Luminescent complexes of the trinuclear silver(I) and copper(I) pyrazolates supported with bis(diphenylphosphino)methane

Supporting Information

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Table S1. Crystal data, data collection and structure refinement parameters for complexes 2a and 2b.

Compound	2a	2b
Molecular formula	C40H25Ag3F18N6P2	C40H25Cu3F18N6P2
Formula weight	1317.21	1184.22
Dimension, mm	0.20×0.18×0.10	0.33×0.28×0.14
Temperature, K	120(2)	120(2)
Crystal system	triclinic	Triclinic
Space group	$P\ \bar{1}$	$P\ \bar{1}$
a, Å	11.6217(8)	10.680(7)
b, Å	11.8522(9)	11.922(8)
c, Å	18.6060(13)	19.238(13)
α, deg.	97.5190(10)	74.079(11)
β, deg.	106.5700(10)	75.740(12)
γ, deg.	107.5490(10)	71.620(11)
V, Å3	2275.2(3)	2201(3)
Z	2	2
ρcalc, g cm^{-3}	1.923	1.787
Linear absorption (μ), cm^{-1}	14.61	16.25
Tmin/Tmax	0.660/0.746	0.574/0.746
2θmax, deg.	60	60
No. unique refl.	42101	39651
No. observed refl. (I>2σ(I))	11870	12260
No. parameters	650	622
R1 (on F for observed refl.)a	0.0308	0.0239
wR2 (on F2 for all refl.)b	0.0746	0.0644
GOOF	1.027	1.029

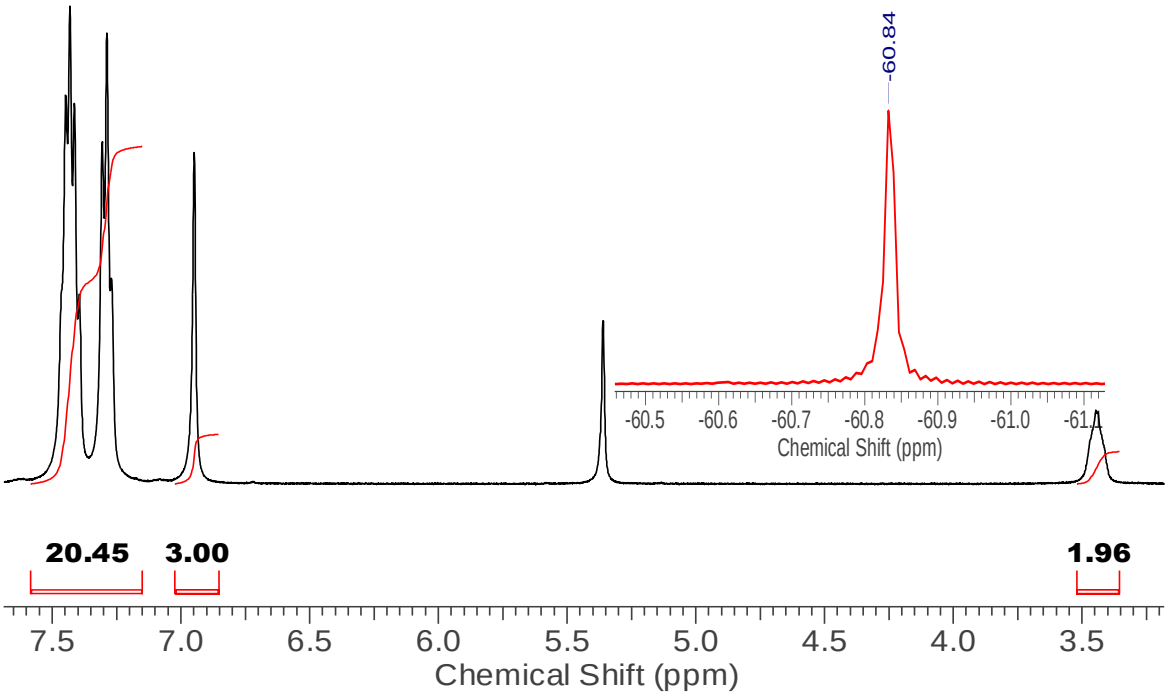


Figure S1. ^{1}H (black) and ^{19}F (red) NMR spectra of complex 2a in CD_2Cl_2, RT.

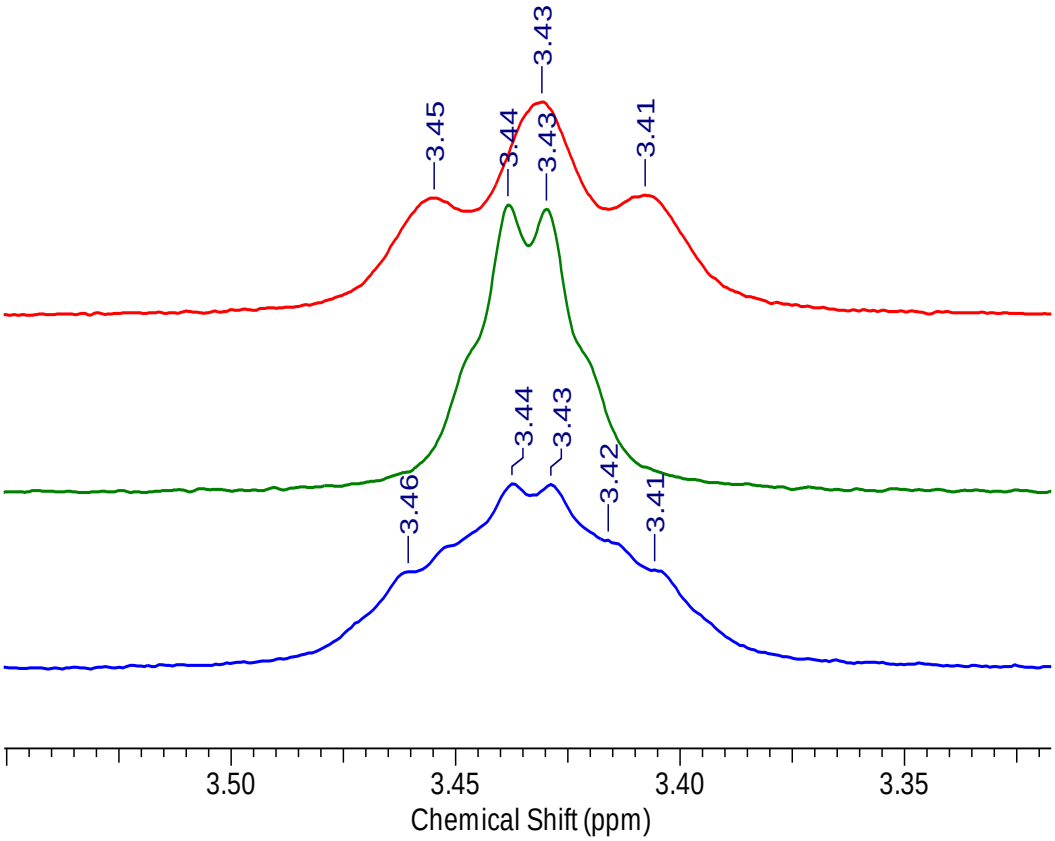


Figure S2. ^{1}H (blue), $^{1}H\{^{31}P\}$ (red) and $^{1}H\{^{109}Ag\}$ (green) NMR spectra of complex 2a in CD_2Cl_2, RT

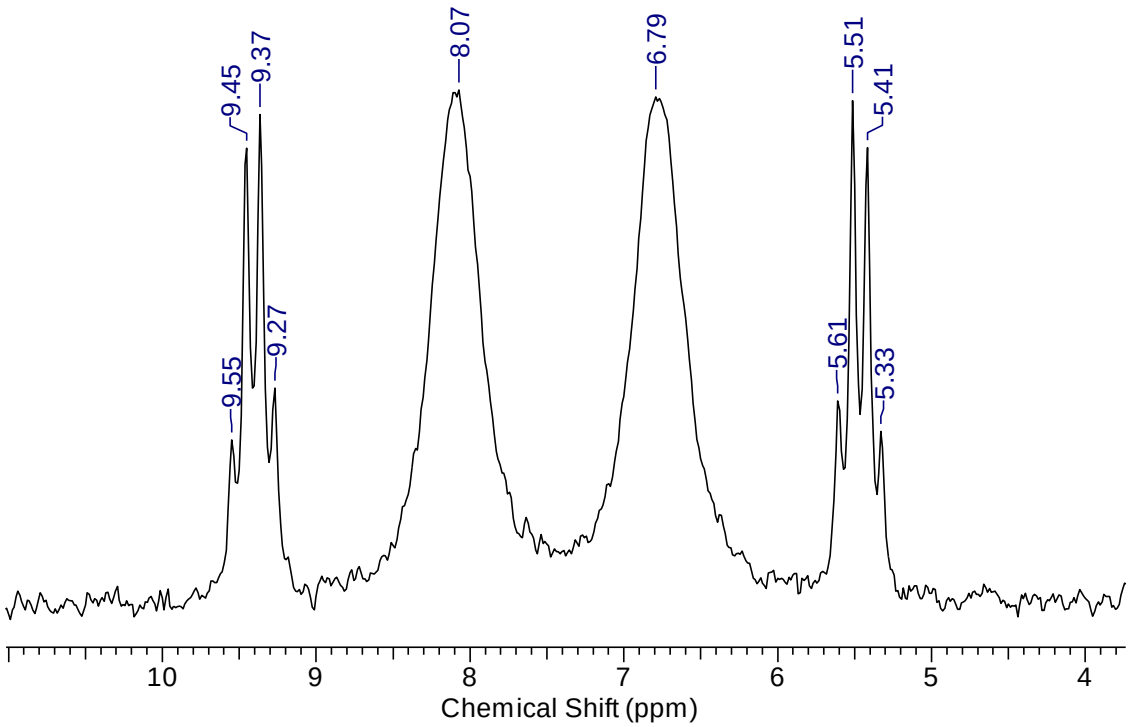


Figure S3. $^{31}P\{^{1}H\}$ NMR spectra of complex **2a** in CD_2Cl_2 at 273 K.

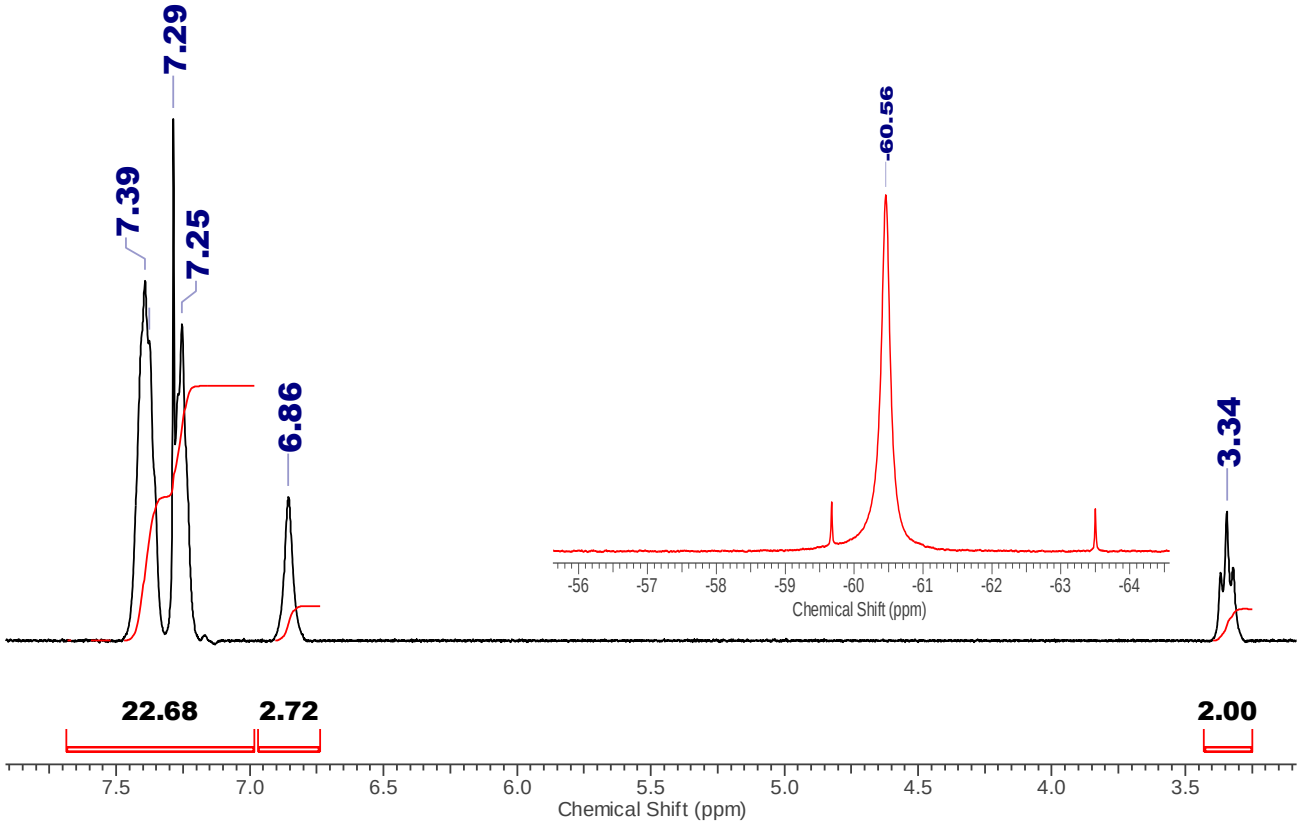


Figure S4. ^{1}H (black) and ^{19}F (red) NMR spectra of complex **2a** in $CDCl_3$, RT.

