

Intramolecular Mobility of η^5 -Ligands in Chiral Zirconocene Complexes and Enantioselectivity of Alkene Functionalization by Organoaluminum Compounds

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Figure S1. VT ^1H NMR study on complex $\text{CpInd}^*\text{ZrCl}_2$ (**1**) in CD_2Cl_2 .

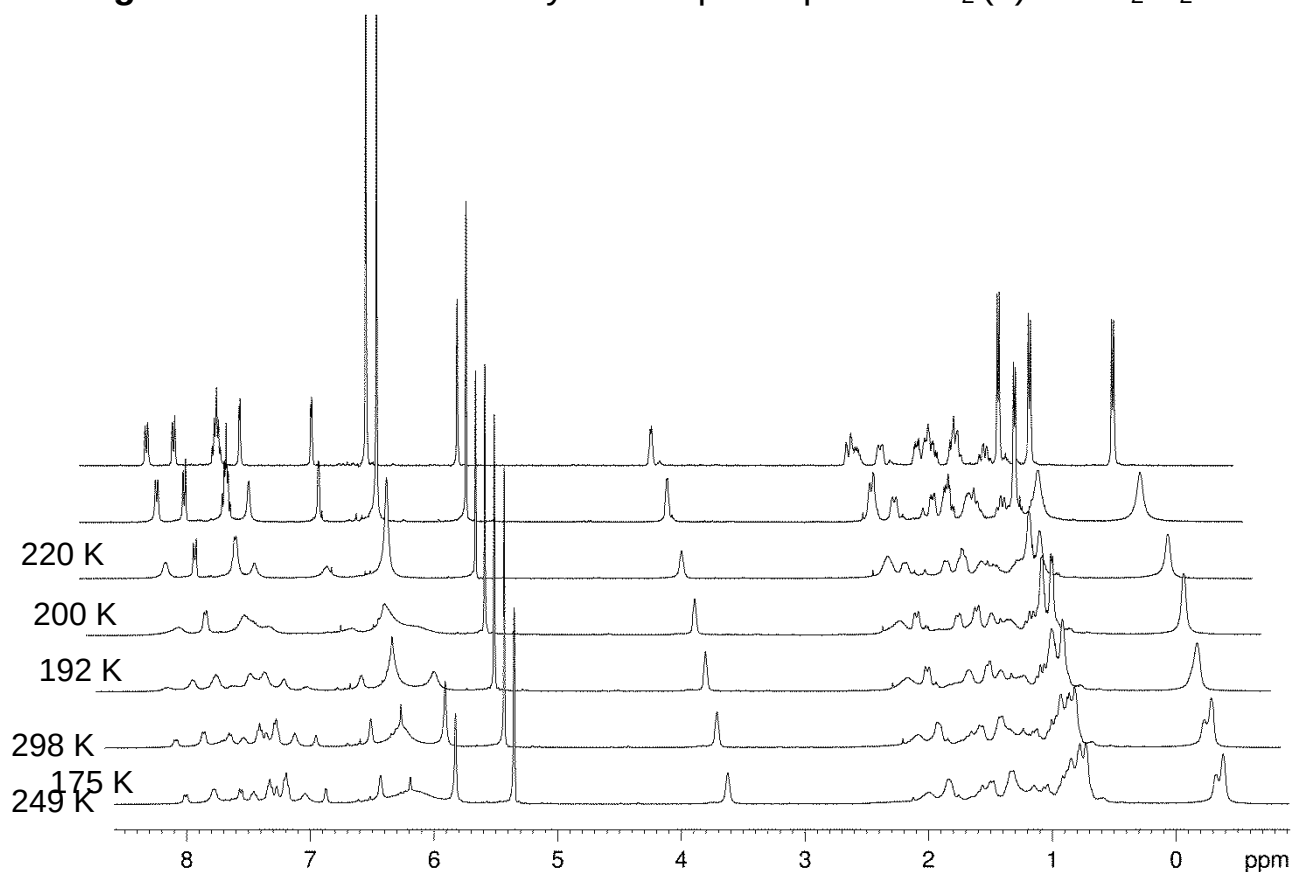


Figure S2. VT ^1H NMR study on complex $\text{CpInd}^*\text{ZrCl}_2$ (**1**) in d_8 -toluene.

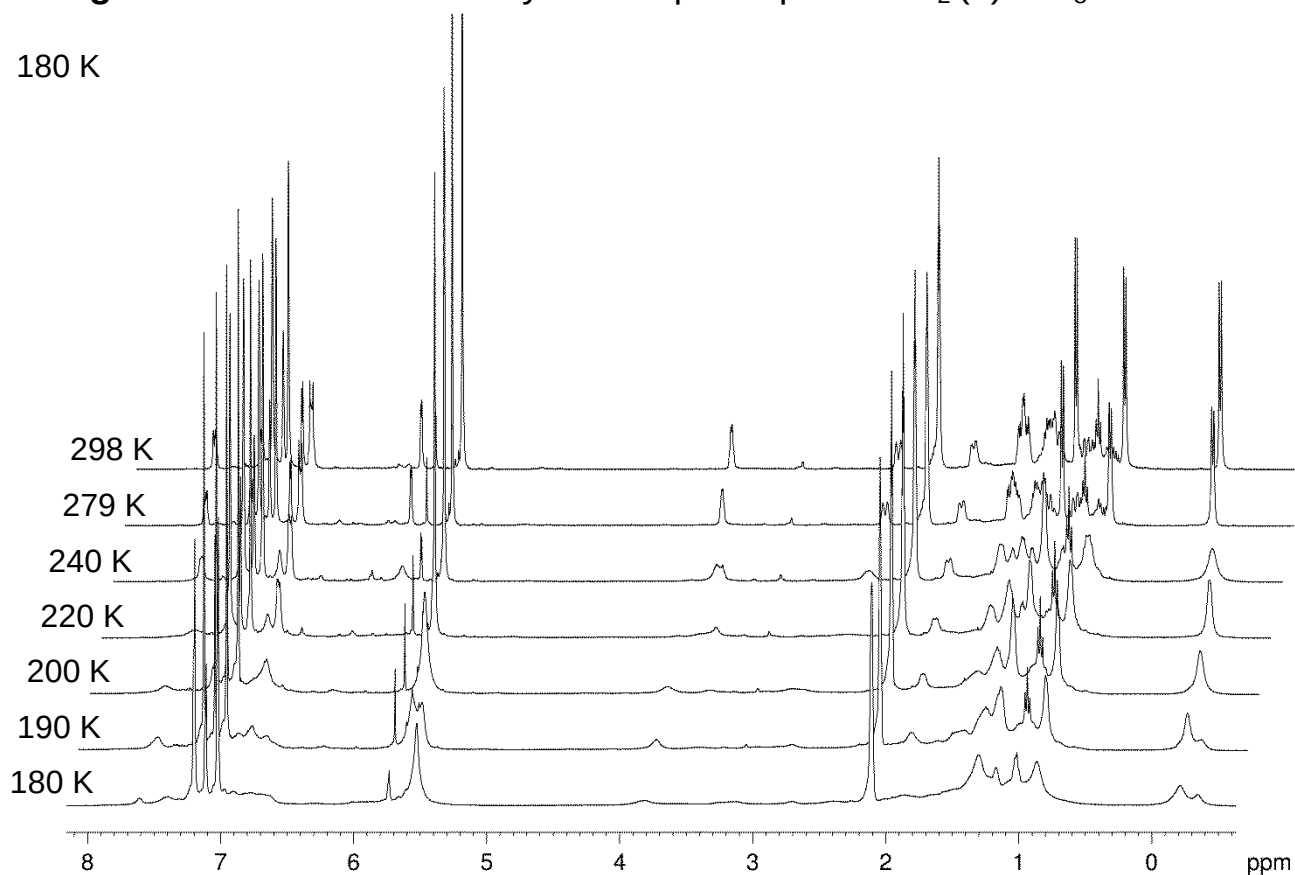


Figure S3. VT ^1H NMR study on complex $\text{CpCp}'\text{ZrCl}_2$ (**2**) in CD_2Cl_2 .

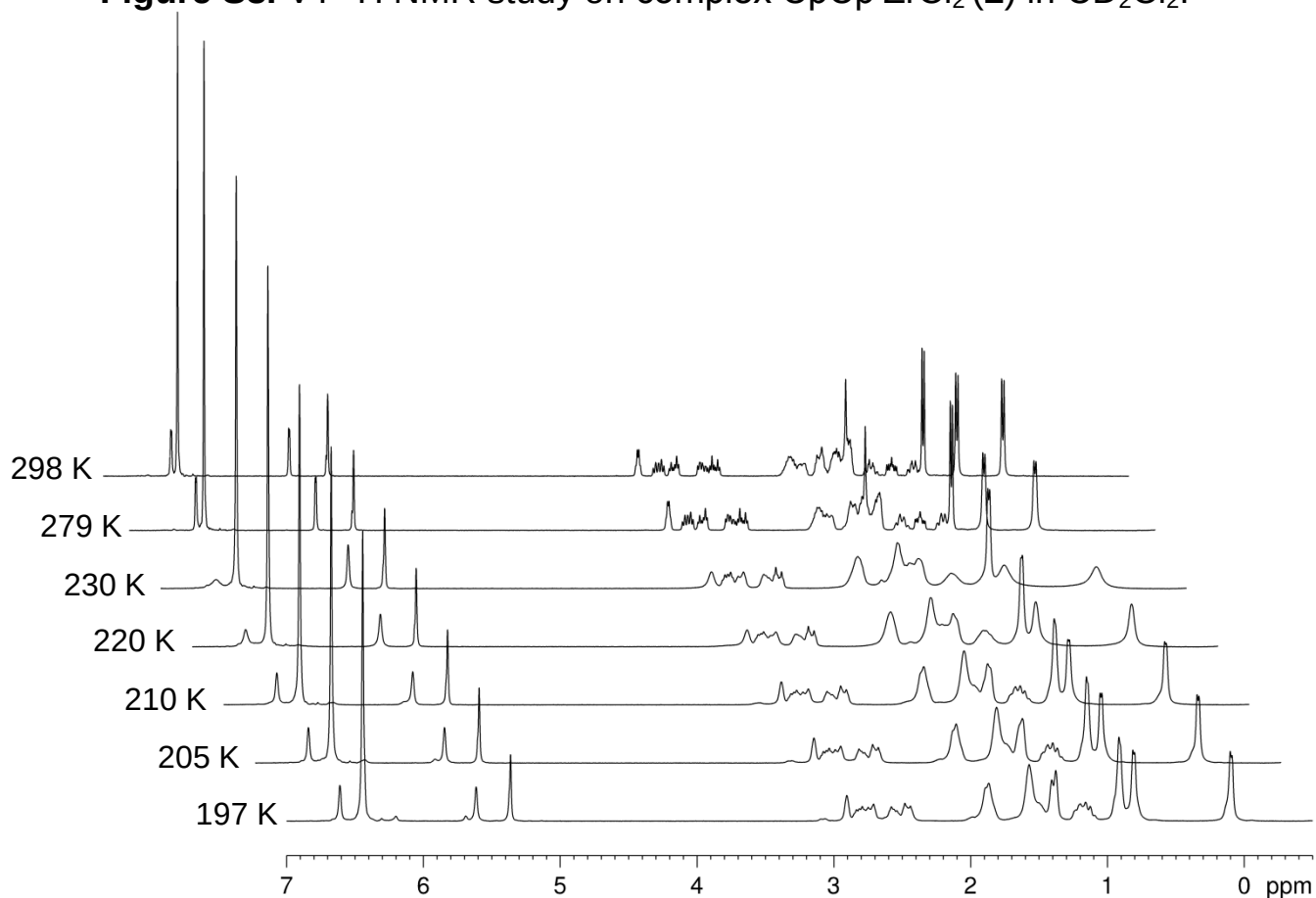


Figure S4. VT ^1H NMR study on complex $\text{CpCp}'\text{ZrCl}_2$ (**2**) in d_8 -toluene.

