215742000	1.483639000
8	6.617595000	0.215781000	-1.483683000
8	5.254193000	2.010835000	0.164852000
6	6.091523000	-2.842413000	0.310164000
6	7.106437000	-2.526635000	1.231577000
6	7.299051000	-1.246645000	1.783008000
6	7.298928000	1.246713000	-1.783063000
6	7.106309000	2.526682000	-1.231588000
6	6.091434000	2.842411000	-0.310113000
1	7.752571000	-3.327691000	1.570239000
1	7.752399000	3.327765000	-1.570270000
6	5.935120000	-4.270838000	-0.165030000
1	4.920719000	-4.617766000	0.059358000
1	6.052940000	-4.300106000	-1.253737000
1	6.658233000	-4.948529000	0.294123000
6	8.375347000	-1.037726000	2.826551000
1	8.923028000	-1.954976000	3.053848000

1	9.077045000	-0.274721000	2.472591000
1	7.916824000	-0.652616000	3.743654000
6	8.375154000	1.037856000	-2.826690000
1	7.916555000	0.652891000	-3.743818000
1	8.922877000	1.955101000	-3.053907000
1	9.076822000	0.274762000	-2.472866000
6	5.935038000	4.270818000	0.165141000
1	6.658019000	4.948563000	-0.294141000
1	4.920568000	4.617687000	-0.059022000
1	6.053089000	4.300067000	1.253824000
6	-5.934944000	-4.270824000	0.165912000
1	-6.657995000	-4.948644000	-0.293148000
1	-4.920512000	-4.617734000	-0.058365000
1	-6.052813000	-4.299896000	1.254619000
6	-8.375185000	-1.038465000	-2.826464000
1	-7.916613000	-0.653655000	-3.743670000
1	-8.922891000	-1.955764000	-3.053501000
1	-9.076865000	-0.275324000	-2.472764000
6	-5.935135000	4.270811000	-0.165915000
1	-4.920667000	4.617726000	0.058184000
1	-6.053191000	4.299874000	-1.254604000
1	-6.658118000	4.948630000	0.293255000
6	-8.375197000	1.038352000	2.826503000
1	-8.922919000	1.955635000	3.053569000
1	-9.076868000	0.275191000	2.472830000
1	-7.916576000	0.653553000	3.743690000

$\text{LsCo}^{\text{III}}\text{-(SQ)}_2\text{-LsCo}^{\text{III}}$ ($\text{R}_1, \text{R}_2=\text{CF}_3$)

$E = -7441.21543 \text{ a.u.}, E^{\text{ZPE}} = -7440.76948 \text{ a.u.}$

8	-3.613762000	-0.020832000	-1.297200000
8	-3.613824000	0.021400000	1.296963000
6	0.000022000	0.000462000	-0.724566000
6	-1.219157000	-0.004059000	-1.453670000
6	0.000084000	0.000498000	-3.552530000
6	1.219232000	0.004989000	-1.453615000
6	-2.457564000	-0.006804000	-0.716587000
6	-2.457603000	0.007523000	0.716408000
6	-1.206841000	-0.002906000	-2.859286000
6	1.206977000	0.003873000	-2.859231000
1	-2.154205000	-0.002338000	-3.387464000
1	2.154363000	0.003302000	-3.387368000
6	-0.000012000	0.000449000	0.724491000
6	1.219168000	-0.004024000	1.453595000
6	2.457574000	-0.006688000	0.716513000
8	3.613774000	-0.020634000	1.297128000
6	2.457614000	0.007659000	-0.716482000
8	3.613833000	0.021610000	-1.297036000
6	1.206851000	-0.002904000	2.859212000
6	-0.000074000	0.000422000	3.552456000
6	-1.206967000	0.003752000	2.859157000
6	-1.219223000	0.004896000	1.453541000
1	-2.154354000	0.003122000	3.387295000
1	2.154215000	-0.002299000	3.387390000
1	0.000108000	0.000512000	-4.637840000
1	-0.000098000	0.000410000	4.637766000
27	4.999654000	0.000160000	0.000088000
8	4.934006000	-1.901051000	-0.043502000
8	6.354469000	0.085544000	1.335387000
8	6.354461000	-0.085942000	-1.335208000
8	4.935037000	1.901401000	0.043666000
6	5.660715000	-2.646531000	0.668554000
6	6.625135000	-2.274305000	1.607487000
6	6.889183000	-0.928261000	1.864376000
6	6.889499000	0.927576000	-1.864411000
6	6.626081000	2.273761000	-1.607612000
6	5.662025000	2.646496000	-0.668503000
1	7.171654000	-3.036683000	2.141328000
1	7.172826000	3.035848000	-2.141634000
6	5.388056000	-4.147191000	0.421844000
9	6.162452000	-4.937120000	1.192102000
9	4.102302000	-4.435520000	0.696958000
9	5.623953000	-4.461721000	-0.862654000

6	7.950585000	-0.554795000	2.922361000
9	8.574297000	-1.640057000	3.422135000
9	8.885069000	0.248197000	2.384386000
9	7.373731000	0.098740000	3.947287000
6	7.950706000	0.553534000	-2.922388000
9	8.885596000	-0.248693000	-2.383879000
9	7.373872000	-0.101088000	-3.946581000
9	8.573982000	1.638552000	-3.423243000
6	5.390194000	4.147304000	-0.421763000
9	5.626295000	4.461692000	0.862726000
9	6.164989000	4.936821000	-1.192038000
9	4.104580000	4.436336000	-0.696838000
27	-4.999642000	0.000120000	-0.000163000
8	-4.934271000	-1.901099000	0.043412000
8	-6.354448000	0.085714000	-1.335464000
8	-6.354456000	-0.085817000	1.335137000
8	-4.934751000	1.901356000	-0.043725000
6	-5.661148000	-2.646469000	-0.668585000
6	-6.625578000	-2.274096000	-1.607451000
6	-6.889403000	-0.928014000	-1.864361000
6	-6.889311000	0.927771000	1.864390000
6	-6.625687000	2.273922000	1.607619000
6	-5.661599000	2.646539000	0.668500000
1	-7.172265000	-3.036391000	-2.141238000
1	-7.172312000	3.036079000	2.141667000
6	-5.388703000	-4.147171000	-0.421894000
9	-6.163294000	-4.936980000	-1.192079000
9	-4.103020000	-4.435704000	-0.697123000
9	-5.624534000	-4.461660000	0.862627000
6	-7.950859000	-0.554388000	-2.922236000
9	-8.574612000	-1.639572000	-3.422129000
9	-8.885309000	0.248524000	-2.384067000
9	-7.374083000	0.099303000	-3.947098000
6	-7.950472000	0.553878000	2.922466000
9	-8.885188000	-0.248730000	2.384266000
9	-7.373478000	-0.100260000	3.946900000
9	-8.573960000	1.638947000	3.422947000
6	-5.389544000	4.147312000	0.421799000
9	-5.625647000	4.461781000	-0.862671000
9	-6.164182000	4.936927000	1.192131000
9	-4.103873000	4.436132000	0.696831000