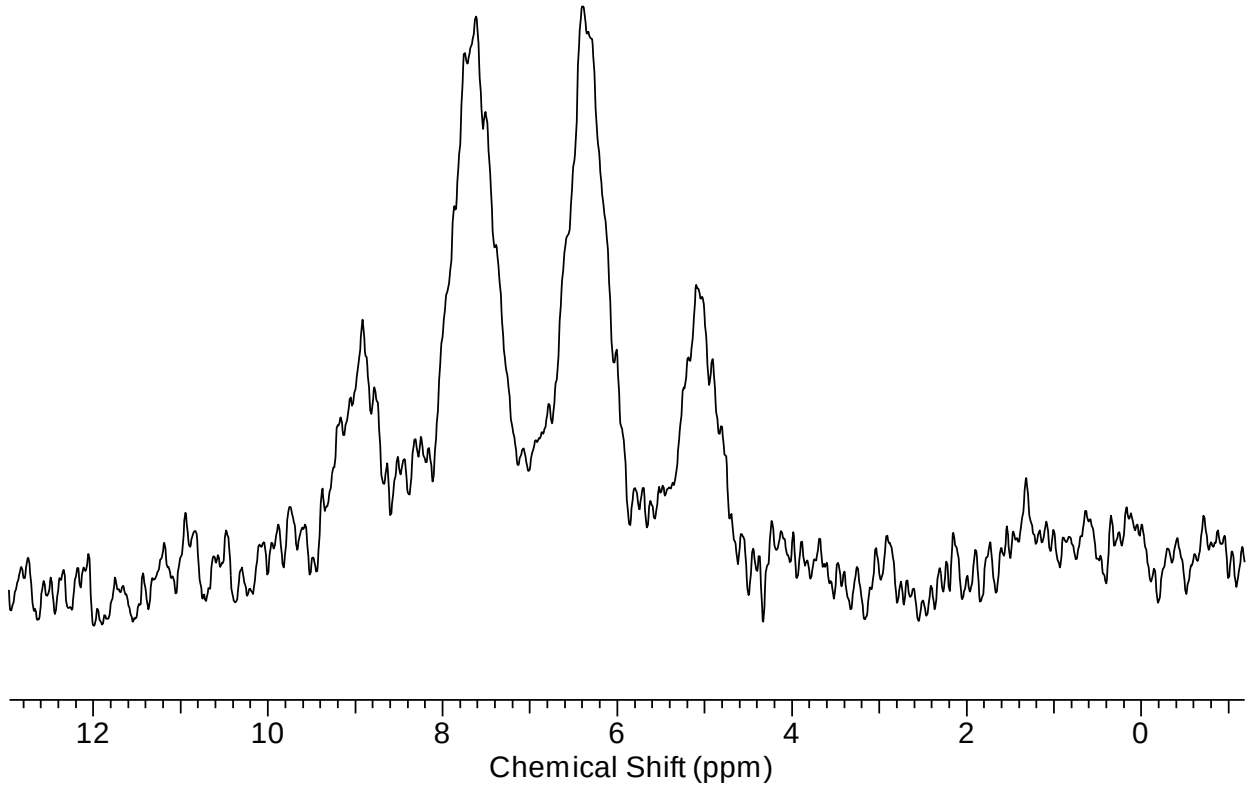


Figure S5. $^{31}P\{^{1}H\}$ NMR spectra of complex **2a** in $CDCl_3$ at 273 K,

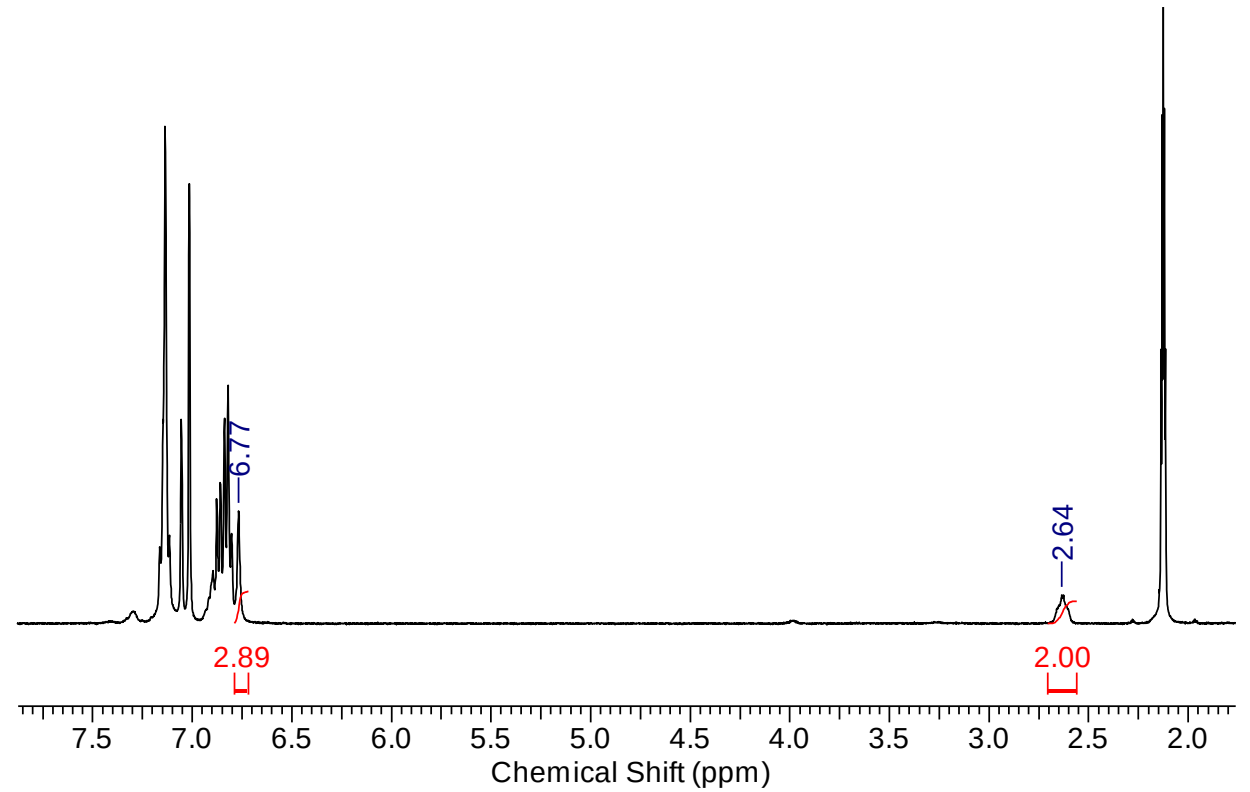


Figure S6. ^{1}H NMR spectrum of complex **2a** in toluene-d_8, RT.

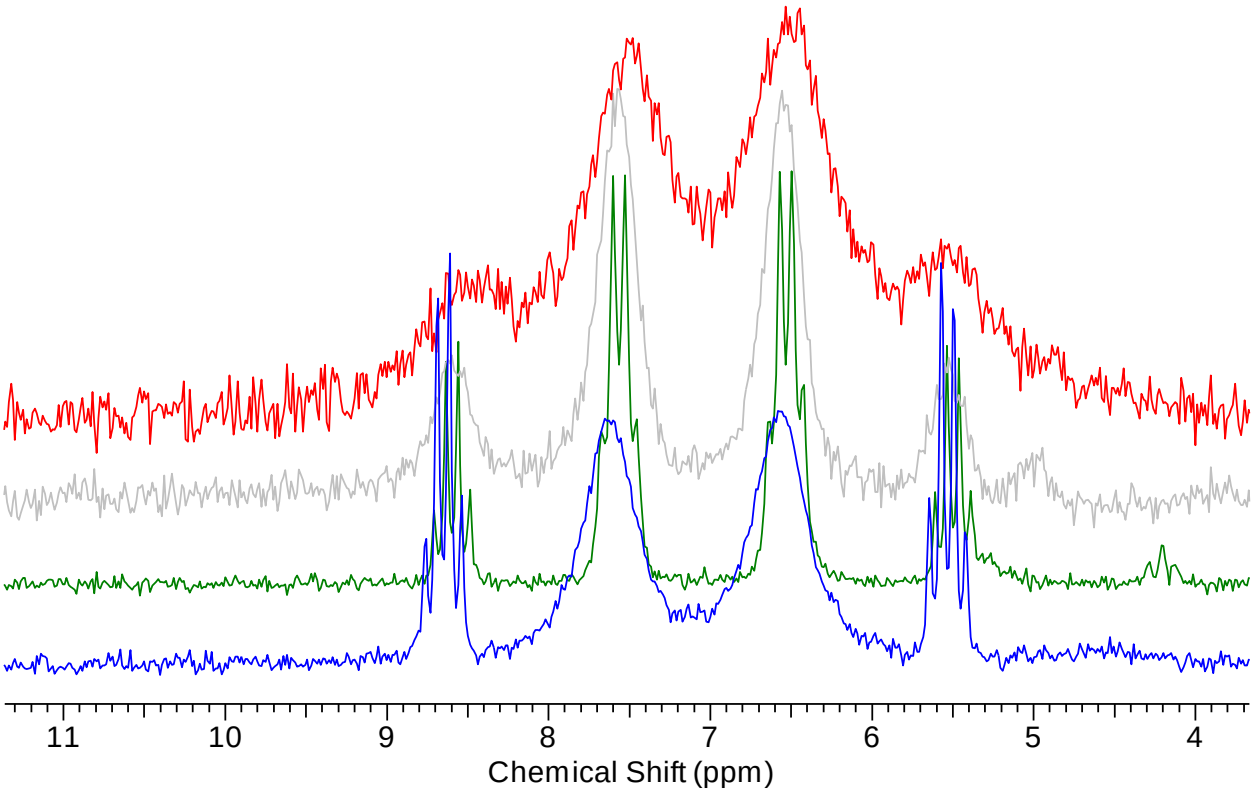


Figure S7. $^{31}P\{^{1}H\}$ NMR spectra of complex **2a** at 273 K(blue), 298 K (green), 333 K (grey), 353 K (red) in toluene-d_8.

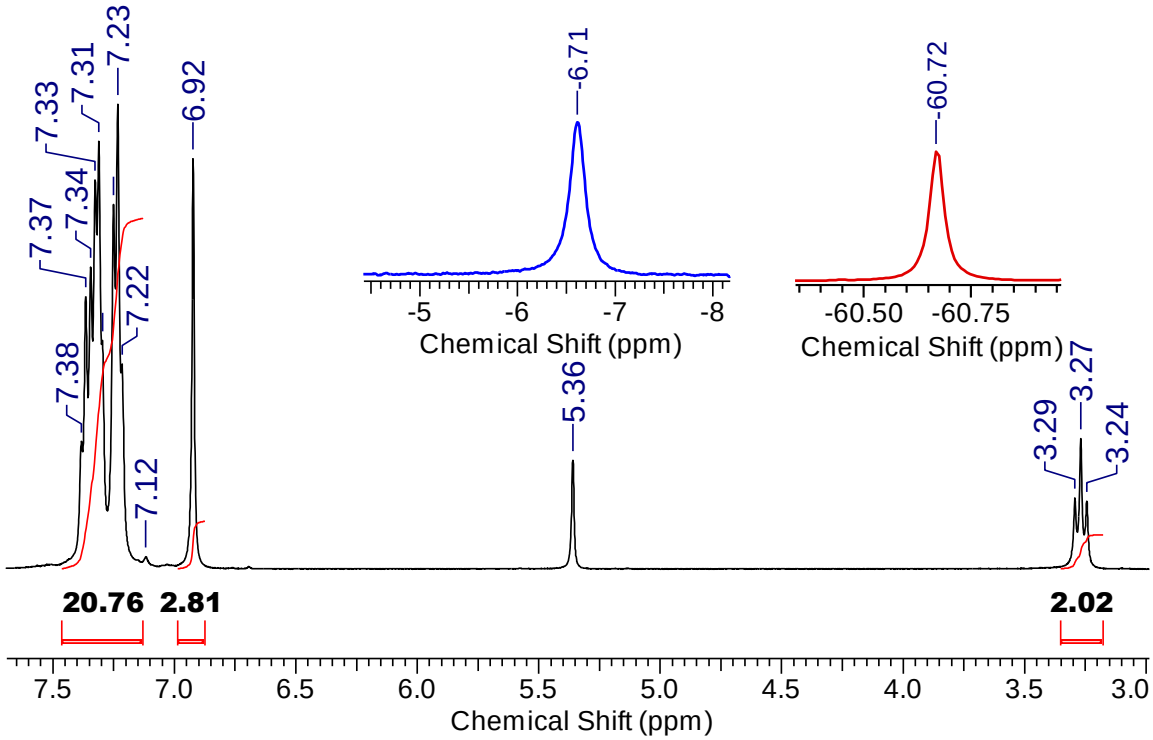


Figure S8. ^{1}H (black),^{19}F (red) and $^{31}P\{^{1}H\}$ (blue) NMR spectra of complex **2b** in CD_2Cl_2, RT.

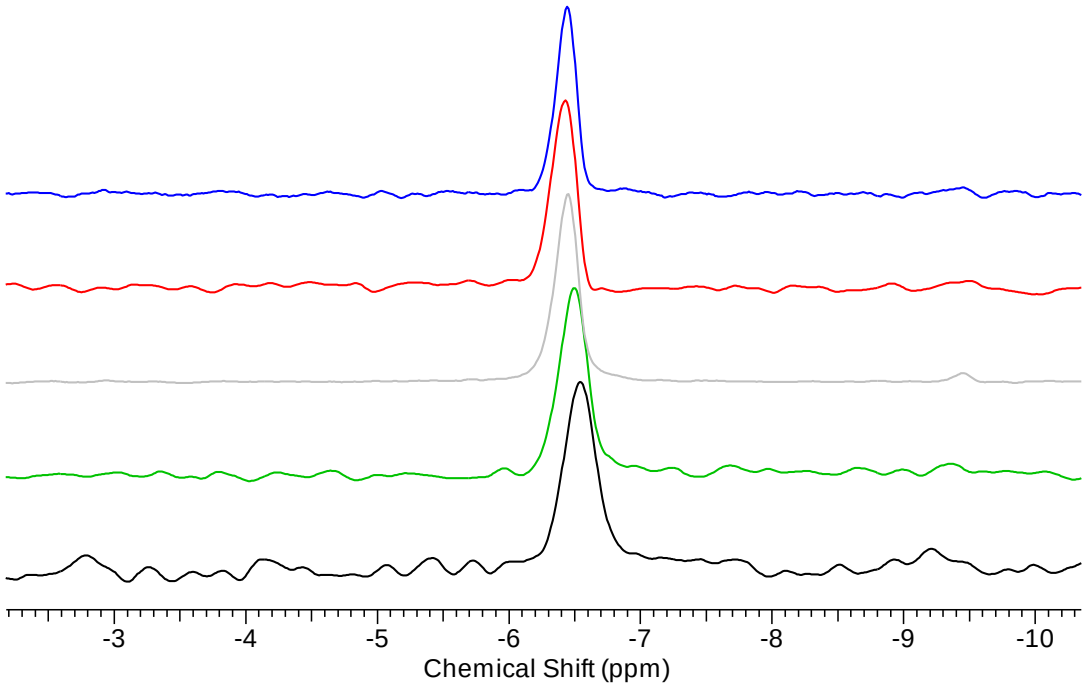
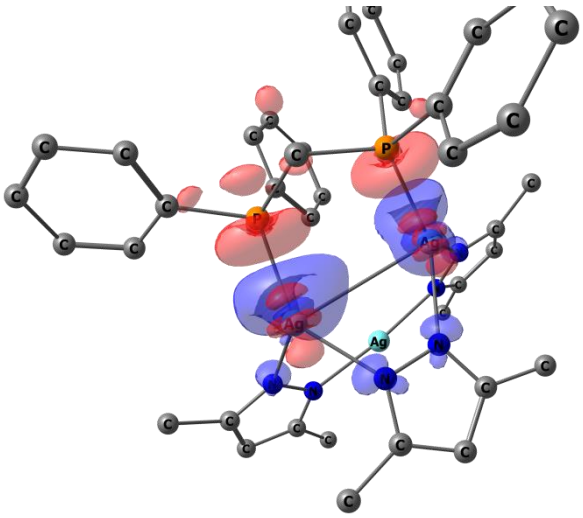
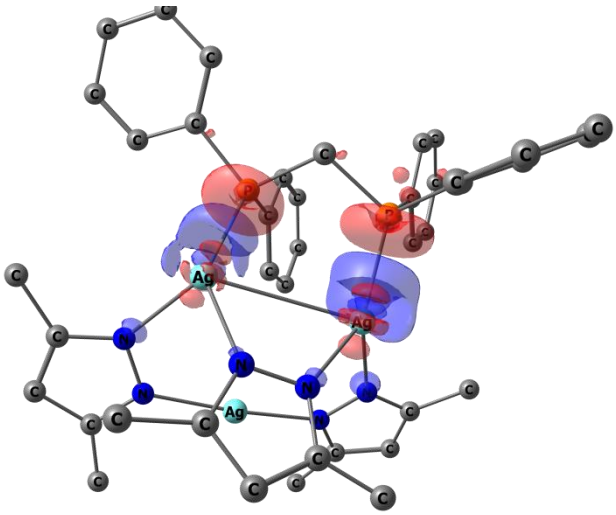


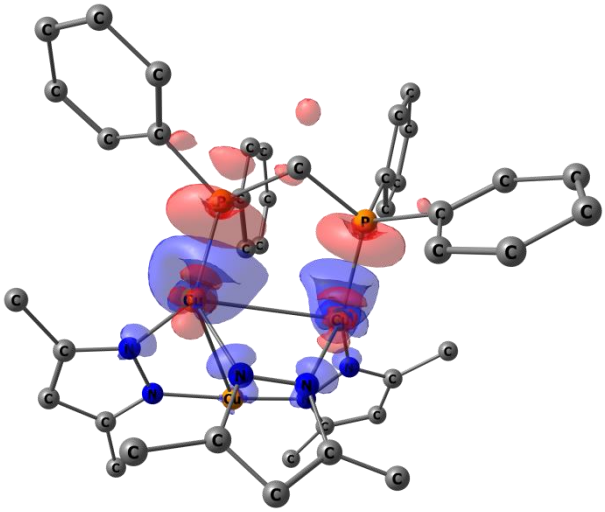
Figure S9. $^{31}P\{^{1}H\}$ NMR spectra of complex **2b** at 292 K (black), 273 K(green), 253 K (grey), 233 K (red), 213 K (blue) in CD_2Cl_2.



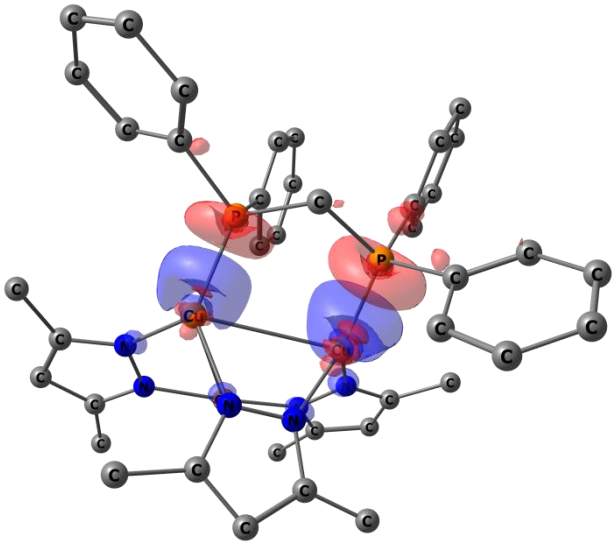
2a/NOCV1



2a/NOCV2

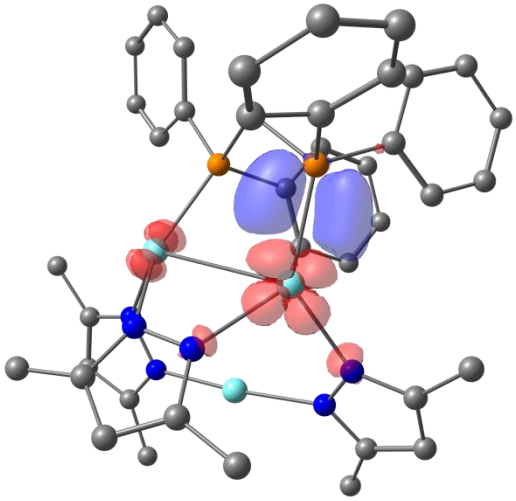


2b/NOCV1

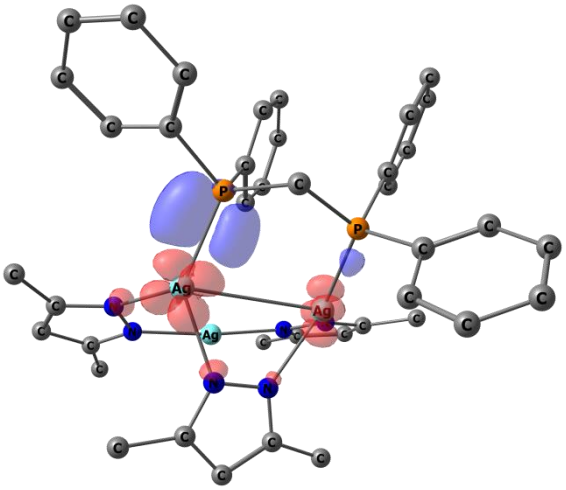


2b/NOCV2

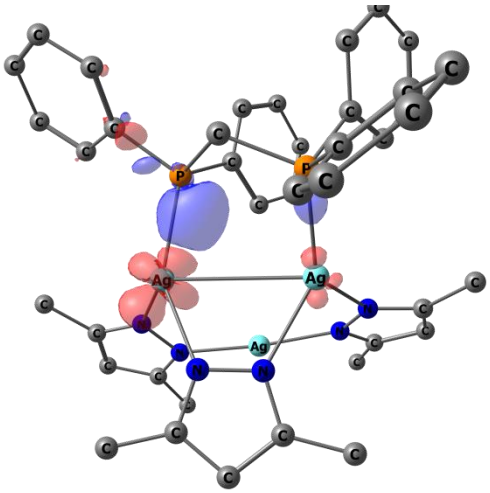
Figure S10. First and second channels of electron density transfer upon formation of complexes **2a** and **2b** as isosurfaces at 0.002 a.u. (red – depletion, blue – concentration of electron density). H and F atoms are omitted.