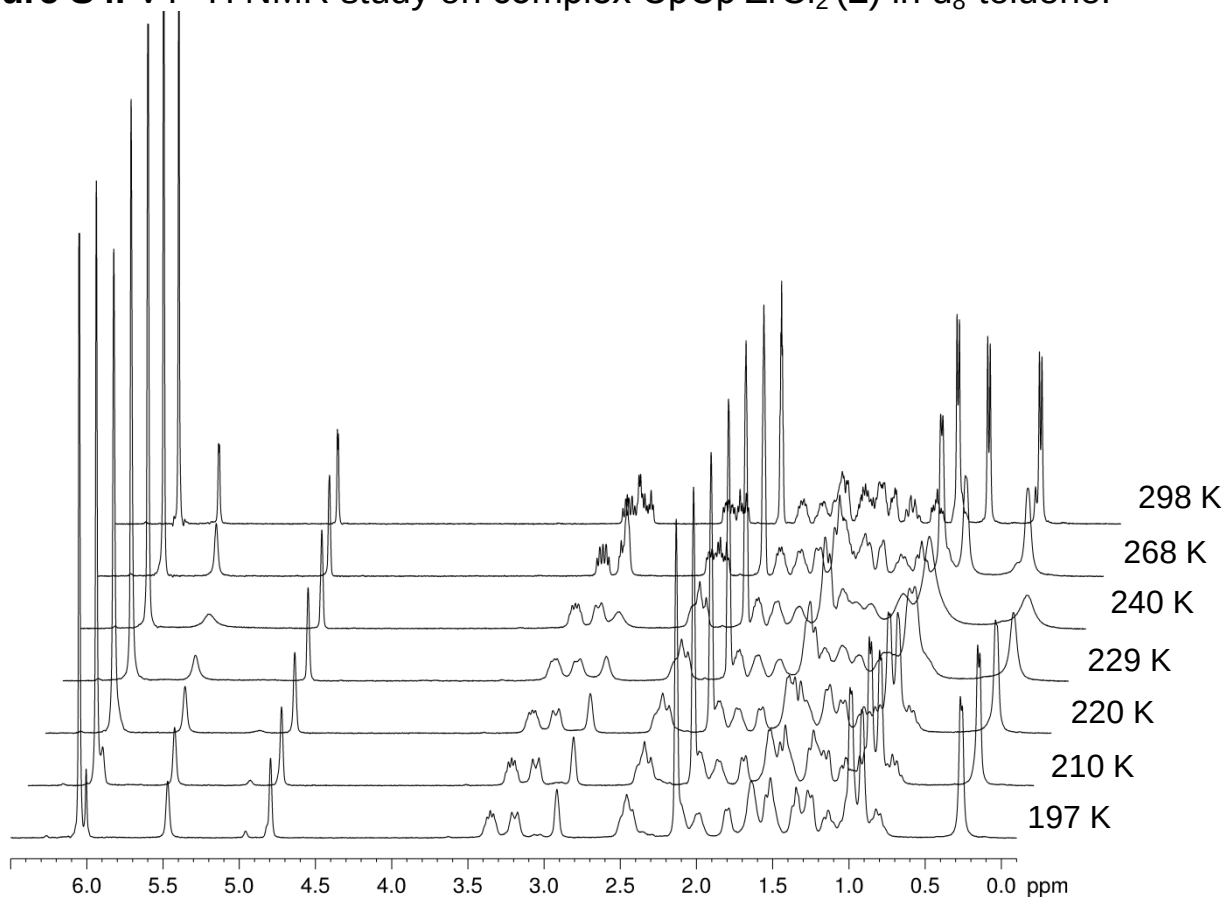


Figure S5. VT ^1H NMR study on complex $\text{CpCp}'\text{ZrCl}_2$ (**2**) in d_8 -THF.

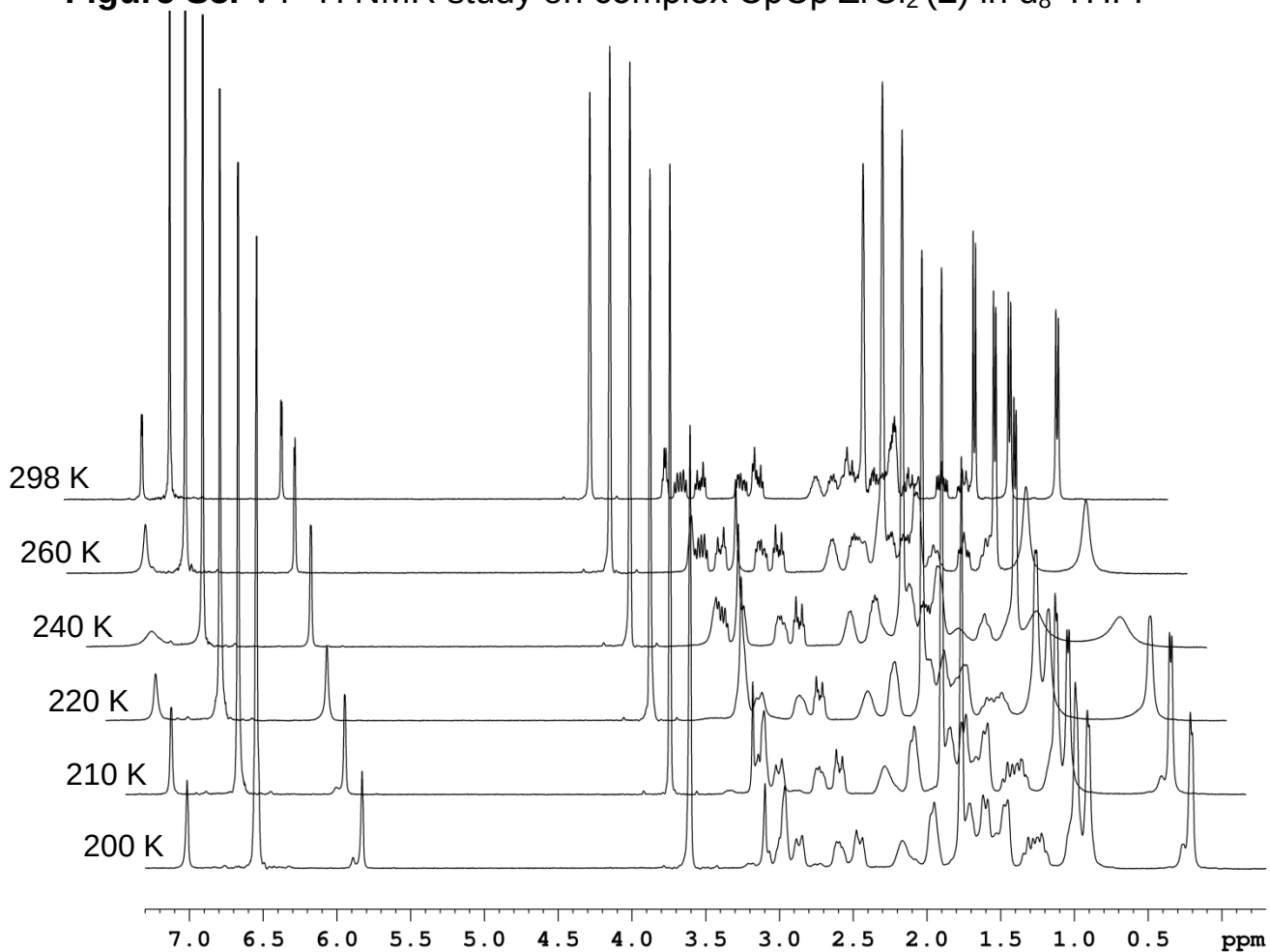


Figure S6. VT ^1H NMR study on complex $\text{Ind}^*_2\text{ZrCl}_2$ (**3**) in CD_2Cl_2 .

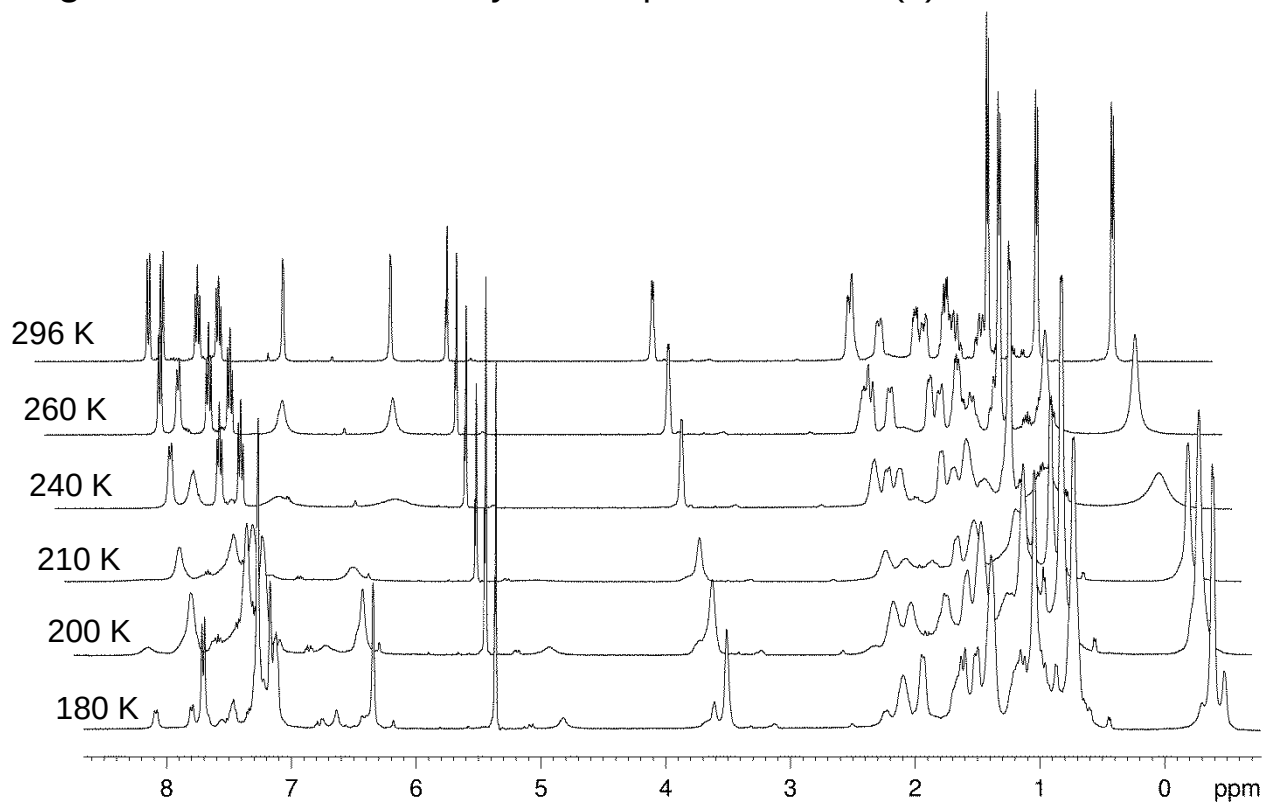


Figure S7. VT ^1H NMR study on complex $\text{Ind}^*_2\text{ZrCl}_2$ (**3**) in d_8 -toluene.