$\text{LSCo}^{\text{III}}\text{-(SQ-Q)}\text{-HS}\text{Co}^{\text{II}}$ ($\text{R}_1, \text{R}_2=\text{CF}_3$)

$E = -7441.21715 \text{ a.u.}, E^{\text{ZPE}} = -7440.77453 \text{ a.u.}$

8	3.777368000	-0.110871000	1.294192000
8	3.777203000	0.110518000	-1.295169000

6	0.160891000	-0.045853000	0.726637000
6	1.382868000	-0.097634000	1.444699000
6	0.182045000	-0.222020000	3.555641000
6	-1.046416000	-0.083747000	1.469216000
6	2.625920000	-0.055604000	0.714240000
6	2.625823000	0.055130000	-0.715082000
6	1.376809000	-0.184878000	2.851379000
6	-1.029694000	-0.172195000	2.865667000
1	2.329864000	-0.219690000	3.368904000
1	-1.977500000	-0.202711000	3.393401000
6	0.160794000	0.045142000	-0.727182000
6	-1.046612000	0.082924000	-1.469613000
6	-2.321841000	0.034763000	-0.763243000
8	-3.422620000	0.050257000	-1.312558000
6	-2.321733000	-0.035745000	0.763004000
8	-3.422433000	-0.051425000	1.312472000
6	-1.030066000	0.171413000	-2.866063000
6	0.181586000	0.221379000	-3.556182000
6	1.376443000	0.184334000	-2.852068000
6	1.382679000	0.097053000	-1.445393000
1	2.329431000	0.219248000	-3.369706000
1	-1.977937000	0.201854000	-3.393685000
1	0.189034000	-0.289447000	4.638380000
1	0.188434000	0.288843000	-4.638920000
27	-5.148709000	-0.000208000	0.000110000
8	-5.101288000	-2.037913000	0.093570000
8	-6.534855000	-0.177262000	-1.481587000
8	-6.533980000	0.178120000	1.482435000
8	-5.099937000	2.037527000	-0.093773000
6	-5.934025000	-2.825515000	-0.425478000
6	-6.975339000	-2.521236000	-1.309915000
6	-7.171260000	-1.217179000	-1.786268000
6	-7.169841000	1.218447000	1.786872000
6	-6.973467000	2.522219000	1.309940000
6	-5.932208000	2.825693000	0.425152000
1	-7.611009000	-3.315701000	-1.671041000
1	-7.608694000	3.317113000	1.670900000
6	-5.697024000	-4.305753000	-0.048060000
9	-4.528185000	-4.735592000	-0.580204000
9	-5.616333000	-4.454663000	1.286279000
9	-6.669927000	-5.127964000	-0.494873000
6	-8.270404000	-0.978911000	-2.848281000
9	-8.991978000	-2.089550000	-3.116390000
9	-9.127802000	-0.025597000	-2.437619000
9	-7.716985000	-0.565650000	-4.008198000
6	-5.694595000	4.305700000	0.047202000
9	-5.613685000	4.454097000	-1.287174000
9	-6.667226000	5.128449000	0.493608000
9	-4.525640000	4.735280000	0.579330000
6	-8.268808000	0.981085000	2.849268000
9	-9.126986000	0.028293000	2.439000000
9	-7.715324000	0.567616000	4.009070000

9	-8.989550000	2.092251000	3.117432000
27	5.171171000	-0.000151000	-0.000582000
8	5.102532000	-1.891489000	-0.178724000
8	6.521210000	-0.008525000	1.334236000
8	6.521078000	0.008160000	-1.335618000
8	5.102611000	1.891210000	0.177793000
6	5.839274000	-2.686511000	0.467953000
6	6.810180000	-2.380768000	1.423568000
6	7.066881000	-1.056865000	1.781045000
6	7.067683000	1.056483000	-1.781330000
6	6.811871000	2.380281000	-1.422857000
6	5.840531000	2.686092000	-0.467712000
1	7.365482000	-3.178157000	1.893664000
1	7.368018000	3.177601000	-1.892071000
6	5.567642000	-4.165077000	0.110648000
9	6.355177000	-5.007255000	0.806228000
9	4.286166000	-4.476286000	0.382445000
9	5.784070000	-4.376684000	-1.197373000
6	8.131039000	-0.755068000	2.859327000
9	8.758076000	-1.870737000	3.278486000
9	9.059779000	0.086759000	2.374794000
9	7.553770000	-0.177104000	3.928021000
6	8.132089000	0.754783000	-2.859412000
9	9.060912000	-0.086817000	-2.374431000
9	7.555302000	0.176556000	-3.928135000
9	8.759076000	1.870501000	-3.278516000
6	5.569939000	4.164620000	-0.109421000
9	5.786791000	4.375119000	1.198742000
9	6.357976000	5.006726000	-0.804525000
9	4.288675000	4.476963000	-0.380735000

MECP_{T-Q} (R₁, R₂=CF₃)

E= -7441.18890 a.u.