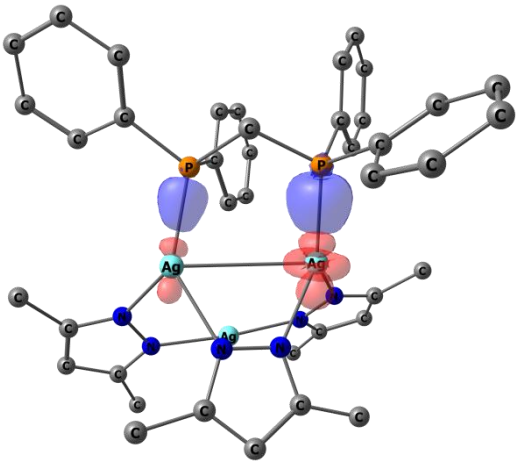
NOCV3



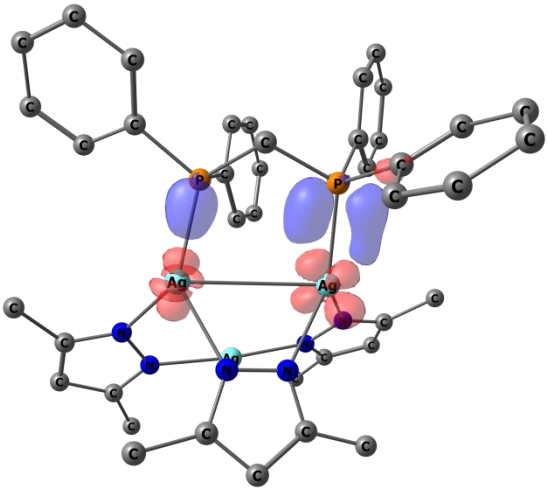
NOCV4



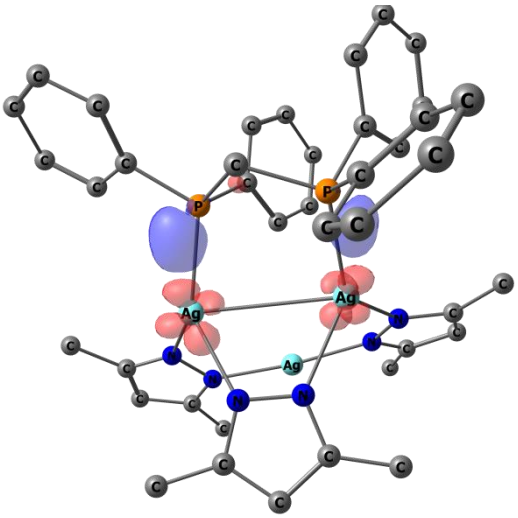
NOCV5



NOCV6



NOCV7



NOCV8

Figure S11. Channels of electron density transfer #3-#8 upon formation of complex **2a** as isosurfaces at 0.001 a.u. (red – depletion, blue – concentration of electron density). H and F atoms are omitted.

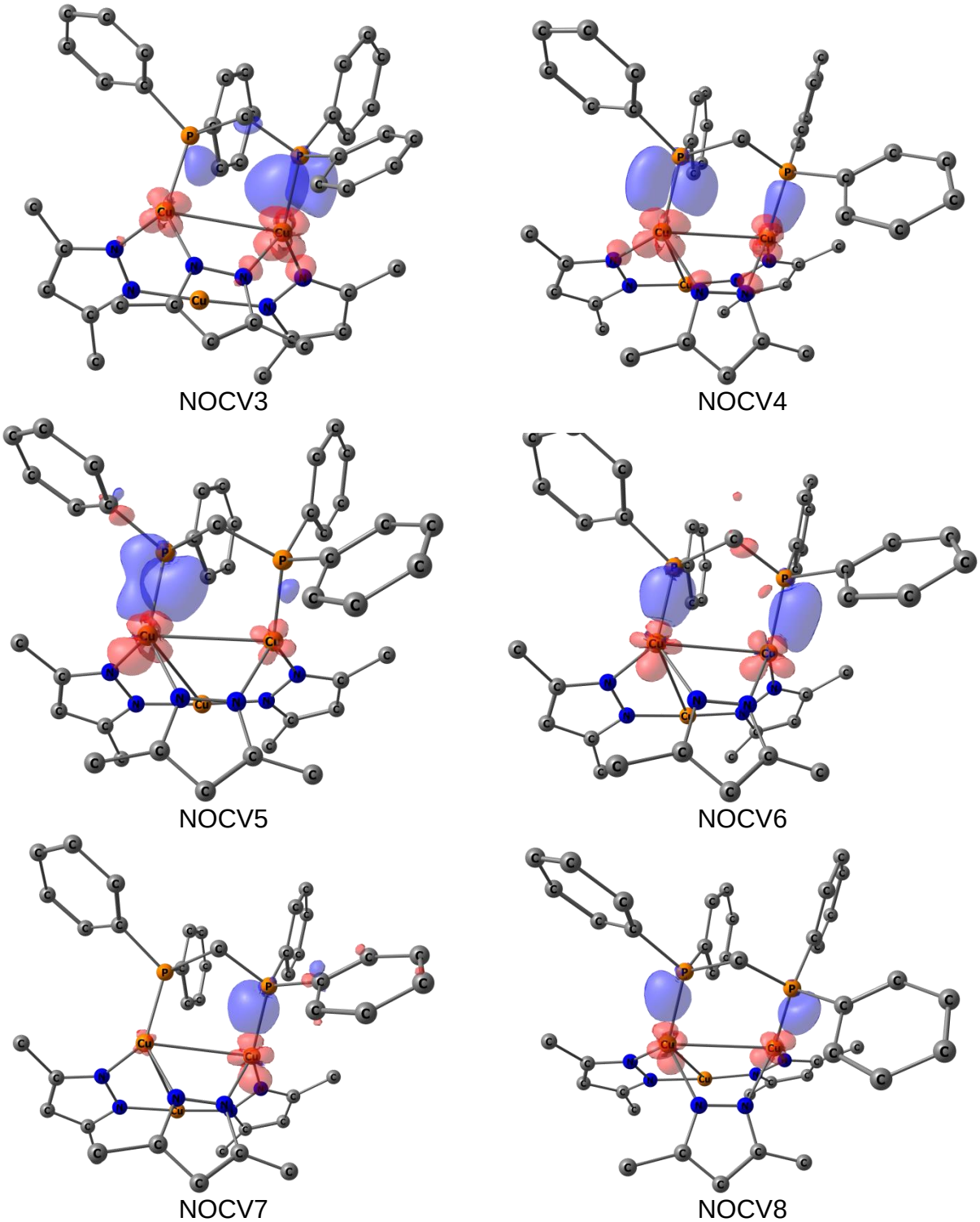


Figure S12. Channels of electron density transfer #3-#8 upon formation of complex **2b** as isosurfaces at 0.001 a.u. (red – depletion, blue – concentration of electron density). H and F atoms are omitted.

Table S2. Rates of the "merry-go-round" intramolecular dppm exchange process

$P(1)Ag(1)Ag(2)P(2) \leftrightharpoons P(1)Ag(1)Ag(3)P(2) \leftrightharpoons P(1)Ag(2)Ag(3)P(2) \leftrightharpoons P(1)Ag(2)Ag(1)P(2) \leftrightharpoons$
$\leftrightharpoons P(1)Ag(3)Ag(1)P(2) \leftrightharpoons P(1)Ag(3)Ag(2)P(2) \leftrightharpoons P(1)Ag(1)Ag(2)P(2) \leftrightharpoons \cdots$
extracted from variable temperature ^{31}P NMR spectra of **2a** by using Spinach program (see Figure 5 and Ref. 20 of the main text).

T / K	***k* / sec^{-1}**
198	$< 0.025\ 10^3$
218	$(0.20 \pm 0.05)\ 10^3$
238	$(3.0 \pm 0.5)\ 10^3$
258	$(25 \pm 5)\ 10^3$
278	$(130 \pm 10)\ 10^3$
298	$(450 \pm 50)\ 10^3$

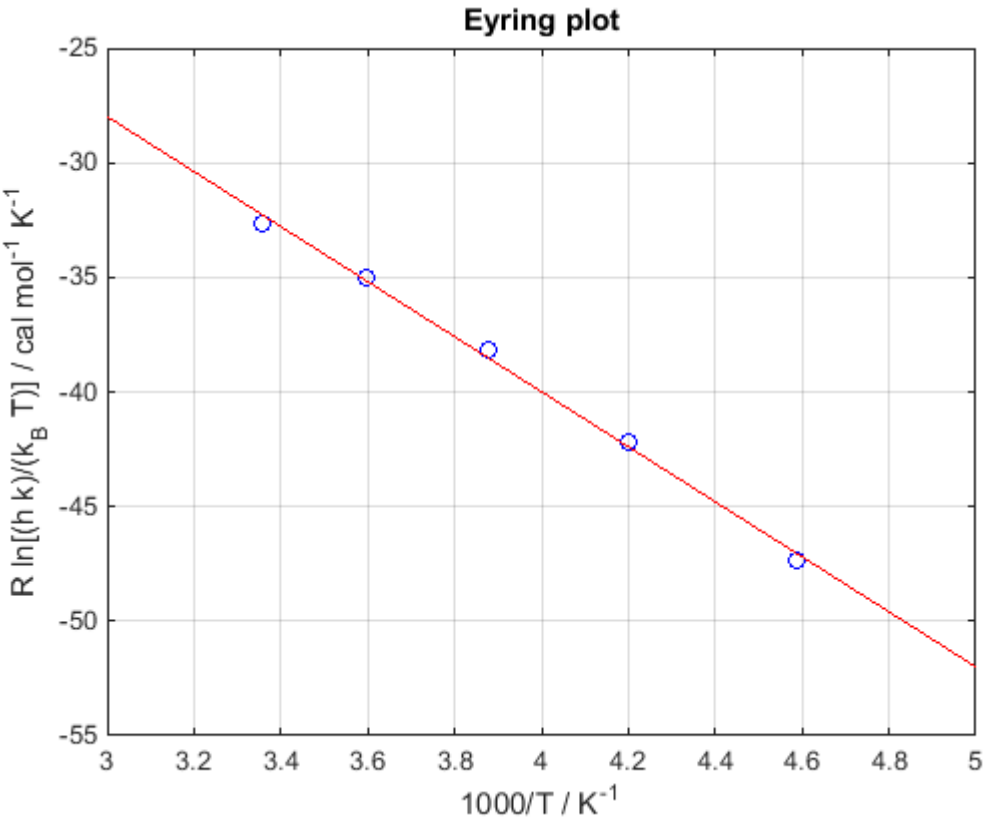


Figure S13. Eyring plot of "merry-go-round" rate temperature dependence (the data of **Table S2** excluding T = 198 K). The best fit corresponds to $\Delta H^{\#}$=12 ± 1 kcal/mol.

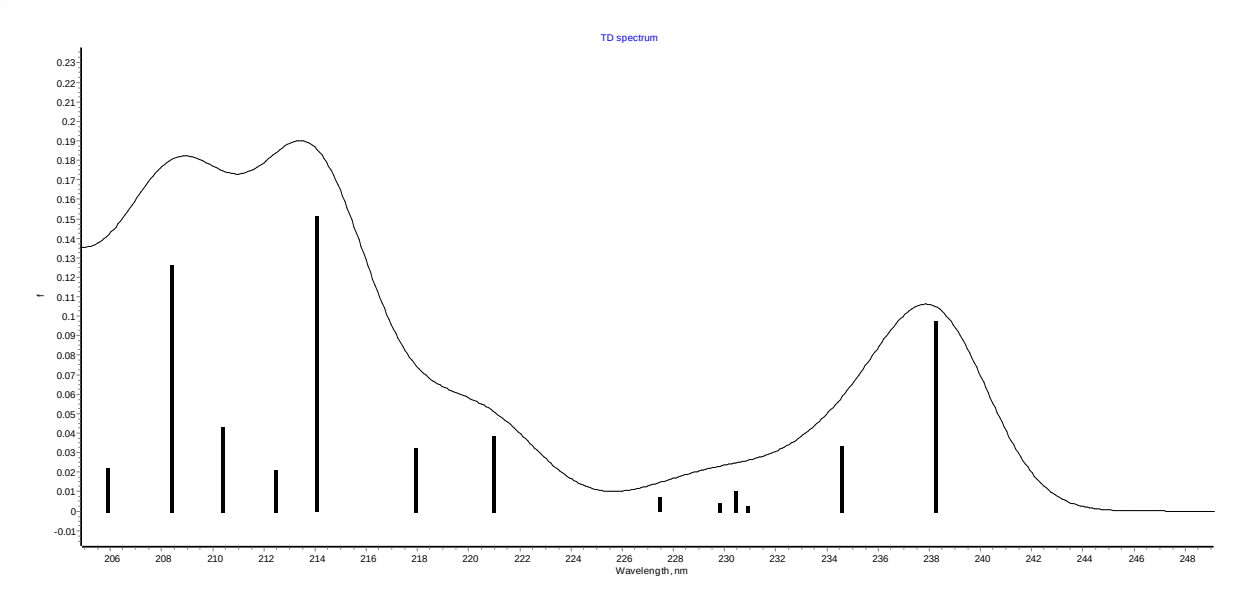


Figure S14. Calculated absorption spectrum of **2a'**.

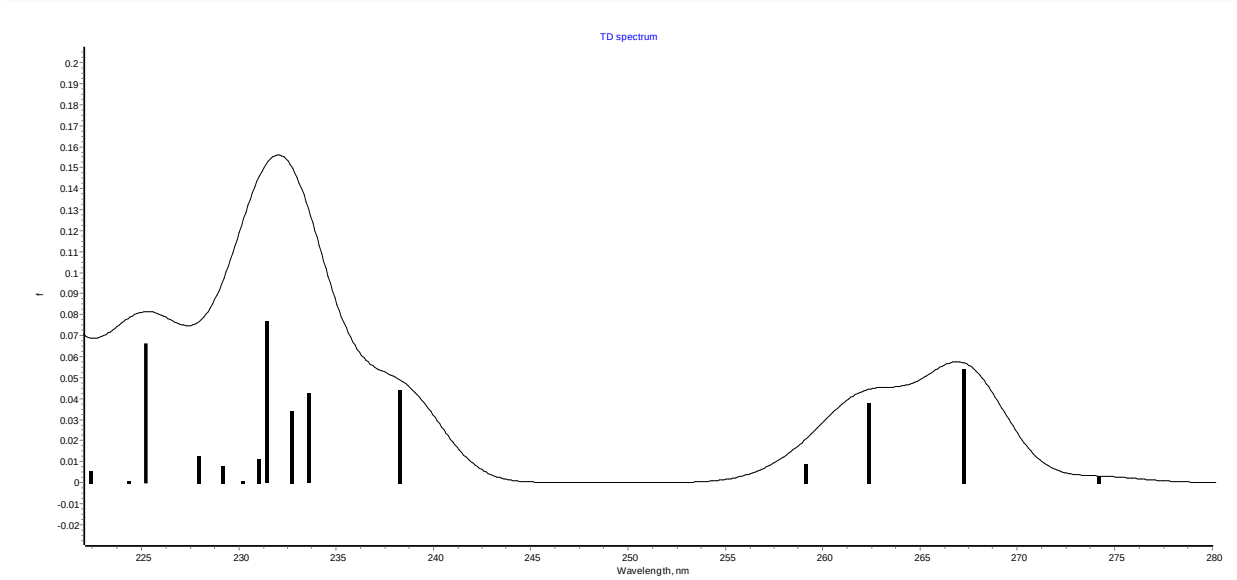


Figure S15. Calculated absorption spectrum of **2b**.