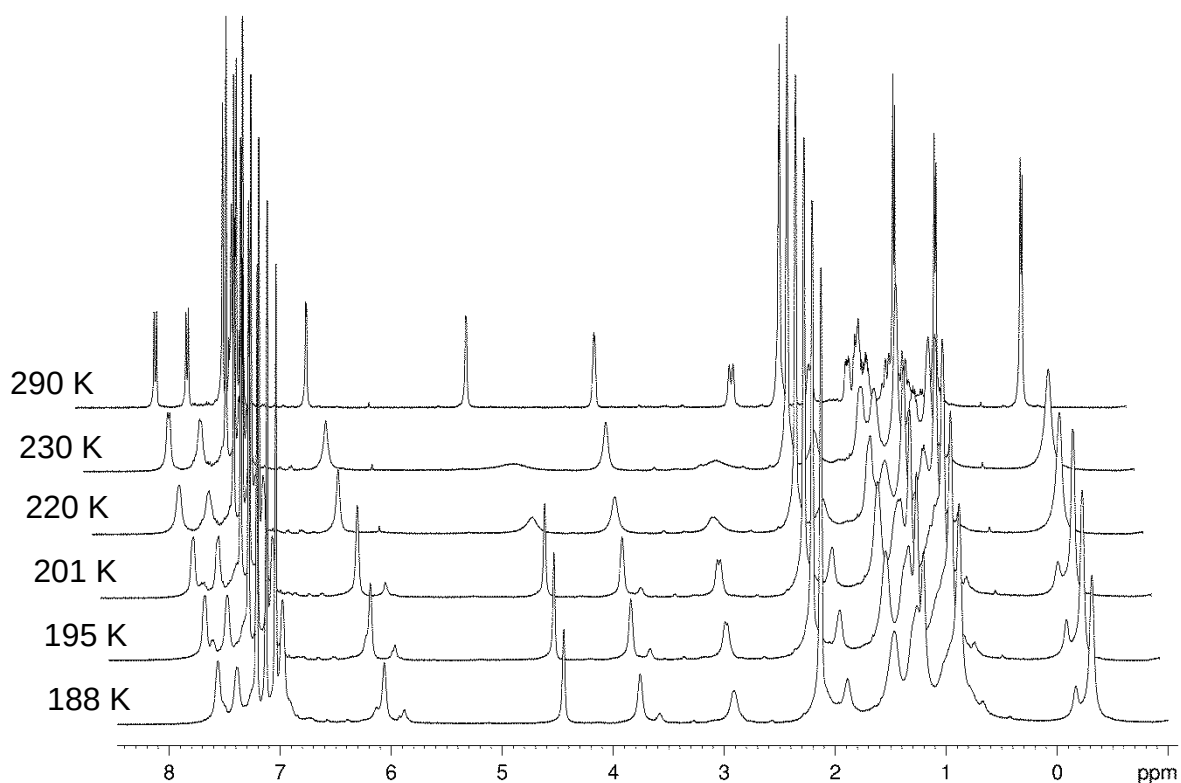


Figure S8. Eyring equation plot for rotamer exchange in complexes: ($\circ$) $\text{Ind}^*_2\text{ZrCl}_2$ in C_7D_8 ; (Δ) $\text{CpCp}'\text{ZrCl}_2$ in CD_2Cl_2 ; ($\square$) $\text{CpCp}'\text{ZrCl}_2$ in d_8 -toluene; ($\diamond$) $\text{CpCp}'\text{ZrCl}_2$ in d_8 -THF.

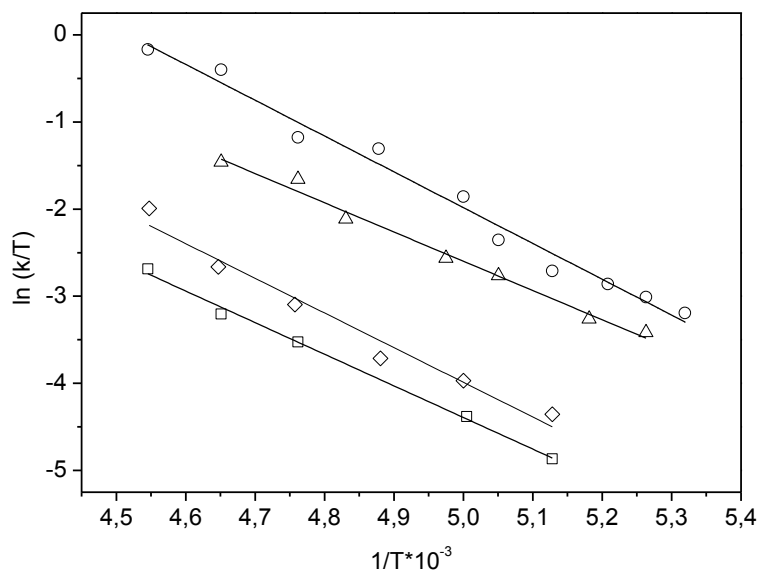


Figure S9. ^1H NMR of *p*-S, *p*-S- (dimethylsilanediyl $\{\eta^5$ -4,5,6,7-tetrahydroindenyl $\}$ zirconium]-S-binaphtholate (**6**) (in $\text{C}_6\text{H}_6+\text{C}_6\text{D}_6$).

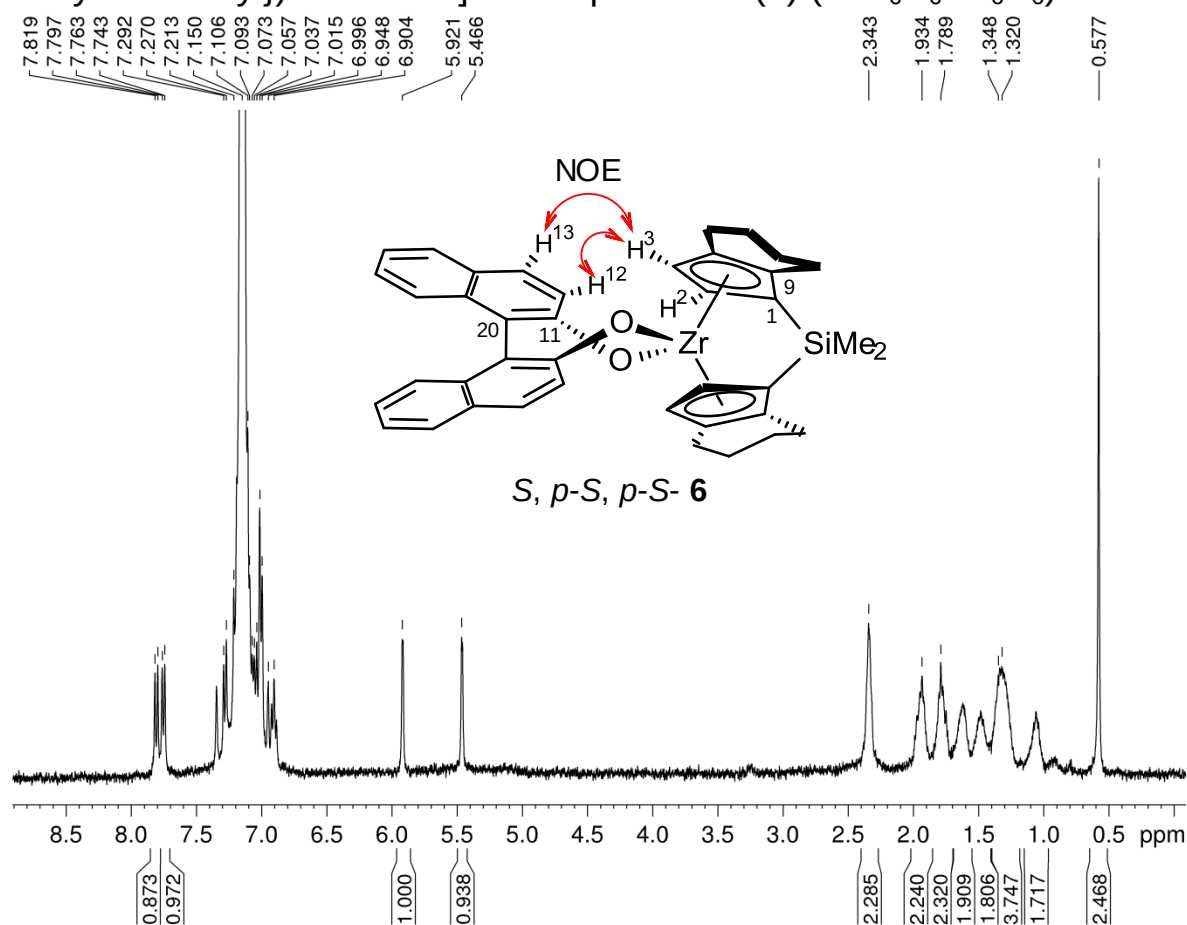


Figure S10. NOESY of reaction mixture of *rac*-(dimethylsilanediyl $\{\eta^5$ -4,5,6,7-tetrahydroindenyl $\}$ zirconium]dichloride (**4**) with lithium *S*-binaphtholate.