8	-3.540960000	0.175729000	1.310833000
8	-3.541685000	-0.174599000	-1.308648000
6	0.038772000	0.025542000	0.731530000
6	-1.168030000	0.078170000	1.469602000
6	0.055168000	0.134538000	3.564692000
6	1.256662000	0.026061000	1.455518000
6	-2.446778000	0.073058000	0.762135000
6	-2.447133000	-0.072022000	-0.760432000
6	-1.152857000	0.134993000	2.869366000
6	1.251381000	0.078734000	2.861842000
1	-2.101872000	0.176282000	3.394242000
1	2.205125000	0.081082000	3.379559000
6	0.038375000	-0.025082000	-0.730942000
6	1.255871000	-0.025970000	-1.455523000
6	2.510962000	0.014908000	-0.732928000
8	3.640249000	0.061206000	-1.299661000
6	2.511339000	-0.015534000	0.732329000
8	3.640853000	-0.062584000	1.298309000
6	1.250036000	-0.078428000	-2.861791000

6	0.053557000	-0.133731000	-3.564038000
6	-1.154064000	-0.133962000	-2.868338000
6	-1.168719000	-0.077320000	-1.468444000
1	-2.103396000	-0.174916000	-3.392751000
1	2.203661000	-0.081020000	-3.379830000
1	0.060363000	0.178345000	4.648476000
1	0.058368000	-0.177375000	-4.648030000
27	5.163728000	-0.000283000	-0.000965000
8	5.144953000	1.962383000	0.202754000
8	6.552944000	0.135517000	-1.391549000
8	6.552523000	-0.135401000	1.390219000
8	5.146017000	-1.962768000	-0.205271000
6	5.989946000	2.758632000	-0.288559000
6	7.029898000	2.468529000	-1.175979000
6	7.208585000	1.174640000	-1.674743000
6	7.207129000	-1.174725000	1.675216000
6	7.028869000	-2.468695000	1.176551000
6	5.990450000	-2.758785000	0.287283000
1	7.680904000	3.261761000	-1.511406000
1	7.679084000	-3.262044000	1.513144000
6	5.766387000	4.224284000	0.149766000
9	4.593465000	4.675154000	-0.343356000
9	5.717503000	4.316235000	1.488556000
9	6.739649000	5.046822000	-0.288718000
6	8.314014000	0.925191000	-2.726171000
9	9.044986000	2.030352000	-2.974976000
9	9.152255000	-0.038052000	-2.302914000
9	7.765885000	0.523087000	-3.888391000
6	5.768092000	-4.224291000	-0.151987000
9	5.721741000	-4.315620000	-1.490901000
9	6.740767000	-5.046770000	0.287948000
9	4.594368000	-4.675654000	0.338750000
6	8.310423000	-0.925399000	2.729049000
9	9.149325000	0.038222000	2.308091000
9	7.759729000	-0.523991000	3.890324000
9	9.041090000	-2.030515000	2.978904000
27	-5.241370000	0.000346000	-0.000116000
8	-5.182359000	1.879306000	-0.297453000
8	-6.651377000	0.175196000	1.426469000
8	-6.651156000	-0.175531000	-1.428954000
8	-5.182662000	-1.878615000	0.297530000
6	-5.999416000	2.719196000	0.183441000
6	-7.027515000	2.510356000	1.099694000
6	-7.258018000	1.244469000	1.666698000
6	-7.257940000	-1.244840000	-1.668123000
6	-7.027718000	-2.510220000	-1.099792000
6	-5.999899000	-2.718581000	-0.183057000
1	-7.644033000	3.344850000	1.397818000
1	-7.644320000	-3.344953000	-1.397120000
6	-5.738135000	4.150785000	-0.325970000
9	-4.545976000	4.596670000	0.136546000
9	-5.692334000	4.184370000	-1.669291000

9	-6.680625000	5.027382000	0.076013000
6	-8.366815000	1.103728000	2.734940000
9	-9.064106000	2.246143000	2.918787000
9	-9.242104000	0.143078000	2.385365000
9	-7.828284000	0.761257000	3.924281000
6	-5.739348000	-4.149740000	0.327640000
9	-5.694789000	-4.182258000	1.671099000
9	-6.681587000	-5.026586000	-0.074437000
9	-4.546807000	-4.596258000	-0.133353000
6	-8.366883000	-1.105117000	-2.736542000
9	-9.242078000	-0.144080000	-2.387844000
9	-7.828447000	-0.763858000	-3.926264000
9	-9.064310000	-2.247649000	-2.919234000

$\text{HSCo}^{\text{II}}\text{-(Q)}_2\text{-HSCo}^{\text{II}}$ ($\text{R}_1, \text{R}_2=\text{CF}_3$)

$E = -7441.21314 \text{ a.u.}, E^{\text{ZPE}} = -7440.77397 \text{ a.u.}$

8	-3.583609000	-0.023034000	-1.312265000
8	-3.583327000	0.023503000	1.312937000
6	-0.000016000	-0.000177000	-0.737299000
6	-1.208419000	-0.007534000	-1.470133000
6	-0.000293000	-0.000323000	-3.576477000
6	1.208238000	0.007174000	-1.470370000
6	-2.485040000	-0.009869000	-0.760553000
6	-2.484870000	0.009897000	0.760995000
6	-1.200610000	-0.006407000	-2.874150000
6	1.200169000	0.005890000	-2.874391000
1	-2.154188000	-0.008694000	-3.392706000
1	2.153656000	0.008163000	-3.393118000
6	0.000134000	-0.000221000	0.737244000
6	1.208539000	-0.007692000	1.470082000
6	2.485162000	-0.010046000	0.760503000
8	3.583736000	-0.023244000	1.312216000
6	2.484979000	0.009769000	-0.761045000
8	3.583443000	0.023338000	-1.312987000
6	1.200736000	-0.006653000	2.874100000
6	0.000417000	-0.000557000	3.576423000
6	-1.200047000	0.005768000	2.874342000
6	-1.208128000	0.007154000	1.470321000
1	-2.153524000	0.008058000	3.393078000
1	2.154312000	-0.009025000	3.392647000
1	-0.000400000	-0.000415000	-4.661097000
1	0.000517000	-0.000721000	4.661053000
27	5.311175000	-0.000083000	-0.000969000
8	5.258416000	-2.021505000	-0.205723000
8	6.689035000	-0.258387000	1.466082000
8	6.686718000	0.259353000	-1.469708000
8	5.259072000	2.021320000	0.205924000
6	6.095890000	-2.839044000	0.260069000
6	7.140055000	-2.585170000	1.155860000
6	7.332720000	-1.311236000	1.708458000
6	7.331792000	1.311831000	-1.710251000
6	7.141056000	2.584934000	-1.155187000