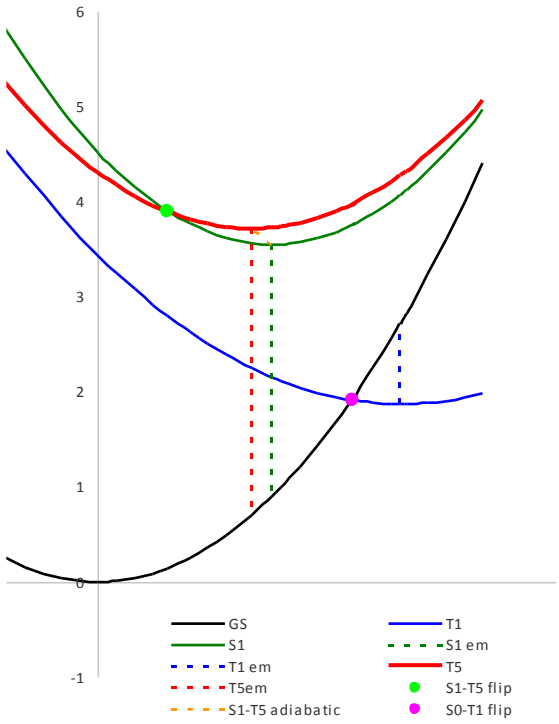


Figure S16. Schematic Jablonsky diagram for **2b**. Ground state (GS) and exited states S_1, T_1 and T_5 potentials represented by idealized parabolas, vertical emissions – by dashed lines.

Table S3. The TD-DFT data of key electronic transitions of complexes **2a'** and **2b**.

		2b		**2a'**	
		eV	nm	eV	nm
S0→S1	Eva	4.52	274	5.20	238
S1→S0	Eve	2.65	468	3.20	388
	Eadia	3.55	349	4.39	282
T1→S0	Eve	-0.84	-1471	2.50	496
	Eadia	1.87	663	3.11	399
T5→S0	Eve	3.02	410	3.11	399
	Eadia	3.72	333	3.84	322

Eva – vertical excitation (absorbance) energy
Eve – vertical emission energy
Eadia – adiabatic energy difference between 2 minima

Table S4. The impacts of atomic fragments to the singlet vertical excitations of 2a' and 2b.

	2b		2a'	
	$S_0 \rightarrow S_2$, E=4.640 eV		$S_0 \rightarrow S_1$, E=5.205 eV	
	hole	electron	hole	electron
dppm	28.46	69.65	41.88	91.08
M3	48.87	26.70	30.89	8.27
Pz3	22.66	3.65	27.24	0.64
	$S_0 \rightarrow S_3$, E=4.726 eV		$S_0 \rightarrow S_2$, E=5.286 eV	
	hole	electron	hole	electron
dppm	23.48	75.85	59.48	97.29
M3	52.87	20.64	24.09	2.50
Pz3	23.65	3.50	16.42	0.21

Table S5. The impacts of atomic fragments of complexes **2a'** and **2b** to the S_0-T_X vertical excitations. Hole corresponds to the distribution in the ground state, electron – to the T_X excited states.

		2b				**2a'**		
	Evex, eV		Hole	Electron	Evex, eV		Hole	Electron
T_1	3.4395	dppm	72	93	3.4622	dppm	85	98
		M3	23	5		M3	4	2
		Pz3	6	2		Pz3	11	0
T_2	3.4617	dppm	80	98	3.4705	dppm	87	96
		M3	14	1		M3	3	4
		Pz3	5	1		Pz3	10	0
T_3	3.4728	dppm	74	97	3.4884	dppm	89	97
		M3	14	2		M3	3	3
		Pz3	12	1		Pz3	7	0
T_4	3.4819	dppm	83	97	3.4919	dppm	91	95
		M3	10	3		M3	3	4
		Pz3	7	1		Pz3	6	0
T_5	4.3097	dppm	22	47	4.5202	dppm	6	5
		M3	50	18		M3	9	9
		Pz3	28	35		Pz3	85	86
T_6	4.3470	dppm	11	13	4.5321	dppm	2	8
		M3	22	9		M3	10	10
		Pz3	68	78		Pz3	87	82
T_7	4.3832	dppm	20	47	4.5531	dppm	6	11
		M3	49	29		M3	10	6
		Pz3	31	24		Pz3	84	83

Table S6. Analysis of fragments impacts to the $T_5 \rightarrow S_0$ vertical emissions.

	2b		**2a'**	
	Hole	Electron	Hole	Electron
dppm	5.27	13.05	1.20	3.20
M3	21.26	7.03	12.25	8.78
Pz3	73.47	79.92	86.55	88.02

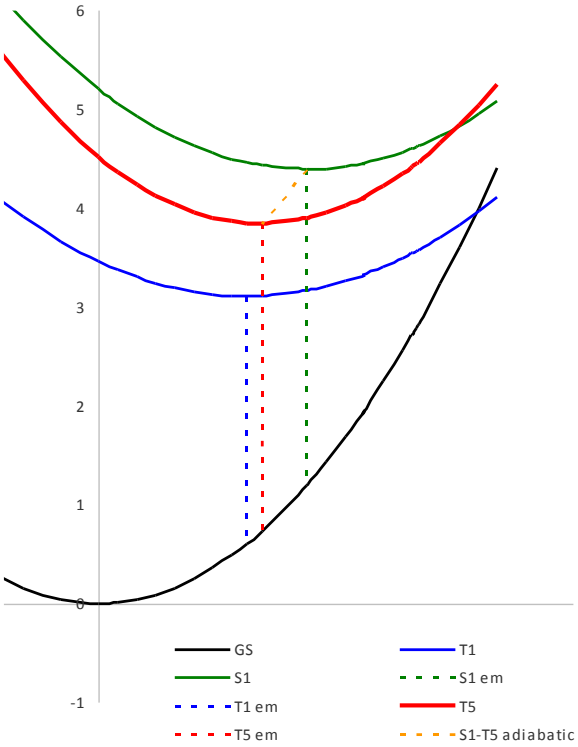


Figure S17. Schematic Jablonsky diagram for **2a'**. Ground state (GS) and exited states S_1, T_1 and T_5 potentials represented by idealized parabolas, vertical emissions – by dashed lines.

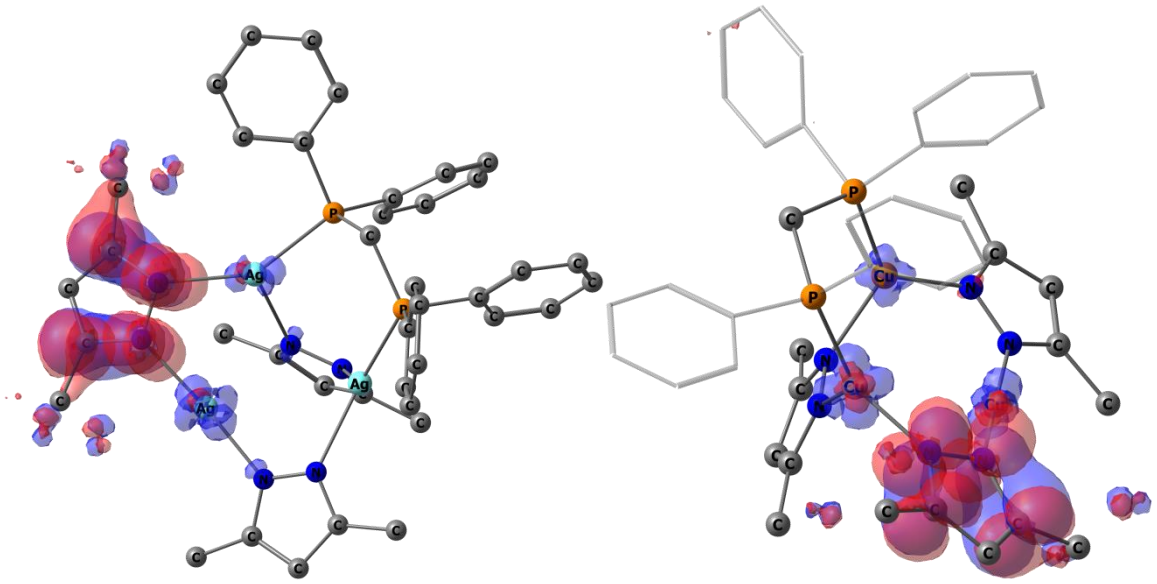


Figure S18. Electron density transfer maps in the $T_5 \rightarrow S_0$, emissions of **2a'** (left) and **2b** (right) as isosurface at 0.002 a.u. Upon the electronic transition the electron density increases in the blue areas and decreases in the red areas. Hydrogen and fluorine atoms are omitted for clarity.

Table S7. XYZ coordinates of all DFT and TD-DFT optimized species.

2a, PBEPBE/def2-TZVP, in DCM, EDCM=-4786.24215783

47	10.303684000	11.457387000	14.998590000
47	9.915223000	8.797855000	13.120727000
47	9.251865000	12.133334000	11.854756000
15	12.498166000	10.623106000	15.257283000
15	11.838767000	7.822770000	14.097541000
9	4.905179000	7.704240000	14.068666000
9	10.778316000	14.079551000	16.928818000
9	5.802196000	12.069675000	17.284874000
9	7.983088000	12.303394000	17.321281000
9	6.797212000	13.324601000	15.799012000
9	6.921934000	6.887194000	13.807431000
9	6.078631000	8.217871000	12.295490000
9	8.521910000	6.388514000	11.203357000
9	9.399570000	16.970543000	11.243715000
9	8.435524000	6.299069000	9.016241000
9	7.410815000	11.408936000	7.433707000
9	10.238261000	15.125602000	10.413447000
9	8.951349000	12.572882000	8.465860000
9	8.107017000	15.244715000	10.865275000
9	11.142900000	16.199271000	16.504875000
9	6.957080000	12.395434000	9.334577000
9	10.349412000	6.599265000	10.032223000
9	9.124797000	15.506500000	16.963816000
7	8.208492000	10.636766000	15.019691000
7	9.144536000	9.229497000	11.003621000
7	9.627368000	13.822909000	13.022237000
7	8.010542000	9.540890000	14.258238000
7	8.856963000	10.490253000	10.625706000
7	9.887579000	13.693579000	14.337323000
6	13.271303000	7.452222000	13.018518000
6	13.402556000	11.289336000	16.707359000
6	12.567896000	8.791299000	15.500846000
6	8.339580000	10.457150000	9.370189000
6	6.709069000	9.184810000	14.377551000
6	13.625248000	10.547623000	17.877727000
6	13.605192000	10.986824000	13.842551000
6	11.398279000	6.221103000	14.886509000
6	7.031860000	10.960562000	15.610115000
6	14.452303000	6.885501000	13.529700000
6	8.806548000	8.411258000	9.980510000
6	6.033556000	10.061026000	15.230925000
6	6.161030000	8.009541000	13.645436000
6	13.185085000	7.740598000	11.649804000
6	13.060156000	11.561529000	12.685490000
6	9.608030000	15.145047000	12.708837000
6	10.036456000	14.937362000	14.843113000
6	6.907715000	12.151098000	16.495840000
6	8.286022000	9.143275000	8.910182000
6	15.242850000	11.574969000	11.644825000
6	14.262340000	7.469179000	10.801269000
6	14.257278000	11.140080000	18.975582000
6	15.794142000	11.003122000	12.797278000
6	13.816674000	12.632493000	16.658205000
6	9.022282000	6.937505000	10.061388000
6	13.876031000	11.854162000	11.589221000
6	10.508531000	6.227081000	15.975705000
6	14.982125000	10.711451000	13.893410000
6	15.432411000	6.907461000	11.315604000
6	9.865391000	15.905591000	13.846619000
6	11.828920000	4.991855000	14.364727000
6	10.272134000	15.169323000	16.297024000
6	15.525706000	6.615504000	12.680860000
6	10.521618000	3.805748000	16.026490000
6	14.671917000	12.472059000	18.917365000
6	9.340044000	15.616848000	11.320447000
6	7.917219000	11.698676000	8.658935000
6	14.450081000	13.216812000	17.754215000
6	10.080336000	5.027607000	16.544770000
6	11.391000000	3.792511000	14.934193000
1	7.923383000	8.779764000	7.955121000
1	9.916772000	16.985502000	13.935986000
1	4.992437000	10.041260000	15.534868000
1	12.505241000	4.963313000	13.509467000
1	11.735627000	2.843649000	14.518139000
1	10.180935000	2.867679000	16.468800000
1	9.392002000	5.048774000	17.392053000
1	10.133353000	7.171183000	16.377882000
1	13.310864000	9.505163000	17.945953000
1	14.426921000	10.552085000	19.879862000
1	15.164809000	12.931177000	19.776417000
1	14.767457000	14.260112000	17.700657000
1	13.640994000	13.225146000	15.757491000
1	15.422549000	10.273603000	14.791968000
1	16.862989000	10.785128000	12.842341000
1	15.882871000	11.805519000	10.790822000
1	13.441317000	12.304743000	10.694766000
1	11.988265000	11.782265000	12.645430000
1	12.271121000	8.185071000	11.249831000
1	14.184724000	7.700852000	9.737333000
1	16.274633000	6.695683000	10.653868000
1	16.438518000	6.174748000	13.086563000
1	14.534445000	6.646648000	14.592403000
1	13.591674000	8.446269000	15.707855000
1	11.943277000	8.581216000	16.382606000

2a', PBEPBE/def2-TZVP, in DCM, EDCM=-4786.24258283

47	10.270367000	11.278744000	15.039732000
47	9.724603000	8.731837000	13.146779000
47	9.289024000	12.003336000	11.856890000
15	11.692453000	7.829402000	14.109858000
15	12.512804000	10.578050000	15.333977000
9	4.617912000	8.006560000	13.907584000
9	11.422362000	14.055377000	16.753102000
9	5.787634000	12.158092000	17.308764000
9	7.976481000	12.175989000	17.439723000
9	6.961480000	13.371841000	15.920850000
9	6.563310000	7.016309000	13.710590000
9	5.908390000	8.443778000	12.195530000
9	8.413770000	6.298158000	11.148065000
9	9.751762000	16.793256000	11.148471000
9	8.401937000	6.217128000	8.958541000
9	7.502025000	11.368736000	7.384326000
9	10.484088000	14.887079000	10.358754000
9	9.061704000	12.478006000	8.446946000
9	8.362186000	15.136263000	10.805041000
9	11.307653000	16.213862000	16.384557000
9	7.048891000	12.363416000	9.281636000
9	10.283284000	6.494642000	10.039929000