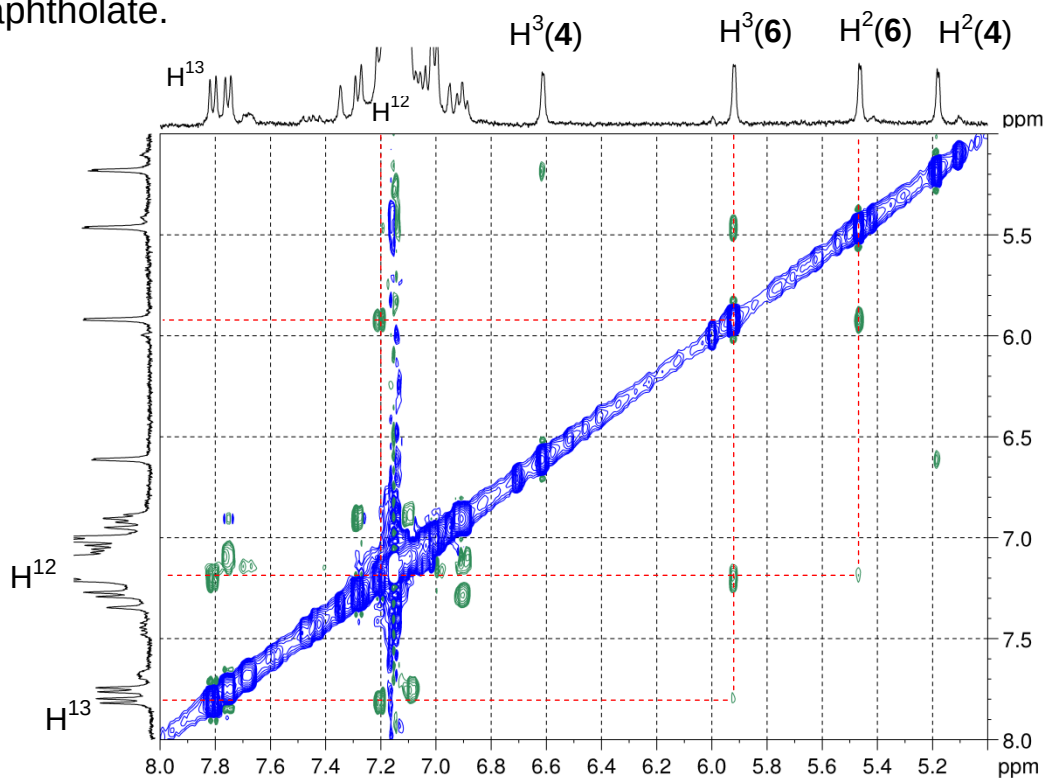
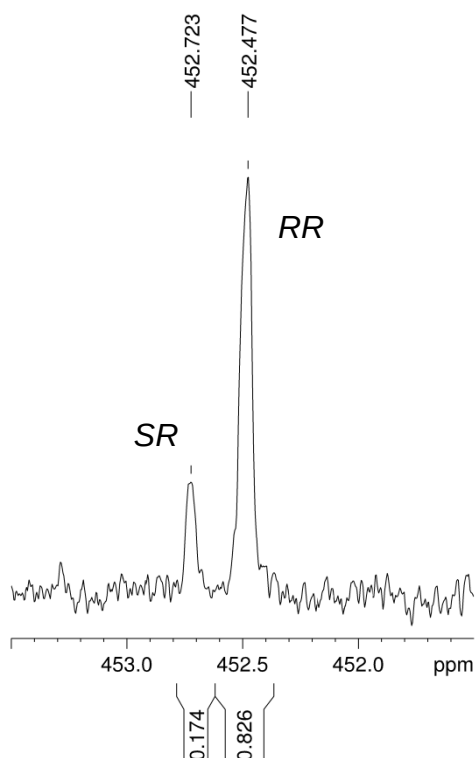
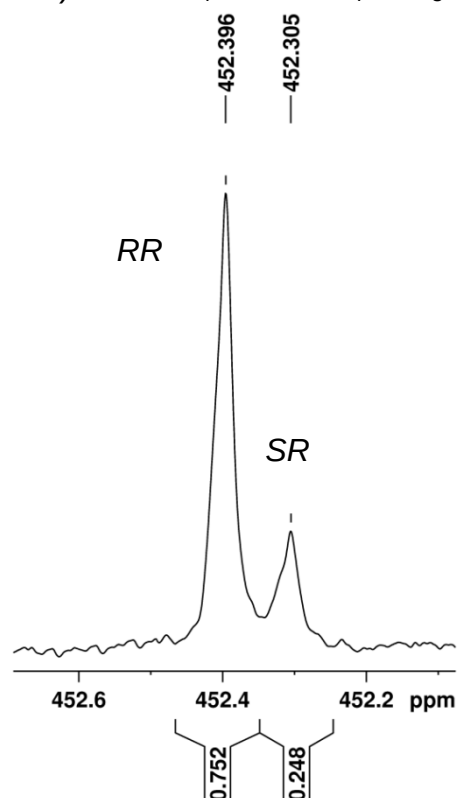


Figure S11. ^{77}Se NMR of (*R*)-PSPA esters of (2*R,S*)-methyl-1-octanol (a,b) and (*R*)-PSPA ester of (2*R,S*)-ethyl-1-hexanol (c,d).

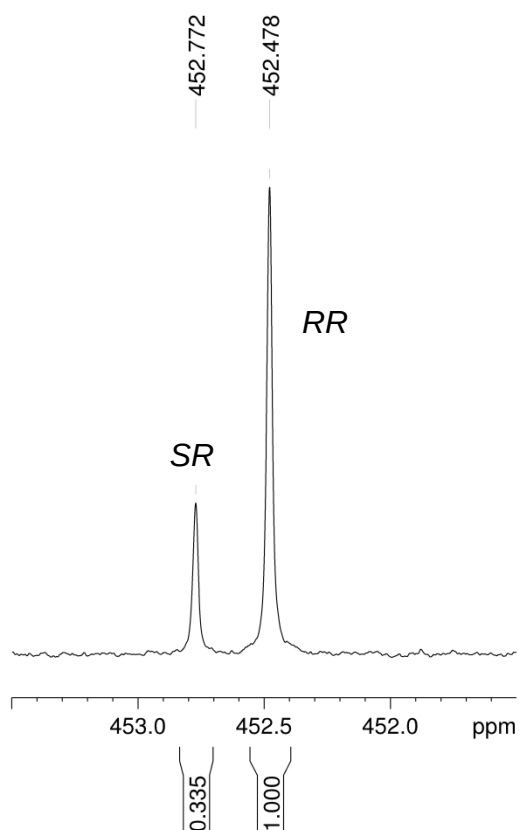
a) 2mol% **4**, 1-octene, AlMe_3 , MAO



c) 2mol% **5**, 1-hexene, AlEt_3



b) 2mol% **3**, 1-octene, AlMe_3 (Ref. [6a])



d) 2mol% **3**, 1-hexene, AlEt_3 (Ref. [6c])

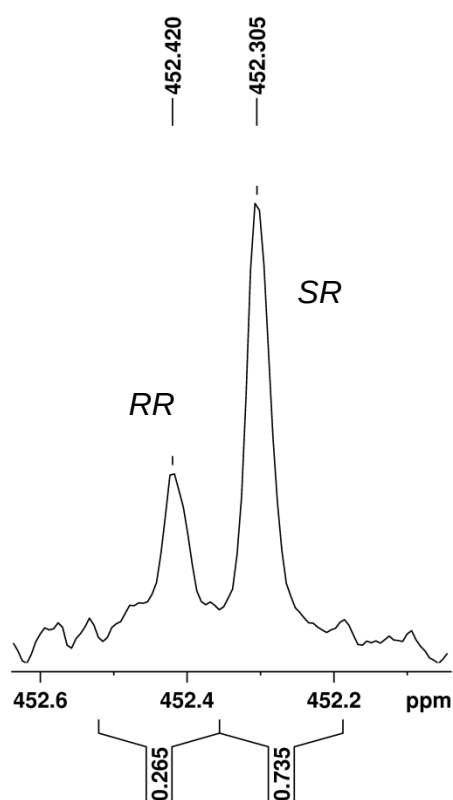


Figure S12. ^{77}Se NMR of (*R*)-PSPA ester of (*2R,S*)- n-butyl-1,4-butanediol.

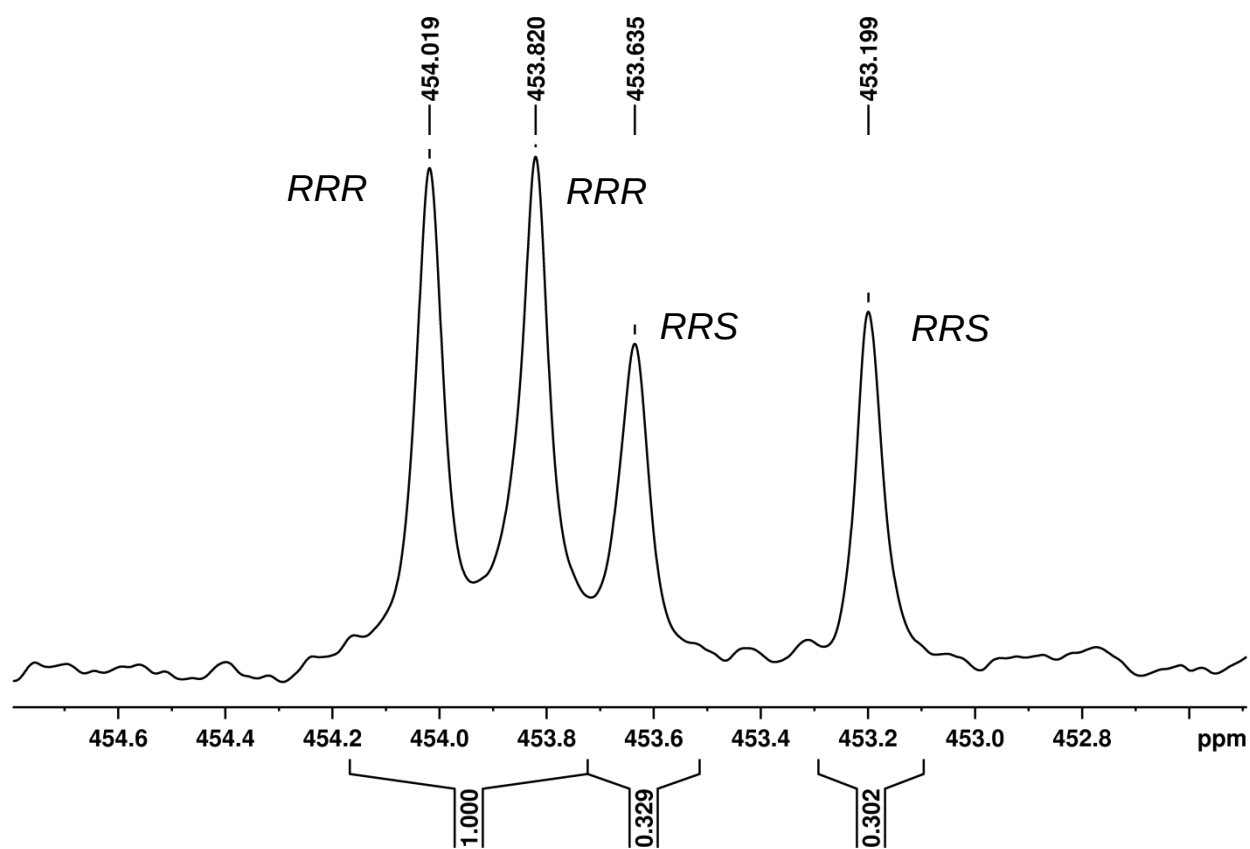


Figure S13. ^1H NMR of 4-methyl-2-n-octyl-1-dodecanol (**11**).