6	6.097409000	2.838595000	-0.258659000
1	7.779553000	-3.397703000	1.466687000
1	7.781535000	3.397183000	-1.464735000
6	5.858870000	-4.293013000	-0.207070000
9	4.683917000	-4.748410000	0.287976000
9	5.790181000	-4.359495000	-1.548511000
9	6.825598000	-5.141088000	0.199096000
6	8.434720000	-1.128509000	2.778233000
9	9.154196000	-2.252146000	2.985222000
9	9.290468000	-0.156183000	2.412401000
9	7.883748000	-0.774574000	3.958028000
6	5.862266000	4.292111000	0.210874000
9	5.793393000	4.356489000	1.552379000
9	6.830197000	5.139565000	-0.193734000
9	4.687999000	4.749878000	-0.283678000
6	8.433272000	1.129568000	-2.780626000
9	9.288802000	0.156622000	-2.415817000
9	7.881790000	0.776745000	-3.960490000
9	9.153123000	2.253076000	-2.986982000
27	-5.311085000	0.000072000	0.000857000
8	-5.258311000	-2.021343000	0.205674000
8	-6.688652000	-0.258302000	-1.466441000
8	-6.687132000	0.259070000	1.469261000
8	-5.258979000	2.021494000	-0.205562000
6	-6.095851000	-2.838855000	-0.260048000
6	-7.139976000	-2.584979000	-1.155884000
6	-7.332481000	-1.311099000	-1.708663000
6	-7.332136000	1.311535000	1.710012000
6	-7.141158000	2.584810000	1.155411000
6	-6.097357000	2.838675000	0.259134000
1	-7.779559000	-3.397482000	-1.466617000
1	-7.781621000	3.397013000	1.465114000
6	-5.858975000	-4.292790000	0.207266000
9	-4.683958000	-4.748292000	-0.287501000
9	-5.790545000	-4.359130000	1.548740000
9	-6.825670000	-5.140862000	-0.198984000
6	-8.434444000	-1.128391000	-2.778476000
9	-9.154103000	-2.251950000	-2.985255000
9	-9.290021000	-0.155855000	-2.412858000
9	-7.883385000	-0.774786000	-3.958345000
6	-5.862139000	4.292278000	-0.210087000
9	-5.793986000	4.356960000	-1.551643000
9	-6.829696000	5.139824000	0.195228000
9	-4.687544000	4.749691000	0.283926000
6	-8.433848000	1.129049000	2.780118000
9	-9.289147000	0.156004000	2.415094000
9	-7.882549000	0.776249000	3.960096000
9	-9.153899000	2.252444000	2.986389000

MECP_{Q-S}(R₁, R₂=CF₃)

E= -7441.20287 a.u.

8	-3.666023000	0.066092000	1.299250000
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8	-3.666677000	-0.068492000	-1.298217000
6	-0.064496000	-0.003644000	0.731327000
6	-1.281433000	0.009701000	1.455985000
6	-0.078328000	-0.024880000	3.567426000
6	1.142973000	-0.023199000	1.470633000
6	-2.537116000	0.024029000	0.733041000
6	-2.537484000	-0.026241000	-0.732522000
6	-1.274996000	-0.001343000	2.863392000
6	1.129245000	-0.034033000	2.871815000
1	-2.228647000	0.004064000	3.381307000
1	2.079059000	-0.047835000	3.396884000
6	-0.064953000	0.002640000	-0.731911000
6	1.142244000	0.022795000	-1.471711000
6	2.418164000	0.021295000	-0.763265000
8	3.518007000	0.047179000	-1.313368000
6	2.418590000	-0.022752000	0.761687000
8	3.518689000	-0.049334000	1.311215000
6	1.127764000	0.035100000	-2.872841000
6	-0.080166000	0.026906000	-3.567947000
6	-1.276573000	0.002382000	-2.863516000
6	-1.282325000	-0.010567000	-1.456089000
1	-2.230397000	-0.002474000	-3.381172000
1	2.077264000	0.049152000	-3.398293000
1	-0.083006000	-0.036141000	4.652132000
1	-0.085180000	0.039212000	-4.652655000
27	5.243978000	-0.000374000	-0.001839000
8	5.199412000	2.021429000	0.246628000
8	6.630112000	0.284267000	-1.461754000
8	6.630387000	-0.283931000	1.460053000
8	5.201208000	-2.021314000	-0.249304000
6	6.046202000	2.841353000	-0.195319000
6	7.093250000	2.600670000	-1.092168000
6	7.280967000	1.338622000	-1.673464000
6	7.279972000	-1.338522000	1.674553000
6	7.092569000	-2.600752000	1.093479000
6	6.047490000	-2.840880000	0.194313000
1	7.740862000	3.415401000	-1.379592000
1	7.739120000	-3.415938000	1.381910000
6	5.823039000	4.285569000	0.308663000
9	4.650908000	4.765411000	-0.169554000
9	5.759923000	4.319616000	1.652046000
9	6.796084000	5.136498000	-0.078834000
6	8.391534000	1.173712000	-2.737169000
9	9.116011000	2.299291000	-2.918353000
9	9.243265000	0.193160000	-2.382051000
9	7.851691000	0.841938000	-3.928678000
6	5.825619000	-4.284495000	-0.311225000
9	5.764360000	-4.317040000	-1.654697000
9	6.798405000	-5.135336000	0.076827000
9	4.652901000	-4.765020000	0.164923000
6	8.388424000	-1.174132000	2.741030000
9	9.240875000	-0.193391000	2.388564000