9	9.527876000	15.107600000	17.003615000	1	8.971948000	6.598453000	18.061126000
7	8.127694000	10.622287000	15.035736000	1	9.375193000	7.651541000	15.838017000
7	9.079000000	9.124944000	10.986556000	1	11.027146000	10.844685000	17.793253000
7	9.754222000	13.681819000	13.006458000	1	11.559150000	10.377156000	20.178535000
7	7.855909000	9.576188000	14.229124000	1	13.788315000	9.446977000	20.798227000
7	8.833696000	10.393790000	10.608053000	1	15.480379000	8.991671000	19.026522000
7	10.037015000	13.562838000	14.317218000	1	14.962181000	9.465546000	16.655331000
6	12.953482000	10.188152000	17.065725000	1	13.933789000	8.650055000	14.759210000
6	12.517579000	6.512479000	13.131813000	1	13.249815000	9.471789000	13.333196000
6	13.018621000	9.095487000	14.341493000				
6	8.364622000	10.381515000	9.333534000				
6	6.530987000	9.313010000	14.323324000	2a_flat, PBEPBE/def2-TZVP, in DCM, EDCM=-4786.22496697			
6	13.727214000	6.703235000	12.446669000				
6	11.445672000	7.046201000	15.749302000	47	14.582612000	11.632989000	11.394513000
6	13.729703000	11.843826000	14.787501000	47	11.618012000	10.188597000	10.477128000
6	6.972220000	11.009237000	15.629927000	47	11.824324000	12.682863000	12.755519000
6	14.208232000	9.663203000	17.420614000	15	11.165757000	11.472676000	8.517058000
6	8.764990000	8.321537000	9.945128000	15	10.262201000	8.889426000	7.119380000
6	5.914138000	10.201225000	15.208152000	9	13.425451000	5.620056000	9.345869000
6	5.911526000	8.206478000	13.542446000	9	16.817224000	14.019411000	10.120139000
6	12.005934000	10.442474000	18.068164000	9	18.066984000	8.306412000	10.815698000
6	10.182790000	7.124848000	16.352692000	9	17.459073000	10.289451000	10.112478000
6	9.856605000	14.990280000	12.652362000	9	17.381721000	9.818300000	12.242574000
6	10.325337000	14.799831000	14.779020000	9	11.760075000	6.930962000	9.902630000
6	6.927032000	12.166142000	16.566032000	9	12.786418000	5.747963000	11.427908000
6	8.302244000	9.072236000	8.860982000	9	10.165196000	6.969494000	12.656475000
6	10.996271000	5.860590000	18.248298000	9	12.685786000	17.514930000	13.450304000
6	12.305148000	10.177657000	19.407055000	9	8.041980000	7.392705000	12.956011000
6	14.263645000	5.675579000	11.664181000	9	8.610515000	11.710551000	16.275010000
6	12.258647000	5.776409000	17.649510000	9	11.264275000	16.324095000	12.286618000
6	11.853485000	5.277974000	13.013955000	9	9.165856000	13.264146000	14.834540000
6	8.960254000	6.845829000	10.024891000	9	11.774105000	15.724299000	14.321274000
6	9.959221000	6.533797000	17.599655000	9	17.433230000	15.670365000	11.420832000
6	13.767511000	12.195500000	13.426127000	9	10.710680000	12.272222000	16.013548000
6	12.484409000	6.363399000	16.404418000	9	9.023221000	7.959266000	11.079653000
6	13.553248000	9.655642000	19.752641000	9	17.436149000	13.613055000	12.171731000
6	10.219636000	15.752913000	13.759933000	7	14.689281000	9.605717000	10.928480000
6	14.535752000	12.547279000	15.694658000	7	10.416398000	10.055576000	12.458054000
6	10.645223000	15.037173000	16.215621000	7	13.295469000	14.119967000	12.379859000
6	14.503527000	9.398951000	18.758313000	7	13.567562000	8.879502000	10.732583000
6	15.426158000	13.898043000	13.889077000	7	10.502468000	11.150602000	13.241349000
6	13.602916000	4.450687000	11.558396000	7	14.469510000	13.660986000	11.896135000
6	9.613839000	15.447056000	11.254813000	6	8.725539000	9.337052000	6.205006000
6	7.996461000	11.637783000	8.619382000	6	12.281371000	12.897494000	8.195769000
6	12.395419000	4.254608000	12.237332000	6	11.300973000	10.442483000	6.990449000
6	14.615941000	13.209281000	12.980590000	6	9.663140000	11.000864000	14.297036000
6	15.379278000	13.567462000	15.244569000	6	13.954540000	7.602337000	10.510413000
1	7.969572000	8.723437000	7.889594000	6	13.516673000	12.714832000	7.550543000
1	10.382787000	16.823788000	13.814825000	6	9.486961000	12.203996000	8.450125000
1	4.871510000	10.247372000	15.503724000	6	11.143668000	7.782719000	5.931710000
1	14.507170000	12.306872000	16.758046000	6	15.766026000	8.783749000	10.834506000
1	16.001309000	14.105252000	15.962979000	6	8.716253000	9.935340000	4.933137000
1	16.085188000	14.695425000	13.540500000	6	9.512738000	9.226107000	13.027886000
1	14.636183000	13.468029000	11.920085000	6	15.347989000	7.484046000	10.566643000
1	13.123168000	11.685977000	12.704862000	6	12.979753000	6.493469000	10.295841000
1	14.265956000	7.648943000	12.514308000	6	7.501320000	9.052081000	6.829345000
1	15.206317000	5.838146000	11.137549000	6	8.616868000	12.021494000	9.533600000
1	14.024847000	3.650534000	10.947265000	6	13.438938000	15.438463000	12.648383000
1	11.869294000	3.301244000	12.157897000	6	15.343648000	14.692698000	11.863351000
1	10.906049000	5.115316000	13.533660000	6	17.156658000	9.294983000	11.000472000
1	13.469848000	6.282738000	15.940067000	6	9.002059000	9.778255000	14.206980000
1	13.069961000	5.248003000	18.154136000	6	6.892687000	13.265223000	8.379141000
1	10.822666000	5.395650000	19.220919000	6	6.290956000	9.357234000	6.198344000

6	14.385076000	13.793292000	7.367812000	9	5.524010000	10.349888000	8.535583000
6	7.756907000	13.452803000	7.294256000	9	7.797278000	14.461101000	10.218163000
6	11.945491000	14.176331000	8.671625000	9	7.213949000	11.715679000	8.788390000
6	9.189436000	7.898919000	12.429791000	9	6.194164000	14.463202000	11.699199000
6	7.323245000	12.550780000	9.498523000	9	12.163099000	14.950362000	14.796810000
6	12.523229000	7.555000000	6.093204000	9	5.610474000	11.686468000	10.269274000
6	9.048520000	12.927735000	7.327894000	9	9.696199000	6.338525000	10.812217000
6	6.293631000	9.952993000	4.935715000	9	10.812358000	16.579383000	15.352092000
6	14.732894000	15.855776000	12.334393000	7	8.686657000	10.822690000	15.522656000
6	10.451780000	7.027714000	4.968830000	7	8.377675000	8.942266000	11.756248000
6	16.748365000	14.500395000	11.395011000	7	8.749975000	13.432279000	12.856939000
6	7.508894000	10.240362000	4.303281000	7	8.352397000	9.630118000	14.979772000
6	12.498184000	5.892324000	4.331189000	7	7.838646000	10.098986000	11.306289000
6	14.038060000	15.064778000	7.832190000	7	9.657760000	13.496580000	13.858762000
6	12.299474000	16.245147000	13.176053000	6	12.748198000	8.241462000	12.341331000
6	9.537843000	12.052765000	15.346365000	6	13.006147000	11.551835000	16.633480000
6	12.818336000	15.250849000	8.488198000	6	12.519682000	9.175046000	15.091625000
6	13.194742000	6.627037000	5.295642000	6	7.077470000	9.817157000	10.215175000
6	11.124530000	6.093091000	4.176548000	6	7.255363000	9.168077000	15.632158000
1	8.266738000	9.359487000	14.885243000	6	12.437571000	11.003400000	17.797510000
1	15.162151000	16.846640000	12.432013000	6	13.654502000	11.534274000	13.794235000
1	15.955663000	6.595679000	10.431106000	6	11.592210000	6.541489000	14.398441000
1	9.378565000	7.169485000	4.831133000	6	7.796032000	11.095692000	16.509831000
1	10.567674000	5.521164000	3.430961000	6	14.070530000	7.783283000	12.469467000
1	13.022176000	5.163567000	3.709718000	6	7.947531000	7.948268000	10.942660000
1	14.266827000	6.472326000	5.435383000	6	6.859981000	10.067114000	16.623176000
1	13.085497000	8.095864000	6.858285000	6	6.624401000	7.866063000	15.281305000
1	13.812422000	11.730082000	7.184566000	6	12.295034000	8.683648000	11.090342000
1	15.337504000	13.636142000	6.857529000	6	13.284586000	12.353519000	12.717862000
1	14.718257000	15.906216000	7.687433000	6	8.419084000	14.702391000	12.501388000
1	12.539183000	16.239174000	8.859437000	6	9.887126000	14.806304000	14.118442000
1	10.994576000	14.339073000	9.182614000	6	7.870355000	12.348039000	17.311299000
1	9.715544000	13.082782000	6.477091000	6	7.114098000	8.452551000	9.941866000
1	7.422116000	14.010075000	6.417050000	6	15.572080000	12.386679000	11.930893000
1	5.881989000	13.677094000	8.348548000	6	13.147523000	8.668942000	9.982373000
1	6.653021000	12.401298000	10.347208000	6	12.840623000	11.442491000	19.059272000
1	8.957496000	11.456700000	10.404602000	6	15.949751000	11.569009000	13.001923000
1	7.498032000	8.590191000	7.819741000	6	13.965162000	12.568910000	16.764075000
1	5.346784000	9.131141000	6.698110000	6	8.380935000	6.535335000	11.140404000
1	5.350416000	10.193197000	4.440575000	6	14.239089000	12.776896000	11.788540000
1	7.514540000	10.704006000	3.314405000	6	11.133127000	6.285254000	15.702917000
1	9.657430000	10.160700000	4.425973000	6	14.997438000	11.141656000	13.927521000
1	11.088815000	11.032644000	6.086095000	6	14.458617000	8.208586000	10.117066000
1	12.348740000	10.110922000	6.945974000	6	9.119472000	15.618772000	13.281407000
				6	11.936048000	5.456190000	13.576364000
				6	10.871978000	15.237224000	15.152056000
2b, PBEPBE/def2-TZVP, in DCM, EDCM=-9266.16797775				6	14.918680000	7.764998000	11.362038000
				6	11.401928000	3.902366000	15.358525000
29	10.291490000	11.787565000	14.729580000	6	13.805413000	12.447243000	19.180409000
29	9.502795000	8.961344000	13.444324000	6	7.427207000	14.983152000	11.426042000
29	8.264873000	11.760394000	12.111549000	6	6.360665000	10.883777000	9.461623000
15	12.363470000	11.020552000	14.990261000	6	14.360993000	13.010668000	18.029695000
15	11.590860000	8.272187000	13.764435000	6	11.046480000	4.976489000	16.179913000
9	5.624107000	7.557398000	16.148657000	6	11.841618000	4.146896000	14.055768000
9	10.673158000	14.640430000	16.360181000	1	6.610092000	7.912457000	9.148232000
9	6.997547000	12.314226000	18.353563000	1	9.073012000	16.701538000	13.248941000
9	9.111451000	12.565015000	17.837646000	1	6.030832000	9.984109000	17.317272000
9	7.567632000	13.465596000	16.583739000	1	12.280778000	5.628092000	12.555762000
9	7.511280000	6.826509000	15.309852000	1	12.115272000	3.314950000	13.403584000
9	6.074624000	7.858880000	14.030116000	1	11.330686000	2.878911000	15.731644000
9	8.247869000	6.114894000	12.428503000	1	10.694178000	4.796606000	17.197648000
9	7.265571000	16.318693000	11.247700000	1	10.830904000	7.107291000	16.355342000
9	7.656982000	5.689198000	10.362372000	1	11.663546000	10.235833000	17.726858000

1	12.391872000	11.001130000	19.951523000
1	14.117715000	12.792261000	20.167932000
1	15.109814000	13.801176000	18.112065000
1	14.409741000	13.022370000	15.877240000
1	15.305202000	10.506774000	14.761358000
1	16.991420000	11.261640000	13.115159000
1	16.319811000	12.719086000	11.208029000
1	13.938956000	13.414264000	10.954481000
1	12.241368000	12.660506000	12.610716000
1	11.267419000	9.039642000	10.985997000
1	12.784098000	9.016883000	9.013468000
1	15.125571000	8.194695000	9.252660000
1	15.944046000	7.405604000	11.470219000
1	14.439326000	7.432053000	13.435759000
1	13.570210000	8.852107000	15.146188000
1	12.027662000	8.895048000	16.035390000

2b', PBEPBE/def2-TZVP, in DCM, EDCM=-9266.16606607

29	-1.248419000	0.915846000	0.759933000
29	1.426261000	-0.492560000	0.882617000
29	-0.927399000	-1.805985000	-0.938238000
15	2.463599000	1.330593000	0.124769000
15	-0.299071000	2.701711000	-0.160011000
9	1.326793000	-2.891327000	5.225015000
9	-3.865006000	2.526960000	0.733892000
9	-3.470778000	-0.301533000	5.000971000
9	-3.231531000	1.243289000	3.464320000
9	-3.977684000	-0.734607000	2.919731000
9	2.621114000	-1.617619000	3.999503000
9	1.689291000	-3.387273000	3.125316000
9	4.166386000	-1.846071000	1.201767000
9	-5.121725000	-2.711557000	-2.964928000
9	4.287973000	-4.028262000	1.237523000
9	1.065011000	-5.352669000	-3.360863000
9	-2.996822000	-2.571051000	-3.472213000
9	0.048401000	-3.455587000	-3.763698000
9	-3.624414000	-3.712422000	-1.720118000
9	-5.403846000	2.486281000	-0.824049000
9	-0.771879000	-4.837670000	-2.286689000
9	5.181052000	-2.920573000	-0.414607000
9	-5.717135000	1.406739000	1.044473000
7	-0.951948000	-0.171011000	2.419928000
7	1.753991000	-2.250578000	-0.128651000
7	-2.640918000	-0.997835000	-0.952888000
7	0.254330000	-0.780356000	2.491157000
7	0.769337000	-2.643122000	-0.971226000
7	-2.863552000	0.148449000	-0.270768000
6	-0.110909000	4.145167000	0.953417000
6	3.863204000	1.013612000	-1.031461000
6	1.380567000	2.435069000	-0.894371000
6	1.231672000	-3.684996000	-1.714924000
6	0.275328000	-1.536641000	3.617031000
6	3.596991000	0.582710000	-2.343659000
6	3.185932000	2.416287000	1.414614000
6	-1.245331000	3.348843000	-1.603422000
6	-1.675761000	-0.552216000	3.502985000
6	0.469026000	5.351825000	0.526230000
6	2.821983000	-3.051518000	-0.351642000
6	-0.934732000	-1.423299000	4.303190000
6	1.466825000	-2.349334000	3.987293000
6	-0.578830000	4.038581000	2.270973000
6	3.125886000	1.998520000	2.751787000
6	-3.790054000	-1.345238000	-1.594009000
6	-4.146985000	0.512438000	-0.495470000
6	-3.073487000	-0.087399000	3.718586000
6	2.540112000	-3.986154000	-1.353730000
6	4.264452000	4.015134000	3.451762000
6	-0.473924000	5.120549000	3.149584000
6	4.641366000	0.248538000	-3.207264000
6	4.327208000	4.439481000	2.119662000
6	5.197846000	1.078466000	-0.599935000
6	4.097491000	-2.949282000	0.417142000
6	3.665020000	2.794014000	3.766822000
6	-1.290691000	2.579988000	-2.780751000
6	3.794873000	3.643983000	1.104844000
6	0.099265000	6.317808000	2.716054000
6	-4.784474000	-0.409251000	-1.332554000
6	-2.025087000	4.513647000	-1.528419000
6	-4.765251000	1.725098000	0.114066000
6	0.572778000	6.431037000	1.404200000
6	-2.837698000	4.149500000	-3.784102000
6	5.967786000	0.326135000	-2.771835000
6	-3.882097000	-2.574617000	-2.430154000
6	0.398920000	-4.329289000	-2.769442000
6	6.240729000	0.737841000	-1.465611000
6	-2.073126000	2.981566000	-3.863927000
6	-2.813886000	4.909433000	-2.612782000
1	3.186472000	-4.760399000	-1.753167000
1	-5.809064000	-0.399918000	-1.688493000
1	-1.224829000	-1.888616000	5.239040000
1	-2.023622000	5.118078000	-0.620252000
1	-3.413846000	5.818603000	-2.536446000
1	-3.454323000	4.460677000	-4.629504000
1	-2.090947000	2.373713000	-4.770822000
1	-0.723579000	1.649245000	-2.856775000
1	2.568321000	0.498821000	-2.702076000
1	4.415389000	-0.076563000	-4.224900000
1	6.783934000	0.062477000	-3.447192000
1	7.272496000	0.796225000	-1.112924000
1	5.429842000	1.395435000	0.418022000
1	3.854930000	3.981003000	0.067904000
1	4.794437000	5.394575000	1.871020000
1	4.682472000	4.640113000	4.243512000
1	3.611991000	2.458727000	4.804394000
1	2.646555000	1.047611000	2.996509000
1	-1.021182000	3.098193000	2.609419000
1	-0.840737000	5.025248000	4.173371000
1	0.180327000	7.164549000	3.400595000
1	1.023657000	7.365251000	1.063391000
1	0.837288000	5.452985000	-0.496847000
1	1.872685000	3.388396000	-1.139950000
1	1.215734000	1.895143000	-1.838661000

2b_flat, PBEPBE/def2-TZVP, in DCM, EDCM=-9266.15009458

29	14.463485000	11.642204000	11.344395000
29	11.656014000	10.197477000	10.602031000
29	12.125627000	12.631623000	12.691937000
15	11.074984000	11.279310000	8.726609000
15	10.177393000	8.817422000	7.053588000
9	13.280113000	5.813703000	9.420681000
9	16.711763000	13.741661000	9.764067000
9	17.798571000	8.363263000	11.466737000