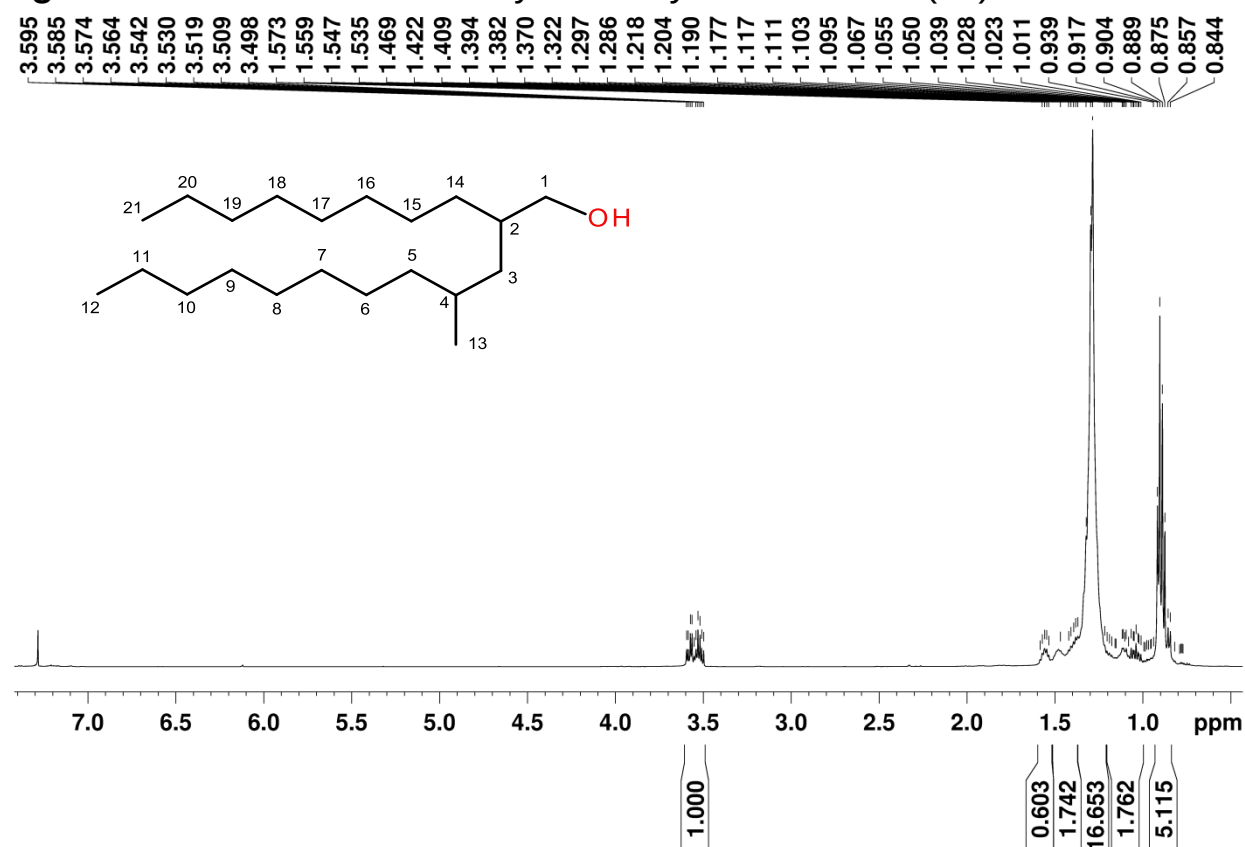


Figure S14. ^{13}C NMR of 4-methyl-2-n-octyl-1-dodecanol (**11**).

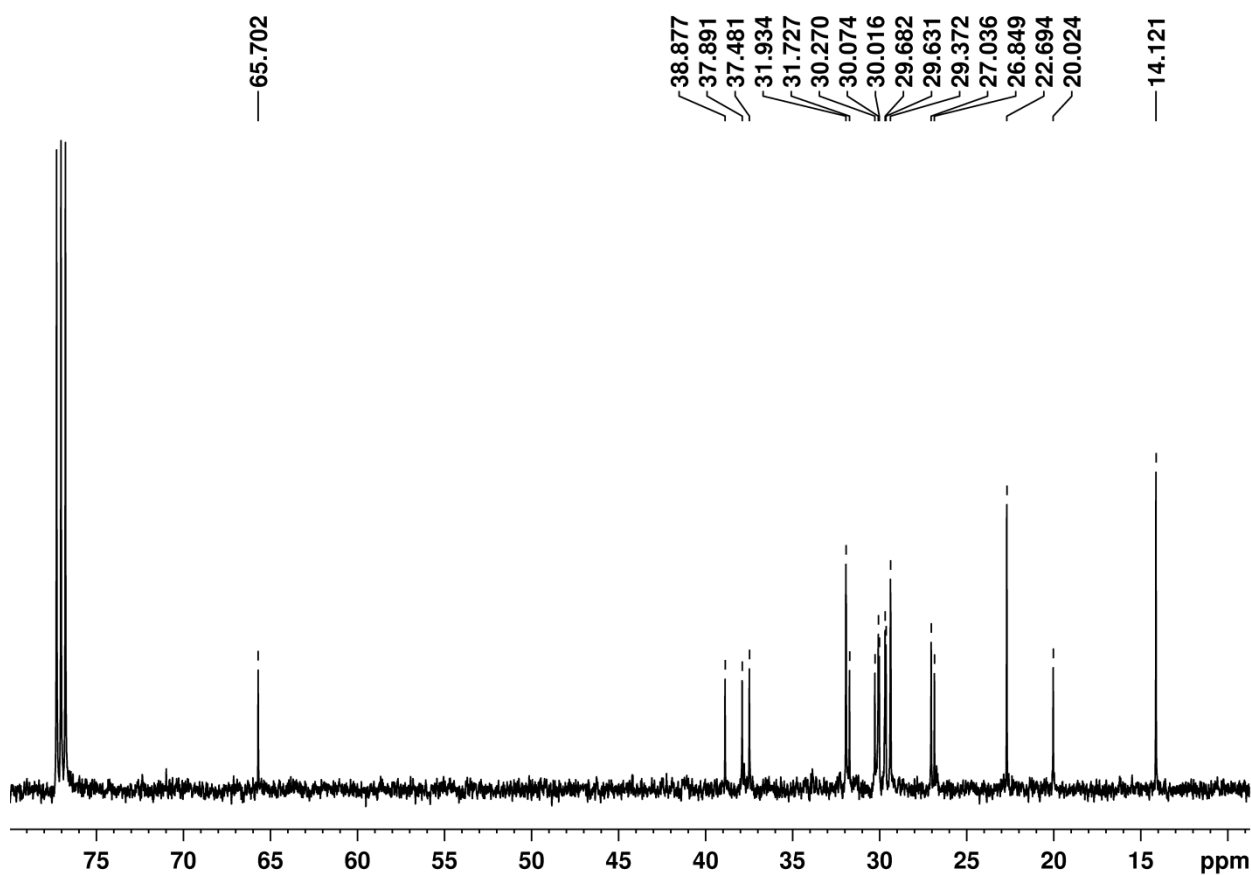
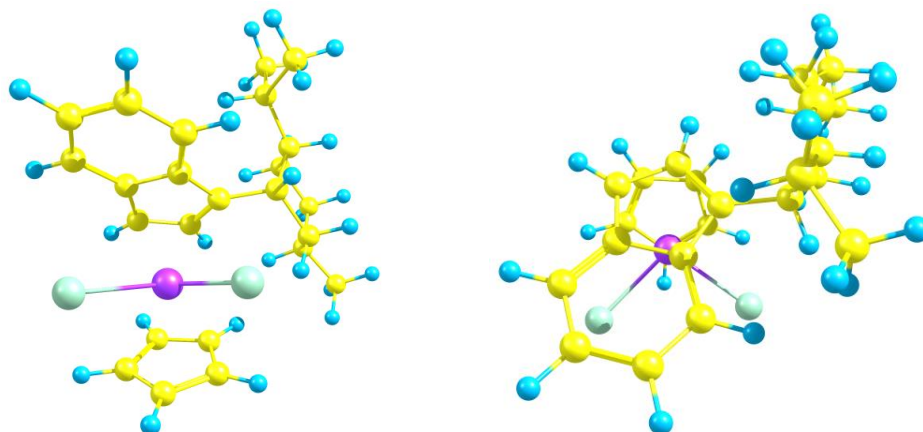


Table S1. Calculated relative Gibbs energies and conformer distribution vs solvents (M062-X, CPCM).

Complex	Solvent	Conformer	ΔG_{180}^0 , kcal/mol	P_{180} , %
1	d ₈ -toluene	1A	1.44	0.4
		1B	0.13	38.7
		1C	0.00	60.9
	CD ₂ Cl ₂	1A	0.93	2.4
		1B	0.18	33.8
		1C	0.00	63.7
	d ₈ -THF	1A	0.98	2.1
		1B	0.18	34.2
		1C	0.00	63.7
2	d ₈ -toluene	2A	0.00	92.5
		2B	0.52	7.1
		2C	1.44	0.4
	CD ₂ Cl ₂	2A	0.00	84.9
		2B	0.50	14.5
		2C	1.43	0.6
	d ₈ -THF	2A	0.00	85.7
		2B	0.73	13.8
		2C	1.58	0.5
3	d ₈ -toluene	3A	1.11	2.1
		3B	0.00	97.9
		3C	6.00	0.0
		3D	7.03	0.0
		3E	3.17	0.0
		3F	12.04	0.0
		3G	13.18	0.0
	CD ₂ Cl ₂	3A	0.00	55.8
		3B	0.07	44.2
		3C	5.58	0.0
		3D	6.52	0.0
		3E	2.66	0.0
		3F	11.47	0.0
		3G	12.24	0.0
	d ₈ -THF	3A	0.03	47.5
		3B	0.00	52.5
		3C	5.55	0.0
		3D	6.50	0.0
		3E	2.64	0.0
		3F	11.46	0.0
		3G	12.24	0.0

Cartesian coordinates of conformers (M062-X, 180 K)