9	7.845982000	-0.843316000	3.931674000
9	9.112626000	-2.299799000	2.923141000
27	-5.191957000	-0.000040000	0.000233000
8	-5.171990000	1.962962000	-0.200927000
8	-6.580369000	0.133339000	1.392001000
8	-6.582975000	-0.133379000	-1.391161000
8	-5.173298000	-1.961916000	0.201769000
6	-6.016423000	2.758283000	0.292727000
6	-7.056140000	2.466534000	1.179999000
6	-7.235671000	1.172167000	1.676951000
6	-7.237183000	-1.172504000	-1.677648000
6	-7.055964000	-2.466984000	-1.181360000
6	-6.017104000	-2.757334000	-0.292665000
1	-7.706260000	3.259639000	1.517190000
1	-7.704462000	-3.261299000	-1.518887000
6	-5.791929000	4.225187000	-0.140714000
9	-4.622616000	4.675796000	0.361474000
9	-5.734395000	4.320546000	-1.478720000
9	-6.768776000	5.045516000	0.293704000
6	-8.340266000	0.921767000	2.729024000
9	-9.073561000	2.025471000	2.976539000
9	-9.176333000	-0.044196000	2.307712000
9	-7.790338000	0.522627000	3.891580000
6	-5.792644000	-4.223080000	0.143009000
9	-5.736100000	-4.315966000	1.481235000
9	-6.768778000	-5.044406000	-0.290886000
9	-4.622549000	-4.673919000	-0.357486000
6	-8.342251000	-0.923254000	-2.730115000
9	-9.178303000	0.043246000	-2.310428000
9	-7.792455000	-0.525967000	-3.893490000
9	-9.075759000	-2.027260000	-2.976170000

$\text{LsCo}^{\text{III}}\text{-(SQ)}_2\text{-LsCo}^{\text{III}}$ ($\text{R}_1=\text{CH}_3$, $\text{R}_2=\text{CF}_3$)
 $E = -6250.48040$ a.u., $E^{\text{ZPE}} = -6249.94295$ a.u.

8	-3.601911000	0.289383000	1.029774000
8	-3.604440000	0.275294000	-1.571771000
6	0.000016000	-0.000027000	0.453192000
6	-1.216647000	0.093051000	1.180989000
6	-0.000136000	-0.000044000	3.279358000
6	1.216600000	-0.093116000	1.181119000
6	-2.455323000	0.190552000	0.446410000
6	-2.455794000	0.186795000	-0.988559000
6	-1.204109000	0.089683000	2.586226000
6	1.203912000	-0.089764000	2.586355000
1	-2.149985000	0.156647000	3.113026000
1	2.149731000	-0.156730000	3.113255000
6	0.000095000	-0.000015000	-0.995081000
6	1.217293000	-0.091678000	-1.722799000
6	2.455983000	-0.186830000	-0.988296000
8	3.604693000	-0.275329000	-1.571385000
6	2.455355000	-0.190613000	0.446673000
8	3.601877000	-0.289472000	1.030161000
6	1.204024000	-0.090944000	-3.128081000
6	0.000248000	0.000009000	-3.821238000
6	-1.203604000	0.090949000	-3.128210000
6	-1.217024000	0.091660000	-1.722929000
1	-2.148923000	0.163842000	-3.655063000
1	2.149400000	-0.163828000	-3.654834000
1	-0.000194000	-0.000048000	4.364931000
1	0.000307000	0.000017000	-4.906889000
27	4.999466000	-0.381078000	-0.269614000
8	5.057018000	1.520016000	-0.249528000
8	6.337822000	-0.584025000	-1.600104000
8	6.348541000	-0.370255000	1.064034000
8	4.790406000	-2.271760000	-0.293377000
6	5.833680000	2.192264000	-0.990251000
6	6.758047000	1.736618000	-1.919493000
6	6.961133000	0.363103000	-2.171864000
6	6.791471000	-1.426684000	1.607688000
6	6.425195000	-2.742983000	1.370939000
6	5.436735000	-3.093498000	0.423722000
1	7.343902000	2.459137000	-2.468946000
1	6.911217000	-3.528686000	1.931049000
6	5.664178000	3.710841000	-0.780721000
9	6.488253000	4.437240000	-1.568685000
9	4.399937000	4.087060000	-1.063347000
9	5.920562000	4.049026000	0.495918000
6	7.885579000	-1.123994000	2.650817000
9	8.938930000	-0.517201000	2.064255000
9	7.418797000	-0.305038000	3.610501000
9	8.348108000	-2.240124000	3.256582000
27	-4.999354000	0.381056000	-0.270155000
8	-4.790228000	2.271733000	-0.293852000
8	-6.348594000	0.370247000	1.063325000

8	-6.337551000	0.584073000	-1.600795000
8	-5.056971000	-1.520034000	-0.250106000
6	-5.436774000	3.093491000	0.423029000
6	-6.425364000	2.742986000	1.370115000
6	-6.791636000	1.426686000	1.606867000
6	-6.960864000	-0.363024000	-2.172604000
6	-6.757888000	-1.736547000	-1.920198000
6	-5.833621000	-2.192241000	-0.990879000
1	-6.911473000	3.528694000	1.930141000
1	-7.343736000	-2.459037000	-2.469696000
6	-7.885893000	1.124011000	2.649845000
9	-8.348406000	2.240135000	3.255630000
9	-8.939226000	0.517355000	2.063091000
9	-7.419316000	0.304941000	3.609521000
6	-5.664218000	-3.710827000	-0.781331000
9	-5.920685000	-4.048989000	0.495297000
9	-6.488297000	-4.437182000	-1.569332000
9	-4.399985000	-4.087120000	-1.063893000
6	5.083136000	-4.543647000	0.210578000
1	4.016031000	-4.686923000	0.409232000
1	5.255548000	-4.804379000	-0.838720000
1	5.664768000	-5.207956000	0.851608000
6	7.997526000	-0.068398000	-3.178165000
1	7.577038000	-0.841560000	-3.827012000
1	8.357249000	0.767955000	-3.779893000
1	8.846490000	-0.512149000	-2.645212000
6	-5.083519000	4.543672000	0.209538000
1	-5.259884000	4.805059000	-0.838970000
1	-5.662712000	5.207753000	0.853004000
1	-4.015653000	4.686591000	0.404170000
6	-7.997129000	0.068527000	-3.179017000
1	-8.846152000	0.512267000	-2.646147000
1	-7.576557000	0.841707000	-3.827786000
1	-8.356793000	-0.767800000	-3.780816000

$\text{LSCo}^{\text{III}}\text{-(SQ-Q)}\text{-HS}\text{Co}^{\text{II}}$ ($\text{R}_1=\text{CH}_3$, $\text{R}_2=\text{CF}_3$)

$E = -6250.47272$ a.u., $E^{\text{ZPE}} = -6249.93896$ a.u.