9	17.393577000	10.267443000	10.466325000	1	15.704958000	6.714563000	10.830713000
9	17.015142000	10.060144000	12.606490000	1	9.466405000	7.265345000	4.605348000
9	11.585393000	7.114322000	9.904978000	1	10.725330000	5.665548000	3.212054000
9	12.530437000	5.905600000	11.465582000	1	13.136916000	5.212044000	3.674635000
9	10.101232000	7.161043000	12.590873000	1	14.262058000	6.376813000	5.576917000
9	12.905673000	17.403882000	13.312502000	1	13.008906000	7.954513000	6.987718000
9	8.055769000	7.803791000	13.008391000	1	13.598074000	11.792316000	7.223107000
9	9.305417000	11.891671000	16.381784000	1	14.905204000	13.837448000	6.795235000
9	11.355691000	16.075096000	12.517192000	1	14.138975000	16.036266000	7.693968000
9	9.744105000	13.459498000	14.917730000	1	12.054432000	16.149000000	9.062556000
9	12.240318000	15.668373000	14.470160000	1	10.734865000	14.108474000	9.495099000
9	17.449518000	15.455507000	10.913005000	1	9.578471000	12.927207000	6.742022000
9	11.380156000	12.395359000	15.893589000	1	7.238658000	13.728226000	6.668009000
9	8.981137000	8.270057000	11.078329000	1	5.663594000	13.174461000	8.519782000
9	17.522143000	13.440117000	11.766058000	1	6.449080000	11.804750000	10.449730000
7	14.490564000	9.779902000	11.063837000	1	8.801831000	10.998797000	10.524611000
7	10.639471000	10.239489000	12.373554000	1	7.325802000	8.552979000	7.313797000
7	13.399615000	13.974643000	12.291419000	1	5.379067000	9.270092000	5.941731000
7	13.371593000	9.072832000	10.773013000	1	5.744152000	10.544763000	3.830123000
7	10.875007000	11.306608000	13.172725000	1	8.064130000	11.083978000	3.092180000
7	14.519352000	13.495471000	11.697480000	1	10.002724000	10.356301000	4.446259000
6	8.796846000	9.408392000	5.981345000	1	11.176381000	10.975923000	6.279827000
6	12.060570000	12.799681000	8.382114000	1	12.326357000	9.949259000	7.170070000
6	11.291131000	10.319465000	7.155318000				
6	10.103292000	11.193743000	14.285533000				
6	13.741521000	7.775309000	10.647600000	2a, BP86-D3/TZ2P,ADF2014 for ETS-NOCV			
6	13.248861000	12.741103000	7.633773000	47	10.358600000	11.563900000	15.433900000
6	9.346209000	11.901175000	8.640831000	47	9.816700000	8.735400000	13.600600000
6	11.143977000	7.754657000	5.889129000	47	8.435300000	11.925700000	12.479000000
6	15.543305000	8.921325000	11.122425000	15	12.547700000	10.852300000	15.027500000
6	8.991214000	10.121740000	4.786238000	15	11.930600000	7.959400000	14.241200000
6	9.710516000	9.472036000	12.994766000	9	4.939800000	8.010900000	14.180600000
6	15.115775000	7.624823000	10.861624000	9	10.727000000	14.110800000	17.208100000
6	12.780499000	6.671630000	10.359805000	9	6.083100000	11.995000000	17.953600000
6	7.487531000	9.106190000	6.385419000	9	8.220500000	12.429500000	17.674000000
6	8.455713000	11.596257000	9.679137000	9	6.722400000	13.387200000	16.394100000
6	13.595242000	15.288138000	12.556364000	9	6.944800000	7.338500000	13.573900000
6	15.409221000	14.510696000	11.597594000	9	5.941100000	8.940800000	12.470700000
6	16.925048000	9.399281000	11.413896000	9	9.406900000	6.348000000	11.731100000
6	9.336697000	10.034759000	14.218376000	9	6.480300000	16.343900000	12.796900000
6	6.694849000	12.817371000	8.554812000	9	8.197800000	6.012900000	9.928200000
6	6.392500000	9.511424000	5.614563000	9	6.900500000	11.107800000	8.010000000
6	13.990292000	13.899879000	7.388006000	9	7.509000000	15.023600000	11.373300000
6	7.578757000	13.129093000	7.515163000	9	8.362000000	12.390300000	9.033600000
6	11.650992000	14.038176000	8.905332000	9	5.951800000	14.213500000	12.675400000
6	9.218589000	8.189015000	12.416014000	9	11.564700000	15.700900000	15.959700000
6	7.133652000	12.050404000	9.635404000	9	6.414000000	12.012300000	9.952400000
6	12.497761000	7.473858000	6.150411000	9	10.289600000	6.623000000	9.744400000
6	8.896317000	12.673617000	7.556021000	9	9.843400000	16.124000000	17.245100000
6	6.597288000	10.225102000	4.432260000	7	8.334100000	10.624200000	15.602200000
6	14.865082000	15.680530000	12.130536000	7	8.943100000	9.077500000	11.513600000
6	10.518975000	7.079918000	4.825628000	7	8.596100000	13.573900000	13.753300000
6	16.763371000	14.290264000	11.011881000	7	8.090500000	9.614400000	14.726600000
6	7.899518000	10.529279000	4.018601000	7	8.475300000	10.298300000	11.163800000
6	12.580642000	5.918359000	4.294000000	7	9.486300000	13.581500000	14.772000000
6	13.562631000	15.130568000	7.892321000	6	13.121200000	7.628100000	12.894300000
6	12.532536000	16.104897000	13.209885000	6	13.856800000	11.783600000	15.896200000
6	10.132842000	12.225538000	15.360446000	6	12.893900000	9.071100000	15.384000000
6	12.394294000	15.193690000	8.657106000	6	7.972400000	10.222100000	9.906100000
6	13.210211000	6.572436000	5.357148000	6	6.749900000	9.445100000	14.647100000
6	11.231409000	6.172875000	4.036440000	6	14.907400000	11.202200000	16.618100000
1	8.619355000	9.659690000	14.939865000	6	12.994500000	10.991400000	13.255400000
1	15.320423000	16.662280000	12.195659000	6	11.820300000	6.416300000	15.222600000

6	7.142200000	11.074300000	16.056500000
6	14.445900000	7.230100000	13.142100000
6	8.720100000	8.247300000	10.471900000
6	6.095400000	10.353100000	15.479600000
6	6.149600000	8.436500000	13.724500000
6	12.687700000	7.788700000	11.574100000
6	11.991200000	11.247200000	12.313300000
6	8.019000000	14.798700000	13.677900000
6	9.456700000	14.811200000	15.325300000
6	7.048200000	12.214700000	17.015100000
6	8.104400000	8.927800000	9.417400000
6	13.592000000	11.035900000	10.523100000
6	13.561800000	7.553100000	10.512300000
6	15.846100000	12.013100000	17.262000000
6	14.604800000	10.796600000	11.458400000
6	13.752500000	13.183200000	15.834200000
6	9.144200000	6.816000000	10.481600000
6	12.283800000	11.263500000	10.950000000
6	11.052000000	6.464500000	16.398600000
6	14.310500000	10.774000000	12.819500000
6	14.876200000	7.161600000	10.763200000
6	8.537200000	15.630800000	14.664600000
6	12.374500000	5.198000000	14.810500000
6	10.382200000	15.177600000	16.435100000
6	15.318300000	7.000400000	12.080700000
6	11.441200000	4.106200000	16.761900000
6	15.743800000	13.402800000	17.186100000
6	6.990900000	15.096100000	12.636600000
6	7.408000000	11.427100000	9.227800000
6	14.694400000	13.986900000	16.470200000
6	10.873500000	5.317700000	17.168700000
6	12.182900000	4.048700000	15.581600000
1	7.793000000	8.542000000	8.455600000
1	8.276700000	16.659600000	14.875000000
1	5.032000000	10.458000000	15.652500000
1	12.947500000	5.139900000	13.886300000
1	12.614500000	3.103500000	15.252300000
1	11.292900000	3.206700000	17.359100000
1	10.276600000	5.366000000	18.079300000
1	10.571000000	7.397900000	16.699000000
1	15.000600000	10.119500000	16.695100000
1	16.657500000	11.554000000	17.826800000
1	16.475400000	14.031700000	17.693100000
1	14.597000000	15.070800000	16.418900000
1	12.922000000	13.643900000	15.298100000
1	15.102100000	10.583300000	13.545200000
1	15.625300000	10.614700000	11.123100000
1	13.827200000	11.042900000	9.458900000
1	11.485100000	11.451300000	10.232800000
1	10.966800000	11.436300000	12.644200000
1	11.668600000	8.117700000	11.377100000
1	13.209400000	7.683600000	9.490100000
1	15.560500000	6.980900000	9.934200000
1	16.344100000	6.690200000	12.279800000
1	14.795000000	7.083900000	14.165000000
1	13.962800000	8.839200000	15.292400000
1	12.570500000	8.865700000	16.412300000

2b, BP86-D3/TZ2P,ADF2014 for ETS-NOCV

29	10.303200000	11.611400000	15.176100000
29	9.851200000	8.989400000	13.422900000
29	8.497900000	11.876600000	12.497600000
15	12.334600000	10.954800000	15.011500000
15	11.698700000	8.150500000	14.116700000
9	5.425000000	7.567000000	14.578300000
9	10.906900000	13.925600000	16.983700000
9	6.408000000	11.791200000	18.037200000
9	8.549600000	12.229800000	17.785200000
9	7.071100000	13.183900000	16.484000000
9	7.422400000	7.050300000	13.813800000
9	6.179600000	8.499800000	12.745700000
9	9.681900000	6.510600000	11.790500000
9	6.792300000	16.271400000	12.515200000
9	8.341400000	6.123500000	10.095200000
9	6.350100000	10.995100000	8.441600000
9	7.613800000	14.748700000	11.161700000
9	7.870000000	12.414200000	9.144300000
9	6.022700000	14.215300000	12.564500000
9	11.719800000	15.525800000	15.728500000
9	6.128400000	11.976200000	10.394600000
9	10.359600000	6.886100000	9.741100000
9	10.006500000	15.930300000	17.028000000
7	8.650000000	10.591100000	15.518100000
7	9.023500000	9.232100000	11.649800000
7	8.693600000	13.376000000	13.568800000
7	8.421700000	9.541100000	14.683700000
7	8.409700000	10.414300000	11.359700000
7	9.588000000	13.372300000	14.595000000
6	13.022500000	7.760700000	12.919600000
6	13.574400000	11.821800000	16.035100000
6	12.583800000	9.163300000	15.400300000
6	7.771700000	10.279300000	10.167700000
6	7.124200000	9.176700000	14.817500000
6	14.148400000	11.257700000	17.182400000
6	12.990800000	11.100500000	13.307600000
6	11.328900000	6.598800000	15.017100000
6	7.490600000	10.868400000	16.161500000
6	14.281600000	7.272400000	13.304400000
6	8.749100000	8.377100000	10.638900000
6	6.486400000	9.990700000	15.753300000
6	6.542700000	8.076400000	13.993900000
6	12.755700000	7.987200000	11.565800000
6	12.099300000	11.389200000	12.267400000
6	8.178100000	14.628900000	13.461700000
6	9.619600000	14.618100000	15.110600000
6	7.384200000	12.012000000	17.114500000
6	7.956500000	8.996500000	9.670500000
6	13.889400000	11.206700000	10.661600000
6	13.730100000	7.725200000	10.602600000
6	15.029800000	12.007600000	17.965200000
6	14.788000000	10.923700000	11.696000000
6	13.881300000	13.147900000	15.690600000
6	9.277900000	6.979800000	10.582300000
6	12.543700000	11.439900000	10.946500000
6	10.360300000	6.688400000	16.032200000
6	14.343500000	10.871500000	13.015000000
6	14.979900000	7.241000000	10.988800000
6	8.737500000	15.457400000	14.426000000
6	11.875700000	5.352100000	14.691100000
6	10.553300000	14.988700000	16.215000000
6	15.255700000	7.015400000	12.341500000
6	10.535500000	4.308800000	16.419100000
6	15.340500000	13.321000000	17.610500000
6	7.152500000	14.964600000	12.427800000
6	7.027400000	11.414500000	9.541700000

6	14.762300000	13.890300000	16.471900000
6	9.975100000	5.550100000	16.736300000
6	11.477200000	4.212000000	15.393700000
1	7.564200000	8.575200000	8.754600000
1	8.527000000	16.502900000	14.607200000
1	5.461300000	9.940200000	16.096200000
1	12.602100000	5.265300000	13.884300000
1	11.903300000	3.243200000	15.132600000
1	10.226100000	3.416000000	16.962400000
1	9.222500000	5.628400000	17.520700000
1	9.887800000	7.650100000	16.243600000
1	13.912700000	10.235700000	17.477600000
1	15.472400000	11.561700000	18.855900000
1	16.026200000	13.904600000	18.224600000
1	14.989900000	14.919800000	16.196800000
1	13.419400000	13.599800000	14.812700000
1	15.045000000	10.649900000	13.819900000
1	15.836700000	10.732400000	11.470300000
1	14.242300000	11.241000000	9.631000000
1	11.836200000	11.660000000	10.147600000
1	11.045200000	11.568100000	12.496700000
1	11.786800000	8.392900000	11.278200000
1	13.511100000	7.909800000	9.551500000
1	15.743800000	7.039700000	10.237600000
1	16.231300000	6.635300000	12.645000000
1	14.500600000	7.082400000	14.356000000
1	13.644900000	8.889200000	15.464300000
1	12.094500000	8.966200000	16.362600000

2a', CAM-B3LYP/SVPFIT, ground state, E=-19942.5420358

47	10.703569000	11.829193000	14.697753000
47	10.118224000	8.870666000	12.477929000
47	8.555876000	11.969834000	11.909766000
15	12.147409000	8.087450000	13.671682000
15	12.937791000	10.814804000	15.057032000
9	5.487148000	7.779758000	13.613272000
9	10.972690000	14.455216000	16.488709000
9	6.635099000	11.788288000	17.359510000
9	8.760183000	12.088703000	17.070347000
9	7.340964000	13.222010000	15.919003000
9	7.495786000	7.257101000	12.995808000
9	6.360327000	8.692102000	11.868322000
9	9.613966000	6.522823000	10.320738000
9	6.997004000	16.451148000	11.768105000
9	8.954377000	6.503699000	8.259849000
9	6.155792000	11.320870000	7.898599000
9	7.613071000	14.639928000	10.756180000
9	7.800510000	12.625685000	8.380019000
9	6.125977000	14.552761000	12.302052000
9	11.954784000	15.834611000	15.165381000
9	6.379979000	12.104128000	9.904770000
9	10.874375000	7.331690000	8.780201000
9	10.282914000	16.502445000	16.343922000
7	8.693710000	10.715488000	14.688801000
7	9.230721000	9.291446000	10.449924000
7	8.918487000	13.762476000	13.095168000
7	8.438839000	9.748170000	13.811966000
7	8.561420000	10.434936000	10.357208000
7	9.819770000	13.831991000	14.068526000
6	13.063456000	10.316224000	16.817667000
6	13.088940000	6.888010000	12.652729000
6	13.468075000	9.311284000	14.108302000
6	7.862223000	10.430662000	9.216340000
6	7.169329000	9.355272000	13.977750000
6	12.863367000	6.922309000	11.273436000
6	11.731748000	7.229091000	15.231194000
6	14.331326000	11.969877000	14.785283000
6	7.586219000	10.937153000	15.405144000
6	14.285642000	10.052709000	17.446209000
6	8.953040000	8.559607000	9.364894000
6	6.561324000	10.084583000	14.996556000
6	6.618236000	8.275751000	13.112103000
6	11.880370000	10.212549000	17.555099000
6	10.396500000	6.849763000	15.410432000
6	8.344925000	14.964191000	12.954890000
6	9.808502000	15.078039000	14.553616000
6	7.572822000	12.011803000	16.437244000
6	8.075215000	9.242133000	8.524752000
6	10.937031000	5.869234000	17.545983000
6	11.915880000	9.831808000	18.894298000
6	13.539621000	6.053073000	10.421858000
6	12.265576000	6.257739000	17.385457000
6	13.996394000	5.957280000	13.171437000
6	9.589143000	7.227342000	9.179085000
6	10.003208000	6.167809000	16.558846000
6	15.650796000	11.575852000	14.532303000
6	12.660467000	6.934382000	16.236529000
6	13.133810000	9.560463000	19.508915000
6	8.876715000	15.861761000	13.874024000
6	14.030405000	13.334185000	14.839953000
6	10.744975000	15.471355000	15.640681000
6	14.319637000	9.673753000	18.783801000
6	16.338888000	13.888767000	14.431970000
6	14.446439000	5.136967000	10.944762000
6	7.265527000	15.156969000	11.944935000
6	7.047034000	11.622027000	8.843272000
6	14.672464000	5.089594000	12.319991000
6	16.647180000	12.531884000	14.356050000
6	15.028022000	14.289259000	14.673618000
1	7.652230000	8.921982000	7.577643000
1	8.622857000	16.906105000	14.027014000
1	5.549454000	10.002596000	15.381722000
1	13.001453000	13.655479000	15.000328000
1	14.765724000	15.347678000	14.724042000
1	17.123575000	14.635361000	14.292551000
1	17.672505000	12.213920000	14.155673000
1	15.915225000	10.518731000	14.463019000
1	12.142440000	7.627990000	10.858300000
1	13.334286000	6.088839000	9.350480000
1	14.973264000	4.447863000	10.281191000
1	15.375051000	4.363274000	12.734064000
1	14.168199000	5.891640000	14.247097000
1	13.702101000	7.245644000	16.142066000
1	12.999256000	6.039931000	18.163991000
1	10.628073000	5.338968000	18.449324000
1	8.958120000	5.877311000	16.682209000
1	9.652152000	7.098048000	14.650734000
1	10.919962000	10.428999000	17.081539000
1	10.984138000	9.755220000	19.457893000
1	13.162999000	9.269068000	20.561071000
1	15.278577000	9.476074000	19.267617000
1	15.222755000	10.159406000	16.895547000
1	14.310908000	8.808728000	14.606038000
1	13.839020000	9.676021000	13.137895000