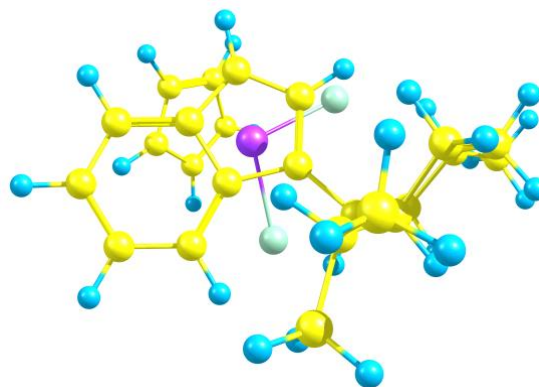
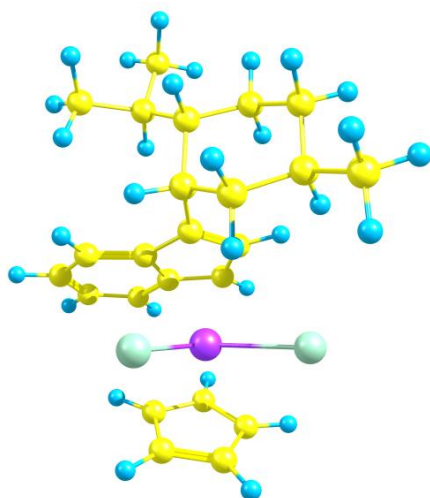
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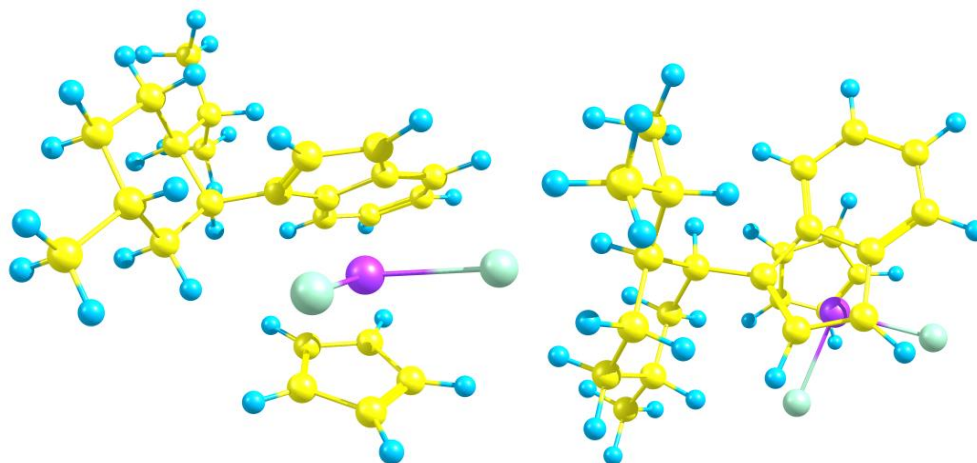
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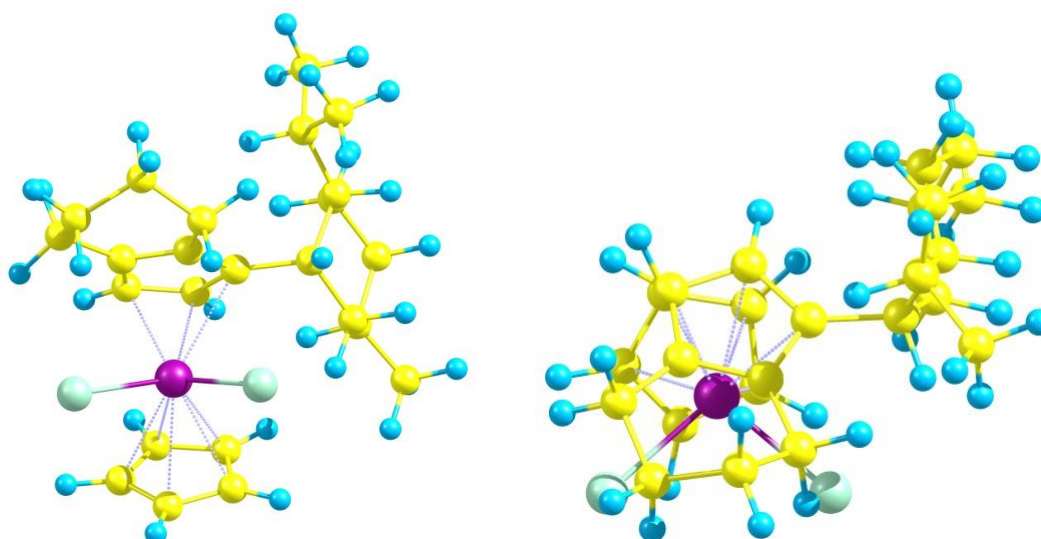
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1	1.642523000	-2.495075000	-0.856112000				
1	0.888240000	-1.905016000	1.422855000				
1	2.569932000	-1.797089000	1.965364000				
1	1.805597000	0.412780000	1.685070000				
1	4.071147000	-0.020389000	1.087219000				
1	4.840567000	-0.456320000	-1.218057000				
1	3.176925000	-0.498901000	-1.795457000				
6	3.567618000	1.733577000	-0.039472000				
1	2.679945000	2.081918000	-0.595740000				

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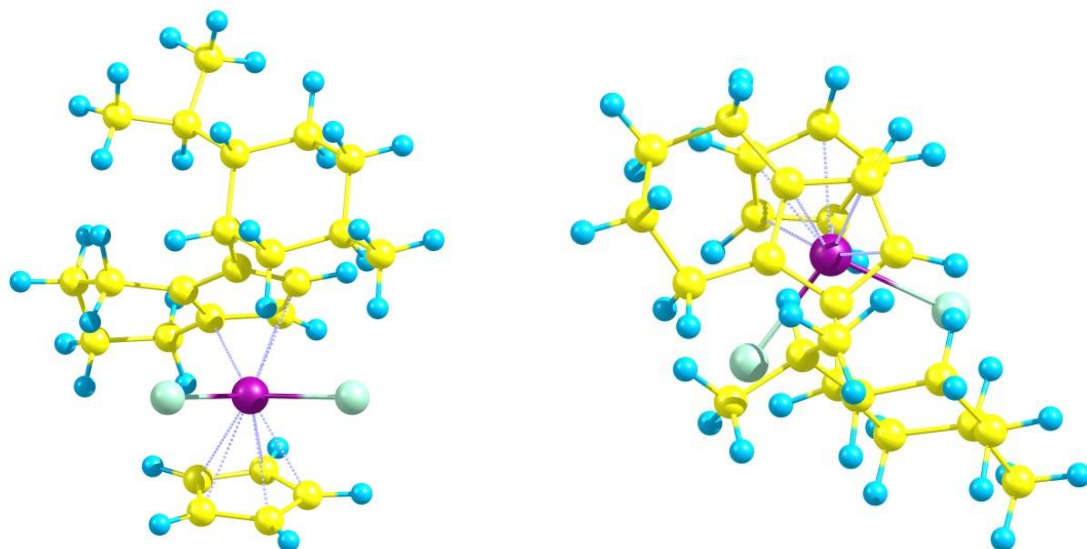


E= -1901.632492 Hartree

ZPE= 0.530647 Hartree

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1	-0.485637000	-3.197289000	-0.556912000	1	2.450252000	-2.063474000	1.842484000
6	-2.226410000	-2.179753000	-1.545501000	1	1.794345000	0.175415000	1.626573000
1	-1.909054000	-2.102370000	-2.582933000	1	4.034524000	-0.421006000	0.965053000
6	-2.255635000	-2.665919000	0.697822000	1	4.702229000	-0.738011000	-1.418573000
1	-1.950459000	-2.987068000	1.690289000	1	3.002742000	-0.708282000	-1.893108000
6	-3.457482000	-1.734130000	-1.017379000	6	3.666265000	1.441281000	-0.019289000
1	-4.241311000	-1.217062000	-1.564944000	1	2.766642000	1.925574000	-0.436808000
6	-3.470783000	-2.020934000	0.374072000	6	3.984468000	2.067537000	1.343126000
1	-4.261608000	-1.754875000	1.071112000	1	4.990081000	1.755806000	1.669191000
17	-1.117694000	-0.238155000	2.407572000	1	3.972473000	3.166842000	1.294112000
6	0.343643000	-0.305439000	-1.468234000	1	3.278074000	1.755055000	2.126177000
1	0.608241000	-1.254531000	-1.923152000	6	4.820479000	1.738036000	-0.978212000
6	0.850966000	0.218178000	-0.247296000	1	4.595791000	1.431798000	-2.009080000
6	-0.581591000	0.623429000	-2.023584000	1	5.031917000	2.817711000	-0.987438000
1	-1.115890000	0.511625000	-2.965762000	1	5.741753000	1.222505000	-0.660114000
6	0.229497000	1.503677000	-0.069376000	6	2.170935000	-4.252145000	0.330336000
6	0.437557000	2.520560000	1.024590000	1	1.169305000	-4.531949000	0.693085000
6	-0.615084000	1.762311000	-1.176549000	1	2.450211000	-4.947681000	-0.474933000
6	-1.285878000	3.085360000	-1.419164000	1	2.876733000	-4.398175000	1.163490000
6	-1.248283000	3.969228000	-0.168966000	17	-3.536374000	1.270328000	0.049644000
6	0.126046000	3.926635000	0.500822000				
1	-0.734687000	3.581874000	-2.236628000				
1	-2.318657000	2.941140000	-1.765765000				
1	1.468081000	2.471210000	1.396283000				
1	-0.213818000	2.290971000	1.883108000				
1	0.900675000	4.228256000	-0.226703000				
1	0.167917000	4.643962000	1.332687000				
1	-1.512486000	5.000438000	-0.443494000				
1	-2.008657000	3.616299000	0.545779000				
6	3.587315000	-2.426904000	-0.690399000				
6	2.209086000	-2.803744000	-0.148966000				
6	1.793393000	-1.853412000	0.979275000				
6	1.922944000	-0.349594000	0.667497000				
6	3.368142000	-0.065421000	0.154229000				
6	3.685678000	-0.946463000	-1.058301000				
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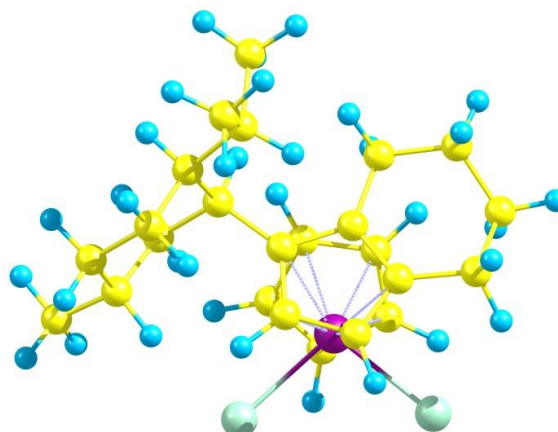
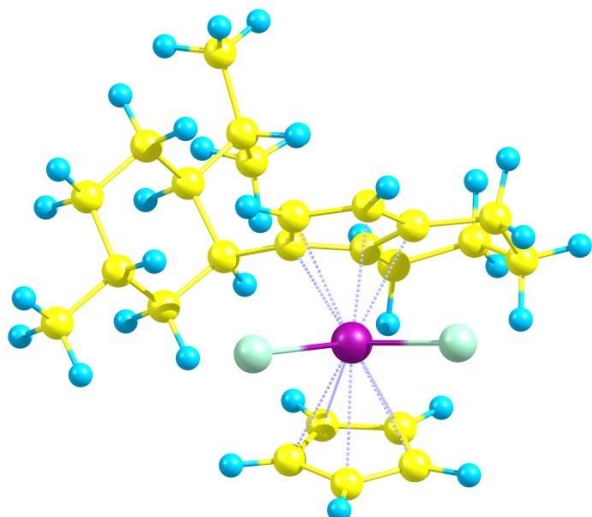
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ZPE= 0.530883 Hartree