8	-3.712229000	0.375548000	0.998397000
8	-3.739671000	0.132841000	-1.596195000
6	-0.117443000	-0.012693000	0.421157000
6	-1.328894000	0.157246000	1.139519000
6	-0.112809000	0.216816000	3.244024000
6	1.092493000	-0.064761000	1.159049000
6	-2.577006000	0.211990000	0.414306000
6	-2.590851000	0.085422000	-1.015264000
6	-1.309910000	0.267498000	2.543738000
6	1.088318000	0.052546000	2.553125000
1	-2.255526000	0.390738000	3.061504000
1	2.037806000	0.013771000	3.077313000
6	-0.130002000	-0.129362000	-1.029528000
6	1.067776000	-0.292541000	-1.771320000
6	2.346223000	-0.350081000	-1.066910000

8	3.437493000	-0.497186000	-1.618428000
6	2.357404000	-0.236092000	0.450967000
8	3.457122000	-0.302805000	1.001549000
6	1.038797000	-0.402568000	-3.165412000
6	-0.174588000	-0.353584000	-3.852598000
6	-1.359679000	-0.195186000	-3.148137000
6	-1.355212000	-0.081399000	-1.744227000
1	-2.314089000	-0.154239000	-3.662652000
1	1.979134000	-0.526993000	-3.692575000
1	-0.109993000	0.304270000	4.325557000
1	-0.190770000	-0.439217000	-4.934224000
27	5.177552000	-0.397285000	-0.301552000
8	5.027396000	1.635247000	-0.326172000
8	6.570165000	-0.237199000	-1.770477000
8	6.520135000	-0.476844000	1.215225000
8	5.197782000	-2.429432000	-0.350004000
6	5.843402000	2.422198000	-0.886669000
6	6.908816000	2.114773000	-1.725569000
6	7.206586000	0.790334000	-2.139845000
6	7.184980000	-1.498787000	1.544353000
6	7.050403000	-2.808527000	1.089737000
6	6.044851000	-3.208904000	0.174559000
1	7.511021000	2.924495000	-2.113585000
1	7.713670000	-3.562780000	1.489566000
6	5.534940000	3.907884000	-0.602270000
9	4.341526000	4.252811000	-1.148905000
9	5.452000000	4.144691000	0.721472000
9	6.460461000	4.756810000	-1.106684000
6	8.261627000	-1.198276000	2.610844000
9	9.137955000	-0.274990000	2.158995000
9	7.697948000	-0.707573000	3.735608000
9	8.981767000	-2.289328000	2.968707000
27	-5.130946000	0.336742000	-0.291267000
8	-4.951754000	2.219306000	-0.486431000
8	-6.462104000	0.422191000	1.049572000
8	-6.483259000	0.396729000	-1.615251000
8	-5.151503000	-1.553535000	-0.098825000
6	-5.629563000	3.092102000	0.136664000
6	-6.620321000	2.810378000	1.104185000
6	-6.944825000	1.515429000	1.476981000
6	-7.112440000	-0.607421000	-2.075030000
6	-6.891163000	-1.947724000	-1.693628000
6	-5.938630000	-2.303416000	-0.749959000
1	-7.137358000	3.634011000	1.574947000
1	-7.484266000	-2.724489000	-2.154239000
6	-8.027309000	1.285210000	2.550404000
9	-8.573866000	2.439406000	2.989677000
9	-9.025913000	0.526164000	2.055942000
9	-7.510073000	0.647305000	3.616588000
6	-5.741471000	-3.792334000	-0.399407000
9	-5.954142000	-4.005417000	0.911033000
9	-6.576956000	-4.599994000	-1.087422000

9	-4.479779000	-4.177196000	-0.683522000
6	5.936582000	-4.668704000	-0.205376000
1	4.928181000	-5.027800000	0.025942000
1	6.073327000	-4.765263000	-1.287987000
1	6.670310000	-5.293489000	0.307875000
6	8.350072000	0.561510000	-3.102244000
1	7.994029000	-0.029988000	-3.951606000
1	8.790450000	1.493541000	-3.462187000
1	9.124161000	-0.028604000	-2.598748000
6	-5.312593000	4.521849000	-0.219513000
1	-5.505955000	4.676116000	-1.286252000
1	-5.901865000	5.231620000	0.362893000
1	-4.246740000	4.708047000	-0.053208000
6	-8.176344000	-0.283137000	-3.091768000
1	-9.028175000	0.177567000	-2.577757000
1	-7.789947000	0.447754000	-3.807078000
1	-8.524009000	-1.173621000	-3.618091000

MECP_{T-Q} (R₁=CH₃, R₂=CF₃)

E= -6250.45946 a.u.

8	-3.643953000	0.404971000	0.993172000
8	-3.711283000	0.070626000	-1.590014000
6	-0.054869000	0.007546000	0.370646000
6	-1.254581000	0.202997000	1.103559000
6	-0.000675000	0.328323000	3.181937000
6	1.169429000	-0.033143000	1.087869000
6	-2.516105000	0.226605000	0.397822000
6	-2.553180000	0.047138000	-1.025255000
6	-1.210475000	0.364112000	2.501873000
6	1.187599000	0.125594000	2.478762000
1	-2.145573000	0.513481000	3.031498000
1	2.143094000	0.092599000	2.992158000
6	-0.093920000	-0.155181000	-1.074974000
6	1.090600000	-0.324279000	-1.832662000
6	2.387955000	-0.316372000	-1.158048000
8	3.467222000	-0.403916000	-1.740920000
6	2.417894000	-0.245923000	0.361481000
8	3.512440000	-0.424265000	0.908280000
6	1.038459000	-0.483654000	-3.220905000
6	-0.187440000	-0.483324000	-3.886614000
6	-1.361396000	-0.311763000	-3.166854000
6	-1.331476000	-0.143399000	-1.769147000
1	-2.325634000	-0.301186000	-3.664286000
1	1.972278000	-0.608176000	-3.759664000
1	0.021694000	0.456806000	4.259500000
1	-0.221589000	-0.613592000	-4.963356000
27	5.162366000	-0.388141000	-0.316857000
8	4.989707000	1.489072000	-0.287802000
8	6.592538000	-0.368825000	-1.653260000
8	6.514293000	-0.307518000	1.233951000
8	5.193867000	-2.273100000	-0.375846000
6	5.737608000	2.287438000	-0.935066000