2a', CAM-B3LYP/SVPFIT, S1, E=-19942.4981353, E(TD)=-19942.3805742

47	10.755562000	11.871034000	14.904075000
47	10.335893000	8.616377000	12.463346000
47	8.758828000	11.875077000	11.791206000
15	12.160743000	8.215019000	14.083067000
15	13.020000000	10.966621000	15.273551000
9	5.925733000	7.407836000	13.369243000
9	10.542409000	14.406358000	16.655364000
9	6.580733000	11.535306000	17.089160000
9	8.677600000	12.033461000	16.880813000
9	7.203743000	13.007287000	15.651216000
9	7.951119000	7.135416000	12.651483000
9	6.621290000	8.498522000	11.651073000
9	9.982376000	6.452996000	10.567960000
9	7.066544000	16.257460000	11.521951000
9	8.871230000	6.096241000	8.743555000
9	6.445352000	11.081830000	7.804292000
9	7.943275000	14.539293000	10.540669000
9	8.121032000	12.366003000	8.234017000
9	6.293413000	14.277263000	11.888061000
9	11.694939000	15.757544000	15.445773000
9	6.674819000	11.959201000	9.770297000
9	10.856737000	6.912925000	8.655453000
9	9.885487000	16.451505000	16.383297000
7	8.861046000	10.560064000	14.584178000
7	9.457596000	9.106323000	10.462206000
7	8.986620000	13.654816000	13.018540000
7	8.712619000	9.573607000	13.706092000
7	8.833121000	10.269068000	10.307489000
7	9.767836000	13.755404000	14.087597000
6	13.254357000	10.401093000	16.995086000
6	12.724367000	7.190707000	12.680547000
6	13.490378000	9.505301000	14.229815000
6	8.117751000	10.215774000	9.178652000
6	7.444646000	9.133283000	13.762927000
6	13.229152000	7.752778000	11.488027000
6	11.737916000	7.379462000	15.509773000
6	14.378781000	12.141297000	14.923629000
6	7.687094000	10.749979000	15.191913000
6	14.512385000	10.263877000	17.591220000
6	9.130748000	8.313532000	9.434979000
6	6.730269000	9.856494000	14.710119000
6	6.975289000	8.044562000	12.858834000
6	12.108230000	10.090028000	17.733370000
6	10.402005000	7.384240000	16.061127000
6	8.376019000	14.831055000	12.821930000
6	9.643855000	14.993847000	14.574561000
6	7.530722000	11.835645000	16.204256000
6	8.269595000	8.975755000	8.564419000
6	11.121639000	5.972262000	17.910365000
6	12.218392000	9.627596000	19.040598000
6	13.499523000	6.945507000	10.391698000
6	12.425309000	5.964505000	17.389802000
6	12.477892000	5.805898000	12.730786000
6	9.704565000	6.942072000	9.342605000
6	10.126723000	6.699629000	17.218614000
6	15.696463000	11.759082000	14.641480000
6	12.756666000	6.638520000	16.234153000
6	13.472715000	9.489083000	19.625993000
6	8.758973000	15.742403000	13.799337000
6	14.057934000	13.502342000	14.940855000
6	10.432177000	15.406748000	15.767310000
6	14.618771000	9.810862000	18.901837000
6	16.344432000	14.075918000	14.437728000
6	13.277790000	5.571526000	10.466146000
6	7.414375000	14.982900000	11.693191000
6	7.336559000	11.408842000	8.738460000
6	12.772729000	5.004876000	11.636479000
6	16.671975000	12.721843000	14.399858000
6	15.035842000	14.464745000	14.707622000
1	7.814941000	8.613919000	7.647300000
1	8.441328000	16.772310000	13.929082000
1	5.691514000	9.745606000	15.006363000
1	13.029866000	13.816207000	15.124256000
1	14.762173000	15.521388000	14.729494000
1	17.112231000	14.828943000	14.247906000
1	17.695750000	12.411999000	14.179787000
1	15.974609000	10.703799000	14.603906000
1	13.413021000	8.826623000	11.412889000
1	13.875602000	7.390597000	9.468996000
1	13.486307000	4.940373000	9.600182000
1	12.596374000	3.929059000	11.691103000
1	12.063581000	5.374072000	13.643764000
1	13.784468000	6.605883000	15.866168000
1	13.209973000	5.409392000	17.911757000
1	10.882755000	5.430952000	18.825309000
1	9.104846000	6.717778000	17.606127000
1	9.609733000	7.930704000	15.551184000
1	11.120554000	10.193700000	17.279192000
1	11.317082000	9.368984000	19.598403000
1	13.559178000	9.128672000	20.653165000
1	15.604114000	9.710547000	19.361772000
1	15.417519000	10.524853000	17.039901000
1	14.368763000	8.990229000	14.652648000
1	13.766582000	9.884489000	13.235219000

2a', CAM-B3LYP/SVPFIT, T1, E=-19942.5196043, E(TD)=-19942.4277879

47	10.693930000	11.834410000	14.678656000
47	10.110505000	8.864440000	12.472419000
47	8.563702000	11.970949000	11.887538000
15	12.156370000	8.096647000	13.645460000
15	12.918569000	10.804361000	15.056427000
9	5.491972000	7.756065000	13.635873000
9	10.945916000	14.465743000	16.473225000
9	6.609198000	11.849432000	17.302586000
9	8.730629000	12.166984000	17.004751000
9	7.297992000	13.256864000	15.828559000
9	7.504466000	7.235554000	13.029067000
9	6.360590000	8.642905000	11.875614000
9	9.572258000	6.503345000	10.345972000
9	7.033847000	16.458950000	11.698414000
9	8.887590000	6.464129000	8.293486000
9	6.115225000	11.297003000	7.912822000
9	7.662987000	14.646266000	10.697245000
9	7.776279000	12.594474000	8.356216000
9	6.156460000	14.561102000	12.224201000
9	11.944114000	15.852035000	15.169150000
9	6.372339000	12.102781000	9.906123000
9	10.818952000	7.285745000	8.780819000
9	10.252046000	16.511249000	16.323041000
7	8.679258000	10.730933000	14.660484000

7	9.207300000	9.273996000	10.448406000	1	10.888929000	10.576618000	17.169375000
7	8.936530000	13.771864000	13.055845000	1	10.993473000	9.865210000	19.522351000
7	8.432311000	9.743096000	13.804650000	1	13.224751000	9.139049000	20.572095000
7	8.544323000	10.420734000	10.351452000	1	15.339591000	9.229494000	19.192639000
7	9.824972000	13.842279000	14.040765000	1	15.265756000	9.973599000	16.841789000
6	13.031933000	10.287753000	16.781471000	1	14.327532000	8.827640000	14.548326000
6	13.092389000	6.892349000	12.627660000	1	13.827048000	9.717897000	13.104392000
6	13.471734000	9.328095000	14.070993000				
6	7.832272000	10.409367000	9.218511000				
6	7.163803000	9.348771000	13.973307000	2a', CAM-B3LYP/SVPFIT, T5, E= -19942.5149542,			
6	12.844853000	6.908222000	11.251812000	E(TD)=-19942.4007355			
6	11.762445000	7.256031000	15.220555000	47	10.801371000	11.825254000	14.720416000
6	14.317351000	11.970359000	14.837282000	47	10.237190000	9.143280000	12.333319000
6	7.567794000	10.963543000	15.367331000	47	8.723566000	11.953898000	11.636570000
6	14.348551000	9.898555000	17.426730000	15	12.180450000	8.269053000	13.645388000
6	8.912679000	8.532874000	9.374320000	15	13.064424000	10.902133000	15.101734000
6	6.548264000	10.097864000	14.973128000	9	5.389078000	8.436929000	12.986417000
6	6.620317000	8.250374000	13.126852000	9	10.740873000	14.248423000	16.534579000
6	11.842200000	10.272930000	17.607934000	9	6.730428000	11.390396000	17.551783000
6	10.429456000	6.881491000	15.427445000	9	8.638798000	10.421938000	17.820257000
6	8.366614000	14.974033000	12.904765000	9	8.557470000	12.387987000	16.959382000
6	9.809116000	15.089652000	14.522445000	9	7.318906000	7.966017000	12.129787000
6	7.543680000	12.061569000	16.374429000	9	6.332276000	9.807988000	11.617110000
6	8.029863000	9.212410000	8.536957000	9	9.319510000	6.442437000	10.488976000
6	11.005227000	5.928459000	17.566499000	9	6.932284000	16.318092000	11.714072000
6	11.897523000	9.875909000	18.911261000	9	8.670215000	6.233008000	8.434879000
6	13.514517000	6.033967000	10.400116000	9	6.055170000	11.049451000	7.762428000
6	12.331057000	6.312381000	17.378417000	9	7.573937000	14.522321000	10.689708000
6	14.015637000	5.975313000	13.143037000	9	7.661470000	12.454636000	8.096477000
6	9.537955000	7.194446000	9.196303000	9	6.071561000	14.409319000	12.219889000
6	10.055006000	6.215814000	16.591111000	9	11.780419000	15.674842000	15.310340000
6	15.637541000	11.592934000	14.564590000	9	6.372793000	11.904367000	9.726876000
6	12.707350000	6.973075000	16.213865000	9	10.672662000	6.910764000	8.883533000
6	13.195399000	9.453330000	19.528941000	9	10.041914000	16.294596000	16.418785000
6	8.887688000	15.873102000	13.828438000	7	8.871504000	10.575209000	14.827956000
6	14.013544000	13.329824000	14.962352000	7	9.510398000	9.333391000	10.233456000
6	10.728279000	15.483907000	15.623806000	7	8.924854000	13.659278000	12.984500000
6	14.384289000	9.501241000	18.737007000	7	8.523519000	9.978257000	13.691668000
6	16.318487000	13.910246000	14.572303000	7	8.901388000	10.529608000	10.020287000
6	14.436828000	5.131506000	10.919506000	7	9.784422000	13.720244000	13.993858000
6	7.300313000	15.165105000	11.880634000	6	13.179449000	10.396223000	16.860763000
6	7.021397000	11.602536000	8.841714000	6	13.068473000	7.000135000	12.659518000
6	14.685085000	5.102730000	12.291465000	6	13.564536000	9.396938000	14.138754000
6	16.630650000	12.559464000	14.431784000	6	7.895632000	10.310552000	8.985639000
6	15.007229000	14.294936000	14.837568000	6	7.231277000	9.625159000	13.782929000
1	7.594175000	8.885301000	7.598015000	6	12.777677000	6.938775000	11.293589000
1	8.633258000	16.918160000	13.975524000	6	11.656976000	7.443851000	15.192215000
1	5.534996000	10.020164000	15.355531000	6	14.468102000	12.043226000	14.831143000
1	12.984693000	13.639564000	15.144982000	6	7.804116000	10.611616000	15.629798000
1	14.741456000	15.348885000	14.938095000	6	14.394100000	10.180941000	17.521248000
1	17.100538000	14.665015000	14.466034000	6	8.910829000	8.391970000	9.279788000
1	17.656564000	12.254513000	14.214885000	6	6.707218000	10.007663000	15.014169000
1	15.905166000	10.541177000	14.444771000	6	6.562985000	8.958422000	12.632121000
1	12.112385000	7.603653000	10.839677000	6	11.983067000	10.239541000	17.566489000
1	13.292232000	6.055397000	9.331740000	6	10.287598000	7.205739000	15.352097000
1	14.958772000	4.438649000	10.255991000	6	8.280779000	14.831317000	12.901126000
1	15.400133000	4.387193000	12.702957000	6	9.675213000	14.926472000	14.561102000
1	14.205365000	5.924065000	14.216458000	6	7.923294000	11.208416000	16.988738000
1	13.748932000	7.278991000	16.098561000	6	7.915142000	8.996436000	8.537073000
1	13.077585000	6.104477000	18.147507000	6	10.691920000	6.158578000	17.485133000
1	10.710683000	5.410425000	18.481666000	6	11.995296000	9.862569000	18.906267000
1	9.011639000	5.929407000	16.736558000	6	13.407130000	6.003786000	10.475168000
1	9.672958000	7.121459000	14.677170000	6	12.056370000	6.404331000	17.343734000

6	13.999841000	6.103005000	13.196551000
6	9.382325000	6.990542000	9.266389000
6	9.807797000	6.563760000	16.490580000
6	15.785047000	11.627721000	14.599354000
6	12.535460000	7.046355000	16.207416000
6	13.206537000	9.642868000	19.554209000
6	8.720220000	15.696073000	13.898546000
6	14.183710000	13.412213000	14.859995000
6	10.549389000	15.290866000	15.707994000
6	14.405663000	9.802317000	18.859947000
6	16.505829000	13.927958000	14.467705000
6	14.335641000	5.121574000	11.016416000
6	7.210884000	15.024336000	11.881089000
6	6.990463000	11.430326000	8.633108000
6	14.631075000	5.172653000	12.378532000
6	16.796840000	12.566179000	14.418237000
6	15.197831000	14.349506000	14.687819000
1	7.286778000	8.546540000	7.773704000
1	8.395818000	16.710451000	14.109159000
1	5.699883000	9.873815000	15.396356000
1	13.157250000	13.752110000	15.002941000
1	14.953732000	15.413217000	14.716365000
1	17.301657000	14.661951000	14.324558000
1	17.819888000	12.230978000	14.235051000
1	16.034188000	10.565592000	14.551370000
1	12.046592000	7.625065000	10.862649000
1	13.150884000	5.964190000	9.415097000
1	14.827417000	4.383934000	10.378581000
1	15.353237000	4.475279000	12.808417000
1	14.228298000	6.113483000	14.263427000
1	13.604662000	7.251883000	16.132620000
1	12.752382000	6.104292000	18.129491000
1	10.316717000	5.658200000	18.380396000
1	8.735837000	6.389369000	16.600444000
1	9.587056000	7.540029000	14.584112000
1	11.026046000	10.399355000	17.067401000
1	11.047793000	9.749350000	19.436293000
1	13.220343000	9.354330000	20.607532000
1	15.358390000	9.642146000	19.369306000
1	15.340839000	10.326102000	16.996825000
1	14.361684000	8.840648000	14.654205000
1	13.983608000	9.760476000	13.187776000

2b, CAM-B3LYP/SVPFIT, ground state, E=-9264.87492670

29	-1.412913000	1.000078000	0.366756000
29	1.550779000	-0.507280000	0.552717000
29	-1.084076000	-2.166329000	-0.653329000
15	-0.299655000	2.820624000	-0.290248000
15	2.519974000	1.457768000	0.092273000
9	1.285720000	-3.046870000	4.497787000
9	-4.156941000	2.213778000	0.664893000
9	-3.424366000	-0.182453000	4.596080000
9	-2.987435000	1.480821000	3.286688000
9	-3.949792000	-0.276549000	2.509482000
9	2.476259000	-1.981552000	3.038030000
9	1.225954000	-3.617760000	2.421974000
9	4.297835000	-2.112120000	0.919957000
9	-5.304894000	-3.502128000	-2.019748000
9	5.050618000	-3.626688000	-0.425089000
9	0.428579000	-6.392370000	-1.625756000
9	-3.174482000	-3.639268000	-2.368060000
9	-0.450966000	-4.859747000	-2.857428000
9	-3.973041000	-4.059141000	-0.418108000
9	-4.279689000	2.499815000	-1.461464000
9	-1.139582000	-5.125079000	-0.838490000
9	4.549706000	-1.662316000	-1.163943000
9	-5.995508000	1.764082000	-0.385003000
7	-0.962531000	-0.071974000	2.017447000
7	1.742981000	-2.291870000	-0.378723000
7	-2.778040000	-1.322254000	-0.749997000
7	0.166043000	-0.780882000	1.992276000
7	0.638164000	-2.957782000	-0.716262000
7	-2.928465000	-0.026947000	-0.476007000
6	3.171791000	1.663445000	-1.607004000
6	-1.036078000	4.329279000	0.452668000
6	1.431950000	2.930691000	0.363550000
6	0.984504000	-4.186994000	-1.125794000
6	0.165460000	-1.612104000	3.043153000
6	-1.681723000	4.188265000	1.686798000
6	-0.205536000	3.158913000	-2.083834000
6	3.982137000	1.824667000	1.141257000
6	-1.674439000	-0.455109000	3.084898000
6	4.036069000	2.709759000	-1.950968000
6	2.786302000	-3.103370000	-0.578228000
6	-0.995733000	-1.445143000	3.790943000
6	1.289684000	-2.568497000	3.252415000
6	2.794068000	0.738726000	-2.582514000
6	-1.220755000	2.622908000	-2.884389000
6	-3.966027000	-1.820538000	-1.127057000
6	-4.211229000	0.289487000	-0.667774000
6	-3.011841000	0.138656000	3.369119000
6	2.363462000	-4.340407000	-1.059119000
6	-0.237635000	3.631325000	-4.842482000
6	3.251480000	0.871849000	-3.891972000
6	-2.235468000	5.296524000	2.320838000
6	0.780539000	4.163239000	-4.054717000
6	-0.973791000	5.591052000	-0.146228000
6	4.172950000	-2.632042000	-0.306667000
6	-1.239025000	2.863480000	-4.255237000
6	3.982371000	2.771935000	2.168821000
6	0.795086000	3.931638000	-2.682759000
6	4.100850000	1.920120000	-4.229291000
6	-4.933794000	-0.824732000	-1.091007000
6	5.136069000	1.057893000	0.927468000
6	-4.668447000	1.692105000	-0.459197000
6	4.497534000	2.837382000	-3.255799000
6	6.255925000	2.193578000	2.739082000
6	-2.162044000	6.551693000	1.723035000
6	-4.107585000	-3.263329000	-1.482804000
6	-0.048571000	-5.147536000	-1.614278000
6	-1.534237000	6.696227000	0.488128000
6	5.114109000	2.954712000	2.961983000
6	6.263186000	1.244611000	1.718535000
1	2.960704000	-5.211973000	-1.307271000
1	-5.990317000	-0.900397000	-1.327506000
1	-1.294219000	-1.952698000	4.702816000
1	5.155514000	0.307417000	0.135527000
1	7.153277000	0.638238000	1.538962000
1	7.141101000	2.336516000	3.362289000
1	5.097344000	3.699700000	3.760182000
1	3.101733000	3.382931000	2.369112000
1	-1.765839000	3.204684000	2.154293000
1	-2.739639000	5.171495000	3.281178000
1	-2.604623000	7.419717000	2.216370000