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1	-3.501956000	0.712484000	-2.266001000	1	4.126326000	-0.168669000	0.940143000
6	-3.725691000	0.867089000	-0.038363000	1	4.775125000	-0.504162000	-1.436846000
1	-3.681122000	1.937821000	0.141101000	1	3.074546000	-0.557940000	-1.899261000
6	-3.767520000	-1.167387000	-1.094452000	6	3.619562000	1.646822000	-0.073757000
1	-3.703078000	-1.941674000	-1.854871000	1	2.680551000	2.061725000	-0.481413000
6	-3.940269000	-0.132938000	0.943199000	6	3.922042000	2.324161000	1.267793000
1	-4.020312000	0.034221000	2.013587000	1	4.952560000	2.087770000	1.578868000
6	-3.942983000	-1.387888000	0.299595000	1	3.835740000	3.419180000	1.196645000
1	-4.022087000	-2.358004000	0.783731000	1	3.255496000	1.981097000	2.072827000
17	-1.115056000	-2.824392000	-0.418980000	6	4.731339000	1.998533000	-1.063662000
6	0.454914000	-0.267430000	-1.474711000	1	4.507935000	1.650703000	-2.081448000
1	0.788648000	-1.186997000	-1.943435000	1	4.869516000	3.089529000	-1.103088000
6	0.893720000	0.251239000	-0.226114000	1	5.690949000	1.553419000	-0.753036000
6	-0.556545000	0.575691000	-2.002294000	6	2.437874000	-4.114209000	0.394202000
1	-1.060672000	0.440290000	-2.957360000	1	1.449835000	-4.425819000	0.763818000
6	0.153620000	1.463954000	-0.011172000	1	2.735741000	-4.802483000	-0.411048000
6	0.311634000	2.479590000	1.092160000	1	3.162725000	-4.222152000	1.217833000
6	-0.728664000	1.668096000	-1.101979000	17	-1.135483000	-0.357614000	2.393363000
6	-1.505737000	2.942687000	-1.303989000				
6	-1.524999000	3.795157000	-0.030693000				
6	-0.136604000	3.861501000	0.606271000				
1	-1.003093000	3.511836000	-2.104598000				
1	-2.525753000	2.746981000	-1.669016000				
1	1.359720000	2.515840000	1.413281000				
1	-0.272172000	2.181043000	1.977180000				
1	0.585058000	4.242906000	-0.137229000				
1	-0.136203000	4.567488000	1.448482000				
1	-1.893817000	4.802733000	-0.269716000				
1	-2.223675000	3.364036000	0.707224000				
6	3.742790000	-2.236642000	-0.682491000				
6	2.398799000	-2.671865000	-0.099650000				
6	1.977932000	-1.733289000	1.033796000				
6	2.009708000	-0.233575000	0.684076000				
6	3.423747000	0.127938000	0.136430000				
6	3.771669000	-0.756013000	-1.066059000				
1	3.995413000	-2.863093000	-1.552830000				
1	4.528951000	-2.418049000	0.074401000				
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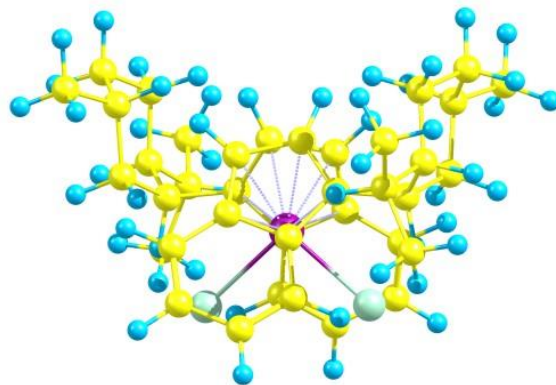
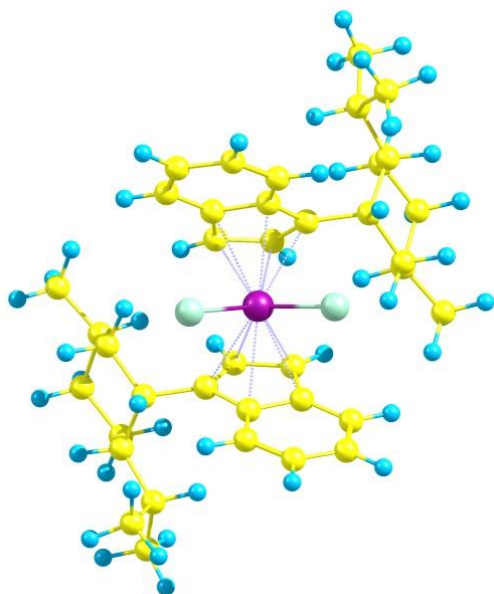
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E= -1901.629468 Hartree
ZPE= 0.530853 Hartree

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6	-1.225621000	-0.449942000	2.315365000	1	4.065254000	-0.100079000	1.061152000
1	-0.235638000	-0.180525000	2.679151000	1	4.811702000	-0.427681000	-1.275132000
6	-1.677278000	-1.756491000	2.020753000	1	3.138231000	-0.463211000	-1.825384000
1	-1.091230000	-2.670168000	2.081117000	6	3.574599000	1.714733000	0.034174000
6	-2.302215000	0.448157000	2.055849000	1	2.650892000	2.114491000	-0.421076000
1	-2.292086000	1.524590000	2.202915000	6	3.800716000	2.397421000	1.387917000
6	-3.020338000	-1.671198000	1.571063000	1	4.811411000	2.162039000	1.758786000
1	-3.626134000	-2.501550000	1.216506000	1	3.720726000	3.491972000	1.305599000
6	-3.410058000	-0.314873000	1.617707000	1	3.087749000	2.062341000	2.155926000
1	-4.371739000	0.082181000	1.305524000	6	4.730914000	2.079177000	-0.898224000
17	-3.556593000	0.089058000	-1.488440000	1	4.562739000	1.729888000	-1.925837000
6	0.539359000	-0.152142000	-1.517838000	1	4.858015000	3.171516000	-0.931091000
1	0.927468000	-1.041553000	-2.001440000	1	5.678592000	1.645069000	-0.539127000
6	0.864066000	0.311400000	-0.207374000	6	2.369463000	-4.053760000	0.378404000
6	-0.438980000	0.694068000	-2.081499000	1	1.363563000	-4.366862000	0.696685000
1	-0.916121000	0.563546000	-3.050295000	1	2.691045000	-4.725224000	-0.431247000
6	0.082803000	1.500776000	0.001441000	1	3.059184000	-4.191109000	1.227416000
6	0.169650000	2.492059000	1.136300000	17	-1.192697000	-2.739259000	-0.990335000
6	-0.720137000	1.728114000	-1.146365000				
6	-1.597847000	2.935728000	-1.323480000				
6	-1.831469000	3.631351000	0.018184000				
6	-0.508699000	3.821121000	0.765101000				
1	-1.083996000	3.631892000	-2.008338000				
1	-2.546026000	2.653664000	-1.801795000				
1	1.227437000	2.681673000	1.364751000				
1	-0.263330000	2.086857000	2.064378000				
1	0.172019000	4.395437000	0.113567000				
1	-0.656896000	4.421619000	1.673899000				
1	-2.314089000	4.605043000	-0.146181000				
1	-2.532031000	3.031540000	0.624300000				
6	3.733853000	-2.165100000	-0.603360000				
6	2.364666000	-2.600508000	-0.083556000				
6	1.917675000	-1.680796000	1.055203000				
6	1.958027000	-0.176065000	0.729110000				
6	3.388922000	0.193661000	0.233725000				
6	3.789081000	-0.678771000	-0.960940000				
1	4.016347000	-2.778439000	-1.473310000				
1	4.486507000	-2.366679000	0.181969000				
1	1.633188000	-2.526178000	-0.902656000				
1	0.909455000	-1.975252000	1.383378000				
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E= -5875.347511 Hartree
ZPE= 0.879605 Hartree

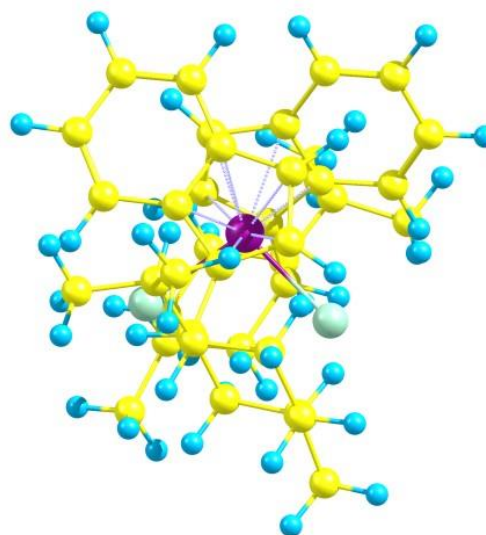
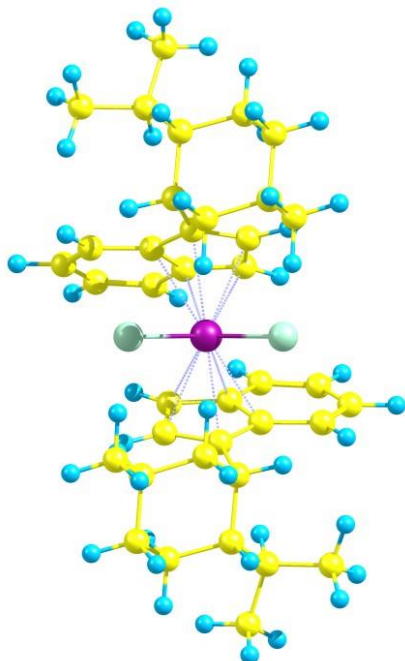
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6	-2.337598000	0.232611000	0.214260000	1	3.753377000	-0.175568000	2.670589000
6	-3.417627000	-0.852941000	0.093169000	1	5.479822000	1.247325000	0.578144000
6	-0.671661000	1.678178000	1.009434000	1	4.978524000	2.648675000	2.523336000
1	0.030181000	2.157745000	1.689017000	1	4.029068000	2.020607000	3.882784000
6	-2.148823000	1.318505000	-0.751116000	1	2.027694000	1.846356000	2.480859000
6	-2.758791000	1.596502000	-2.027604000	1	2.896253000	-2.988466000	-3.641994000
6	-1.170945000	2.238324000	-0.224411000	1	1.290289000	-4.618303000	-2.671847000
6	-0.865723000	3.453440000	-0.931297000	1	0.136880000	-4.153895000	-0.514304000
17	-1.106911000	-1.370639000	-2.230367000	1	3.467066000	-0.883606000	-2.455581000
6	-1.499661000	3.697956000	-2.118660000	17	1.106940000	1.370706000	-2.230355000
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1	-3.466706000	0.883223000	-2.455889000	1	5.462097000	0.245774000	2.883264000
1	-2.895955000	2.988081000	-3.642288000	1	2.000511000	2.508129000	0.086250000
1	-1.290408000	4.618197000	-2.671933000	6	-5.327129000	0.897975000	0.320310000
1	-3.634782000	-0.933333000	-0.982202000	1	-4.492827000	1.601317000	0.188418000
6	-4.749075000	-0.463425000	0.833726000	6	-6.023754000	0.687311000	-1.049266000
6	-4.537110000	-0.531288000	2.369053000	1	-5.381351000	0.137863000	-1.744008000
6	-4.157443000	-1.970762000	2.792912000	1	-6.947142000	0.113127000	-0.912630000
6	-2.962265000	-2.269350000	0.559132000	1	-6.280200000	1.651582000	-1.501555000
6	-2.859323000	-2.451420000	2.097167000	6	-6.340377000	1.537472000	1.302962000
1	-3.701527000	-2.989122000	0.181770000	1	-6.790325000	2.423543000	0.841240000
1	-3.753002000	0.174982000	2.671018000	1	-7.143096000	0.831467000	1.543989000
1	-5.480050000	-1.246895000	0.578364000	1	-5.852987000	1.846281000	2.233011000
1	-4.978543000	-2.649049000	2.523032000	6	5.327449000	-0.897482000	0.319358000
1	-4.028811000	-2.021552000	3.882550000	1	4.493318000	-1.600985000	0.187265000
1	-2.027610000	-1.847066000	2.480254000	6	6.023863000	-0.686063000	-1.050207000
6	1.462068000	-0.517013000	1.302066000	1	6.280544000	-1.650074000	-1.502919000
1	1.367494000	0.069810000	2.213957000	1	5.381224000	-0.136510000	-1.744653000
6	2.337541000	-0.232696000	0.214267000	1	6.947097000	-0.111662000	-0.913441000
6	3.417426000	0.853007000	0.093192000	6	6.340957000	-1.537125000	1.301643000
6	0.671451000	-1.678141000	1.009371000	1	5.853748000	-1.846337000	2.231653000
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6	1.170788000	-2.238328000	-0.224421000	1	3.381492000	4.571527000	2.080234000
6	0.865534000	-3.453446000	-0.931301000	1	1.635789000	4.261942000	1.963037000
6	1.499578000	-3.698067000	-2.118578000	1	2.471958000	4.066988000	3.522086000