6	6.767315000	1.994708000	-1.814465000
6	7.137469000	0.661778000	-2.137501000
6	7.122010000	-1.333477000	1.621004000
6	6.940196000	-2.660427000	1.210495000
6	5.983000000	-3.049140000	0.255006000
1	7.306577000	2.811750000	-2.272480000
1	7.550088000	-3.430141000	1.661946000
6	5.358140000	3.755189000	-0.678962000
9	4.129851000	4.017698000	-1.193648000
9	5.306321000	4.025785000	0.638397000
9	6.219678000	4.631642000	-1.240942000
6	8.198471000	-1.036467000	2.691305000
9	9.109968000	-0.159773000	2.216778000
9	7.641298000	-0.487334000	3.792387000
9	8.878264000	-2.137516000	3.095461000
27	-5.081354000	0.320069000	-0.277008000
8	-4.905792000	2.194844000	-0.538682000
8	-6.402491000	0.451967000	1.070828000
8	-6.444066000	0.335744000	-1.592594000
8	-5.101558000	-1.562808000	-0.019691000
6	-5.594270000	3.087171000	0.043609000
6	-6.590277000	2.837815000	1.014524000
6	-6.901847000	1.557292000	1.444111000
6	-7.066163000	-0.684849000	-2.024655000
6	-6.838401000	-2.011995000	-1.603668000
6	-5.886136000	-2.334655000	-0.647631000
1	-7.118886000	3.675741000	1.445512000
1	-7.427645000	-2.804919000	-2.041021000
6	-7.990072000	1.362680000	2.518845000
9	-8.545092000	2.530077000	2.910499000
9	-8.982153000	0.580992000	2.046124000
9	-7.478154000	0.767475000	3.611570000
6	-5.686654000	-3.811263000	-0.249127000
9	-5.898371000	-3.981906000	1.067592000
9	-6.521442000	-4.642309000	-0.909911000
9	-4.424716000	-4.203702000	-0.521453000
6	5.824428000	-4.510902000	-0.091978000
1	4.803007000	-4.828993000	0.144427000
1	5.961965000	-4.639758000	-1.170347000
1	6.532523000	-5.144734000	0.444307000
6	8.256815000	0.422781000	-3.123956000
1	7.890482000	-0.204391000	-3.943249000
1	8.658131000	1.352793000	-3.530728000
1	9.060470000	-0.130029000	-2.625846000
6	-5.284316000	4.503529000	-0.368520000
1	-5.480707000	4.615639000	-1.439681000
1	-5.875240000	5.232889000	0.187375000
1	-4.218541000	4.700296000	-0.212122000
6	-8.128860000	-0.395919000	-3.053542000
1	-8.981926000	0.081731000	-2.557606000
1	-7.741099000	0.310233000	-3.792514000
1	-8.474892000	-1.303959000	-3.550492000

$\text{HS-Co}^{\text{II}}\text{-(Q)}_2\text{-HS-Co}^{\text{II}}$ ($\text{R}_1=\text{CH}_3$, $\text{R}_2=\text{CF}_3$)
 $E = -6250.46048$ a.u., $E^{\text{ZPE}} = -6249.93043$ a.u.

8	3.569956000	-0.370393000	-1.660150000
8	3.566234000	-0.381967000	0.962839000
6	0.000169000	-0.000131000	-1.084852000
6	1.204877000	-0.120628000	-1.816371000
6	0.000522000	-0.000257000	-3.920937000
6	-1.204356000	0.120305000	-1.816682000
6	2.474948000	-0.251401000	-1.105512000
6	2.472356000	-0.257999000	0.406569000
6	1.195687000	-0.119379000	-3.219493000
6	-1.194817000	0.118931000	-3.219802000
1	2.144656000	-0.214809000	-3.737481000
1	-2.143657000	0.214317000	-3.738034000
6	-0.000014000	-0.000065000	0.385658000
6	-1.203732000	0.127462000	1.116812000
6	-2.472389000	0.257860000	0.405926000
8	-3.566412000	0.381850000	0.961911000
6	-2.474602000	0.251154000	-1.106151000
8	-3.569471000	0.370131000	-1.661070000
6	-1.195439000	0.123156000	2.520364000
6	-0.000368000	0.000072000	3.221392000
6	1.194877000	-0.123083000	2.520674000
6	1.203520000	-0.127526000	1.117125000
1	2.143791000	-0.217071000	3.039161000
1	-2.144481000	0.217195000	3.038606000
1	0.000658000	-0.000306000	-5.005798000
1	-0.000504000	0.000126000	4.306204000
27	-5.284254000	0.357984000	-0.322356000
8	-5.346395000	2.369181000	-0.535249000
8	-6.601985000	0.532398000	1.196850000
8	-6.695296000	0.059363000	-1.740829000
8	-5.099703000	-1.659429000	-0.193971000
6	-6.211436000	3.172258000	-0.076402000
6	-7.202107000	2.826843000	0.875952000
6	-7.297101000	1.558947000	1.443298000
6	-7.326378000	-1.001519000	-2.016692000
6	-6.998192000	-2.284747000	-1.507528000
6	-5.911252000	-2.506155000	-0.670836000
1	-7.884470000	3.594510000	1.213089000
1	-7.594078000	-3.132016000	-1.817084000
6	-8.361220000	1.317559000	2.536472000
9	-9.101765000	2.417365000	2.811902000
9	-9.217843000	0.344013000	2.158873000
9	-7.781454000	0.926192000	3.690452000
6	-5.565944000	-3.956866000	-0.273740000
9	-5.457929000	-4.082948000	1.062784000
9	-6.480406000	-4.859747000	-0.693935000
9	-4.373638000	-4.317020000	-0.811774000
27	5.284410000	-0.358055000	-0.321015000
8	5.099602000	1.659348000	-0.192751000