1	-1.484680000	7.676889000	0.010137000
1	-0.496985000	5.714765000	-1.120079000
1	1.604505000	4.353242000	-2.085769000
1	1.573291000	4.759639000	-4.510592000
1	-0.247579000	3.813591000	-5.919251000
1	-2.039413000	2.442100000	-4.866673000
1	-2.006021000	2.018015000	-2.428022000
1	2.146250000	-0.097604000	-2.311583000
1	2.948407000	0.144891000	-4.647993000
1	4.466202000	2.019626000	-5.253740000
1	5.176509000	3.652492000	-3.515559000
1	4.362708000	3.423080000	-1.189998000
1	1.928494000	3.866135000	0.065026000
1	1.270296000	2.979723000	1.450806000

2b, CAM-B3LYP/SVPFIT, S1, E=-9264.84165720, E(TD)=-9264.74439003

29	-1.424402000	0.461902000	0.331397000
29	1.210654000	-0.245582000	0.571539000
29	-0.669099000	-2.286956000	0.092743000
15	-1.011180000	2.056448000	-1.231720000
15	2.045392000	1.440472000	-0.804998000
9	2.973854000	1.466041000	4.858838000
9	-4.661837000	1.295917000	1.218175000
9	-2.405097000	2.223050000	5.044048000
9	-2.861443000	2.837641000	3.029257000
9	-3.135146000	0.785425000	3.610014000
9	3.451922000	1.693231000	2.765984000
9	3.039922000	-0.259390000	3.563131000
9	4.466900000	-0.857569000	1.222060000
9	-4.681295000	-4.934696000	-0.315230000
9	5.548562000	-2.695621000	0.864843000
9	1.620110000	-6.481028000	0.129981000
9	-2.605917000	-4.723945000	-0.886552000
9	0.390643000	-5.480096000	-1.331315000
9	-3.138788000	-4.885199000	1.188699000
9	-4.808444000	1.186454000	-0.921501000
9	-0.148297000	-5.401761000	0.748337000
9	4.969796000	-1.440484000	-0.786645000
9	-6.357394000	0.316596000	0.304241000
7	-0.610503000	1.076787000	2.176979000
7	2.109874000	-2.029394000	0.233099000
7	-2.583779000	-2.092798000	0.168003000
7	0.705244000	0.868428000	2.152145000
7	1.151768000	-2.949511000	0.089241000
7	-2.980094000	-0.823314000	0.247590000
6	2.443983000	0.801830000	-2.466381000
6	-1.939703000	3.644734000	-1.180133000
6	0.717773000	2.702388000	-1.009461000
6	1.718784000	-4.157901000	0.078105000
6	1.227444000	1.207142000	3.344251000
6	-2.692292000	3.905456000	-0.031877000
6	-1.139660000	1.520640000	-2.977069000
6	3.504202000	2.412625000	-0.288622000
6	-0.925933000	1.542639000	3.385638000
6	3.254723000	1.519843000	-3.353878000
6	3.289197000	-2.663187000	0.301730000
6	0.217497000	1.651682000	4.184093000
6	2.679818000	1.028041000	3.634323000
6	1.896808000	-0.420402000	-2.868941000
6	-2.123164000	0.564993000	-3.258419000
6	-3.666718000	-2.878067000	0.087717000
6	-4.314869000	-0.802280000	0.217554000
6	-2.339697000	1.842666000	3.765332000
6	3.101091000	-4.037726000	0.205381000
6	-1.547070000	0.629671000	-5.599867000
6	2.158611000	-0.919394000	-4.141062000
6	-3.401343000	5.098358000	0.090521000
6	-0.560792000	1.574784000	-5.328517000
6	-1.924958000	4.586385000	-2.215559000
6	4.572181000	-1.912973000	0.411152000
6	-2.328537000	0.126426000	-4.563212000
6	3.388398000	3.670572000	0.313393000
6	-0.358945000	2.018813000	-4.024835000
6	2.965488000	-0.202259000	-5.019411000
6	-4.819270000	-2.099526000	0.115728000
6	4.775647000	1.835759000	-0.412393000
6	-5.039614000	0.499569000	0.211428000
6	3.511511000	1.018117000	-4.625530000
6	5.777701000	3.764296000	0.636522000
6	-3.374873000	6.033588000	-0.938839000
6	-3.522558000	-4.361330000	0.020468000
6	0.886560000	-5.388671000	-0.093968000
6	-2.638089000	5.774355000	-2.093943000
6	4.519200000	4.341156000	0.770375000
6	5.901952000	2.510507000	0.042245000
1	3.848134000	-4.825213000	0.231466000
1	-5.854682000	-2.421856000	0.067947000
1	0.294019000	1.988100000	5.213286000
1	4.891261000	0.851617000	-0.866227000
1	6.884941000	2.047058000	-0.062550000
1	6.663411000	4.290226000	0.998721000
1	4.410997000	5.322189000	1.237144000
1	2.415789000	4.146106000	0.438693000
1	-2.731366000	3.170276000	0.772040000
1	-3.983770000	5.286123000	0.994816000
1	-3.936725000	6.965742000	-0.847265000
1	-2.624135000	6.501125000	-2.909135000
1	-1.366172000	4.389445000	-3.132582000
1	0.427332000	2.751099000	-3.834277000
1	0.060442000	1.967423000	-6.136074000
1	-1.704643000	0.281819000	-6.623101000
1	-3.101595000	-0.616919000	-4.768185000
1	-2.733928000	0.167788000	-2.445061000
1	1.250158000	-0.974526000	-2.186083000
1	1.726288000	-1.874496000	-4.444937000
1	3.172707000	-0.596136000	-6.016736000
1	4.147296000	1.581622000	-5.311646000
1	3.696948000	2.470516000	-3.049232000
1	1.010516000	3.442818000	-1.769248000
1	0.653245000	3.230315000	-0.046592000

2b, CAM-B3LYP/SVPFIT, T1, E=-9264.85052223, E(TD)=-9264.75830382

29	-1.708537000	0.378341000	0.361373000
29	1.540448000	0.143068000	0.524054000
29	-0.051294000	-2.436611000	-0.710191000
15	-1.451410000	2.483392000	-0.355745000
15	1.660952000	2.318634000	0.045443000
9	2.319007000	-2.318091000	4.507491000
9	-4.627378000	0.367244000	0.625482000
9	-3.108177000	-1.434783000	4.651708000
9	-3.342013000	0.298276000	3.381816000
9	-3.580263000	-1.674855000	2.562277000

9	3.021540000	-0.811564000	3.123505000
9	2.517773000	-2.775655000	2.411108000
9	4.628739000	0.023186000	0.942293000
9	-3.349821000	-5.370094000	-2.062664000
9	6.089845000	-1.096687000	-0.194042000
9	3.206231000	-5.614471000	-1.656820000
9	-1.335163000	-4.628999000	-2.348530000
9	1.773479000	-4.611495000	-2.917379000
9	-1.952798000	-5.349917000	-0.418883000
9	-4.981401000	0.467978000	-1.492799000
9	1.217490000	-5.177316000	-0.918233000
9	4.872258000	0.400063000	-1.156810000
9	-6.158554000	-0.869045000	-0.279701000
7	-0.897395000	-0.389478000	2.043150000
7	2.532716000	-1.356308000	-0.380129000
7	-1.942433000	-2.336649000	-0.780477000
7	0.419279000	-0.618305000	2.005549000
7	1.843188000	-2.441192000	-0.754109000
7	-2.617430000	-1.214128000	-0.494319000
6	2.253511000	2.813508000	-1.612167000
6	-2.744401000	3.544537000	0.309579000
6	0.101185000	3.297758000	0.275219000
6	2.716721000	-3.393976000	-1.144390000
6	0.748330000	-1.372634000	3.070264000
6	-3.263652000	3.237931000	1.672381000
6	-1.482026000	2.752255000	-2.164064000
6	2.828497000	3.112301000	1.219596000
6	-1.399084000	-0.998361000	3.131157000
6	2.555996000	4.142910000	-1.934183000
6	3.842957000	-1.622644000	-0.535436000
6	-0.383480000	-1.645969000	3.837808000
6	2.155057000	-1.821931000	3.279439000
6	2.388286000	1.826727000	-2.590507000
6	-2.200205000	1.827117000	-2.930311000
6	-2.831385000	-3.293375000	-1.141184000
6	-3.932525000	-1.465441000	-0.661479000
6	-2.859030000	-0.955377000	3.431778000
6	4.025316000	-2.921346000	-1.025195000
6	-1.672925000	3.050834000	-4.940867000
6	2.802217000	2.163491000	-3.877949000
6	-4.170200000	4.054455000	2.266746000
6	-0.951824000	3.973854000	-4.187022000
6	-3.291592000	4.735783000	-0.390126000
6	4.863179000	-0.577241000	-0.230671000
6	-2.299311000	1.979853000	-4.310431000
6	2.433063000	3.363128000	2.538865000
6	-0.859902000	3.827956000	-2.806364000
6	3.095220000	3.485996000	-4.191309000
6	-4.133772000	-2.788268000	-1.080628000
6	4.154562000	3.365654000	0.852933000
6	-4.932201000	-0.378939000	-0.448177000
6	2.975862000	4.476837000	-3.216107000
6	4.637587000	4.183228000	3.073120000
6	-4.668588000	5.254786000	1.585717000
6	-2.367471000	-4.669275000	-1.492541000
6	2.227817000	-4.707141000	-1.661256000
6	-4.193110000	5.542914000	0.225875000
6	3.328646000	3.903097000	3.455995000
6	5.049777000	3.901726000	1.774293000
1	4.953501000	-3.439099000	-1.245463000
1	-5.066970000	-3.297944000	-1.298496000
1	-0.455939000	-2.214877000	4.759322000
1	4.500073000	3.125964000	-0.153582000
1	6.081646000	4.093318000	1.472755000
1	5.339252000	4.612291000	3.791339000
1	3.002411000	4.095554000	4.480074000
1	1.422357000	3.118268000	2.873055000
1	-2.913387000	2.336621000	2.178417000
1	-4.548228000	3.814207000	3.262652000
1	-5.392222000	5.909549000	2.070512000
1	-4.582795000	6.421436000	-0.293159000
1	-2.956423000	4.951195000	-1.405214000
1	-0.290580000	4.562282000	-2.235733000
1	-0.453803000	4.813397000	-4.676062000
1	-1.744282000	3.166468000	-6.024509000
1	-2.865952000	1.252100000	-4.894643000
1	-2.689787000	0.983696000	-2.441381000
1	2.174007000	0.786304000	-2.338879000
1	2.901583000	1.383965000	-4.635751000
1	3.425691000	3.749072000	-5.198516000
1	3.215746000	5.514690000	-3.457252000
1	2.474568000	4.924220000	-1.174208000
1	0.209672000	4.329533000	-0.089656000
1	-0.066378000	3.356394000	1.360658000

2b, CAM-B3LYP/SVPFIT, T5, E=-9264.84925250, E(TD)=-9264.73817742

29	-1.554634000	0.749148000	0.386144000
29	1.625080000	-0.262573000	0.515158000
29	-0.770524000	-2.279949000	-0.737578000
15	-0.755700000	2.711900000	-0.329464000
15	2.254111000	1.839926000	0.024421000
9	1.906561000	-2.599981000	4.576459000
9	-4.457471000	1.526940000	0.789751000
9	-3.251887000	-0.674591000	4.681861000
9	-3.131450000	1.034735000	3.365122000
9	-3.774793000	-0.868074000	2.600947000
9	2.868094000	-1.308993000	3.130981000
9	1.988453000	-3.164554000	2.499001000
9	4.624240000	-1.552077000	0.957710000
9	-4.725905000	-4.234430000	-2.083735000
9	5.597007000	-2.919650000	-0.406727000
9	1.453340000	-6.298271000	-1.675315000
9	-2.569551000	-4.112325000	-2.224419000
9	0.192609000	-4.907827000	-2.745006000
9	-3.499978000	-4.628983000	-0.357634000
9	-4.672002000	1.818838000	-1.328238000
9	-0.245208000	-5.382130000	-0.693546000
9	4.784996000	-1.046709000	-1.124170000
9	-6.229718000	0.814569000	-0.227961000
7	-0.887914000	-0.169821000	2.054640000
7	2.041212000	-1.951820000	-0.400501000
7	-2.583509000	-1.730189000	-0.737164000
7	0.354603000	-0.648054000	2.033187000
7	1.031041000	-2.759148000	-0.829153000
7	-2.924843000	-0.479880000	-0.430406000
6	2.848318000	2.100864000	-1.688771000
6	-1.714166000	4.098213000	0.398782000
6	0.946503000	3.123272000	0.281024000
6	1.618184000	-4.048100000	-1.111991000
6	0.529669000	-1.420953000	3.112335000
6	-2.309708000	3.882590000	1.647227000
6	-0.754359000	3.020575000	-2.131164000
6	3.651111000	2.458340000	1.042369000
6	-1.497675000	-0.637993000	3.152102000

6	3.528751000	3.262665000	-2.072320000
6	3.282100000	-2.734830000	-0.540663000
6	-0.631239000	-1.449661000	3.879473000
6	1.823815000	-2.126410000	3.332094000
6	2.617425000	1.097917000	-2.632752000
6	-1.700212000	2.324073000	-2.892425000
6	-3.690970000	-2.403097000	-1.084946000
6	-4.247953000	-0.364969000	-0.574583000
6	-2.916162000	-0.290549000	3.449225000
6	3.009134000	-4.011726000	-0.951992000
6	-0.923700000	3.418739000	-4.896596000
6	3.036148000	1.265877000	-3.951314000
6	-3.023723000	4.901876000	2.270338000
6	0.025457000	4.110857000	-4.148293000
6	-1.863512000	5.340571000	-0.224895000
6	4.577649000	-2.073744000	-0.274836000
6	-1.787665000	2.527631000	-4.266489000
6	3.541033000	3.491364000	1.977012000
6	0.107628000	3.916043000	-2.772856000
6	3.700478000	2.427956000	-4.328832000
6	-4.801539000	-1.571752000	-0.996917000
6	4.883948000	1.807352000	0.894866000
6	-4.909031000	0.947537000	-0.331566000
6	3.951782000	3.425409000	-3.386268000
6	5.861119000	3.221529000	2.588848000
6	-3.161061000	6.139459000	1.647689000
6	-3.623089000	-3.851597000	-1.437337000
6	0.753355000	-5.168599000	-1.557605000
6	-2.583542000	6.355679000	0.398731000
6	4.641260000	3.869688000	2.745280000
6	5.979219000	2.189276000	1.659859000
1	3.711616000	-4.822132000	-1.124354000
1	-5.841084000	-1.807491000	-1.201400000
1	-0.813768000	-1.967592000	4.815699000
1	4.990752000	0.994855000	0.174079000
1	6.931789000	1.670860000	1.533149000
1	6.721271000	3.517625000	3.192864000
1	4.538122000	4.678696000	3.471454000
1	2.597341000	4.017915000	2.122604000
1	-2.228498000	2.908471000	2.134742000
1	-3.486642000	4.718765000	3.242065000
1	-3.729100000	6.936208000	2.132743000
1	-2.698832000	7.321161000	-0.098480000
1	-1.427414000	5.517318000	-1.209685000
1	0.861555000	4.464643000	-2.207389000
1	0.711352000	4.805184000	-4.637654000
1	-0.986924000	3.572304000	-5.976040000
1	-2.532929000	1.980174000	-4.846933000
1	-2.376460000	1.621605000	-2.402328000
1	2.116550000	0.175775000	-2.329029000
1	2.847985000	0.478180000	-4.683539000
1	4.035179000	2.555732000	-5.360616000
1	4.487201000	4.331765000	-3.677401000
1	3.741936000	4.041151000	-1.335266000
1	1.275488000	4.118643000	-0.053195000
1	0.800727000	3.176381000	1.370567000