8	6.695808000	-0.059326000	-1.739110000
8	6.601802000	-0.532236000	1.198530000
8	5.346758000	-2.369247000	-0.533746000
6	5.911213000	2.506140000	-0.669395000
6	6.998426000	2.284815000	-1.505752000
6	7.326898000	1.001601000	-2.014773000
6	7.296816000	-1.558762000	1.445348000
6	7.201984000	-2.826739000	0.878152000
6	6.211650000	-3.172266000	-0.074508000
1	7.594326000	3.132132000	-1.815151000
1	7.884222000	-3.594371000	1.215624000
6	5.565647000	3.956827000	-0.272435000
9	4.373409000	4.316814000	-0.810727000
9	5.457342000	4.082951000	1.064063000
9	6.480086000	4.859802000	-0.692477000
6	8.360609000	-1.317232000	2.538808000
9	9.217437000	-0.343843000	2.161267000
9	7.780516000	-0.925563000	3.692521000
9	9.100971000	-2.417043000	2.814711000
6	-6.141451000	4.593078000	-0.585517000
1	-6.871172000	5.248554000	-0.106386000
1	-5.133329000	4.987031000	-0.420223000
1	-6.313951000	4.591159000	-1.667507000
6	-8.495061000	-0.860897000	-2.963464000
1	-9.279788000	-0.274555000	-2.471726000
1	-8.179065000	-0.300402000	-3.848606000
1	-8.909339000	-1.824836000	-3.265202000
6	6.141877000	-4.593134000	-0.583517000
1	5.133602000	-4.986973000	-0.418901000
1	6.315146000	-4.591339000	-1.665387000
1	6.871210000	-5.248626000	-0.103818000
6	8.495960000	0.861059000	-2.961089000
1	8.180574000	0.299874000	-3.846005000
1	8.909838000	1.825048000	-3.263220000
1	9.280844000	0.275443000	-2.468727000

MECP_{Q-S} (R₁=CH₃, R₂=CF₃)

E= -6250.44872 a.u.

8	-3.618114000	0.307693000	-1.733721000
8	-3.621082000	0.498304000	0.890344000
6	-0.041897000	-0.005919000	-1.115108000
6	-1.243785000	0.108566000	-1.852302000
6	-0.014667000	0.069656000	-3.947774000
6	1.172301000	-0.093161000	-1.838427000
6	-2.522279000	0.198324000	-1.154874000
6	-2.528528000	0.254942000	0.335586000
6	-1.218063000	0.142844000	-3.256336000
6	1.177636000	-0.051580000	-3.239355000
1	-2.163378000	0.234531000	-3.781380000
1	2.132498000	-0.115967000	-3.751285000
6	-0.059154000	-0.025044000	0.350322000
6	1.136046000	-0.161782000	1.096980000

6	2.415299000	-0.272885000	0.399389000
8	3.503510000	-0.401800000	0.962875000
6	2.434923000	-0.230410000	-1.116971000
8	3.536539000	-0.327890000	-1.660578000
6	1.108890000	-0.175406000	2.498516000
6	-0.098059000	-0.055774000	3.182774000
6	-1.282349000	0.085702000	2.468865000
6	-1.275834000	0.104881000	1.063144000
1	-2.235847000	0.180080000	2.978321000
1	2.049496000	-0.278275000	3.030184000
1	-0.004593000	0.106716000	-5.031968000
1	-0.113509000	-0.070784000	4.267554000
27	5.247627000	-0.347436000	-0.312818000
8	5.310716000	-2.357436000	-0.568612000
8	6.568760000	-0.553246000	1.205778000
8	6.672485000	-0.029269000	-1.723096000
8	5.070876000	1.669891000	-0.144575000
6	6.187161000	-3.162825000	-0.137497000
6	7.181542000	-2.834446000	0.817273000
6	7.271335000	-1.581600000	1.418759000
6	7.307299000	1.035337000	-1.971748000
6	6.982677000	2.308368000	-1.434532000
6	5.892470000	2.518872000	-0.598898000
1	7.872316000	-3.605617000	1.128432000
1	7.584930000	3.158992000	-1.722025000
6	8.342785000	-1.364324000	2.510213000
9	9.086661000	-2.469353000	2.757071000
9	9.197436000	-0.382243000	2.148975000
9	7.771801000	-0.998788000	3.677098000
6	5.558321000	3.964017000	-0.172281000
9	5.450193000	4.064126000	1.166767000
9	6.480400000	4.869307000	-0.572409000
9	4.369687000	4.346187000	-0.703390000
27	-5.238945000	0.347627000	-0.332881000
8	-5.064753000	-1.523783000	-0.147186000
8	-6.689395000	0.206517000	-1.628685000
8	-6.573536000	0.394823000	1.222197000
8	-5.316698000	2.231002000	-0.534134000
6	-5.836200000	-2.375355000	-0.694396000
6	-6.891259000	-2.157222000	-1.564210000
6	-7.262284000	-0.858813000	-1.998257000
6	-7.253641000	1.418112000	1.486217000
6	-7.143292000	2.696363000	0.932183000
6	-6.165591000	3.032161000	-0.022329000
1	-7.450536000	-3.008585000	-1.925870000
1	-7.809879000	3.472873000	1.279468000
6	-5.463639000	-3.821435000	-0.315680000
9	-4.260416000	-4.145244000	-0.846979000
9	-5.373315000	-3.968048000	1.017011000
9	-6.358032000	-4.726295000	-0.768195000
6	-8.328796000	1.176943000	2.570945000
9	-9.199870000	0.226568000	2.167223000

9	-7.763481000	0.753590000	3.718900000
9	-9.050945000	2.284804000	2.860641000
6	6.130514000	-4.570266000	-0.685697000
1	6.864000000	-5.232784000	-0.222049000
1	5.125029000	-4.976801000	-0.536039000
1	6.308065000	-4.536855000	-1.766469000
6	8.479594000	0.914412000	-2.918104000
1	9.262215000	0.316303000	-2.437309000
1	8.165795000	0.374504000	-3.816760000
1	8.896271000	1.884299000	-3.197065000
6	-6.057934000	4.455877000	-0.513797000
1	-5.042253000	4.825848000	-0.339560000
1	-6.227982000	4.474017000	-1.595693000
1	-6.773710000	5.118178000	-0.023852000
6	-8.415302000	-0.694929000	-2.957785000
1	-8.089894000	-0.103675000	-3.819342000
1	-8.812013000	-1.652504000	-3.299566000
1	-9.214414000	-0.132808000	-2.461968000