S18

6	2.437236000	-2.757590000	-2.676737000
1	3.634309000	0.933753000	-0.982210000
6	4.749104000	0.463571000	0.833369000
6	4.537359000	0.530900000	2.368747000
6	4.157554000	1.970190000	2.793112000

6	-2.566863000	-3.933285000	2.437708000
1	-2.471843000	-4.067898000	3.521059000
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E= -5875.350101 Hartree
ZPE= 0.879704 Hartree

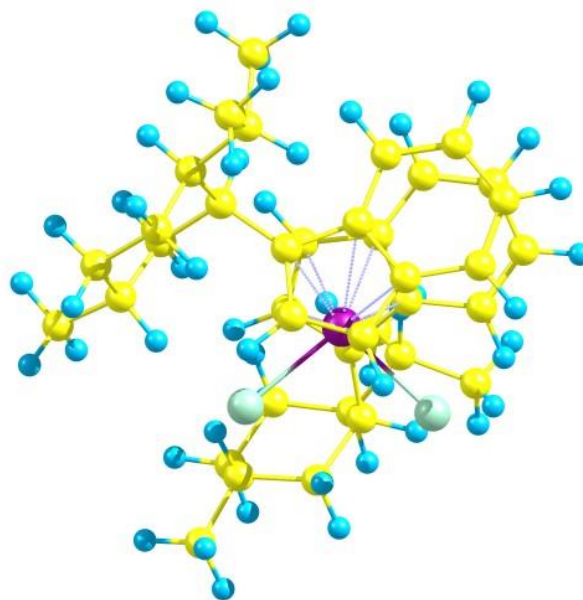
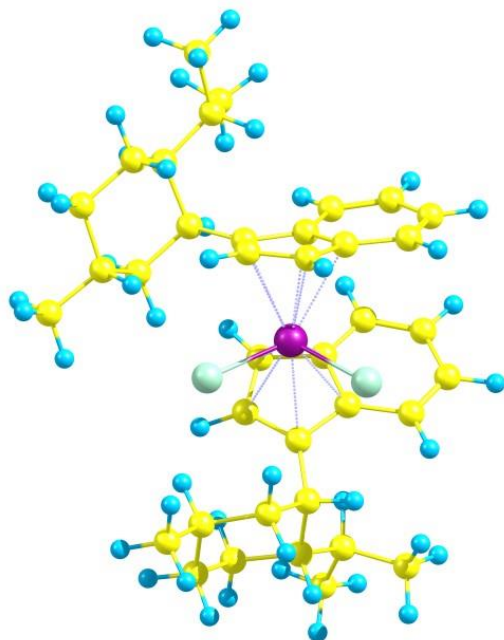
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6	-2.497319000	0.170560000	0.044777000
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6	-1.454693000	1.985618000	1.100230000
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6	-2.192784000	1.189880000	-0.960235000
6	-2.409877000	1.232047000	-2.385182000
6	-1.593474000	2.326369000	-0.302849000
6	-1.311769000	3.519605000	-1.059179000
17	0.260818000	-1.175847000	1.784964000
6	-1.578542000	3.534363000	-2.401144000
6	-2.109216000	2.376809000	-3.072083000
1	-0.918907000	4.402771000	-0.551169000
1	-2.816242000	0.354962000	-2.894634000
1	-2.281951000	2.429401000	-4.150499000
1	-1.388977000	4.438507000	-2.986722000
1	-3.218838000	-1.252798000	-1.342421000
6	-4.818302000	-0.951262000	0.107949000
6	-4.998155000	-0.936403000	1.649164000
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1	5.049866000	-3.089113000	-1.890011000
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1	-6.027065000	0.824999000	-2.664041000
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1	4.770651000	1.119900000	0.563287000

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6	2.410094000	1.231985000	2.385196000
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1	7.505576000	-0.131409000	-0.075588000
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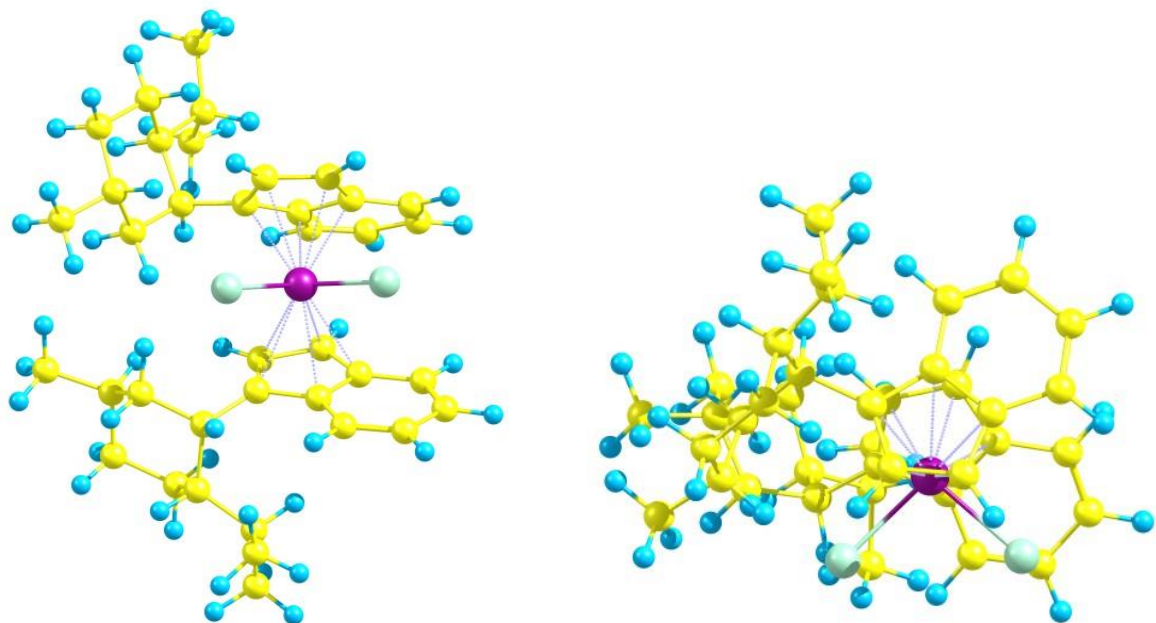
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6	1.819208000	-1.709461000	1.603959000
6	1.560434000	-3.074140000	1.987551000
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1	-2.339621000	-4.815558000	0.268570000
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1	0.511754000	-2.963728000	-2.406648000
1	-3.227410000	-2.601603000	0.961592000
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6	2.709029000	3.268218000	-0.466459000	6	2.093257000	4.597065000	-0.966369000
1	2.594864000	2.390197000	-2.444438000	1	1.000566000	4.519816000	-0.996495000
1	4.591874000	1.705237000	1.012095000	1	2.364905000	5.419965000	-0.295953000
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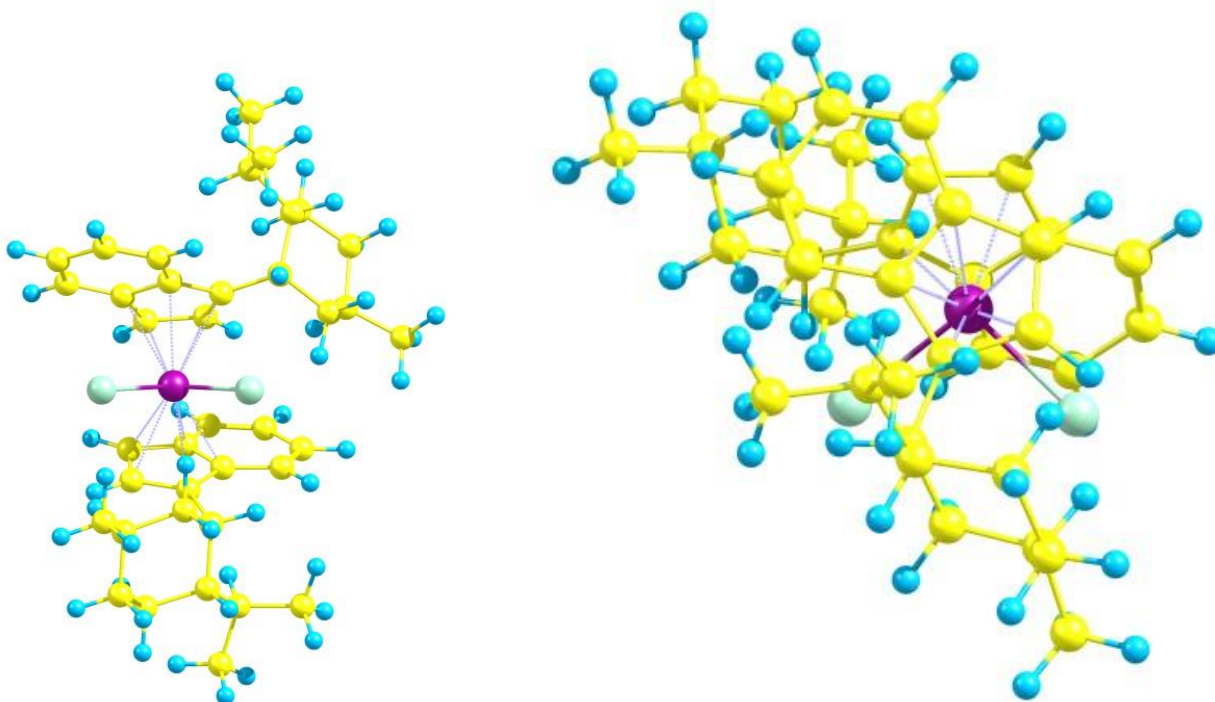


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6	-2.662695000	1.060412000	0.431460000	6	1.096386000	3.503622000	0.862880000
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6	-1.498600000	-3.906958000	0.592525000	1	0.386499000	2.802027000	1.319708000
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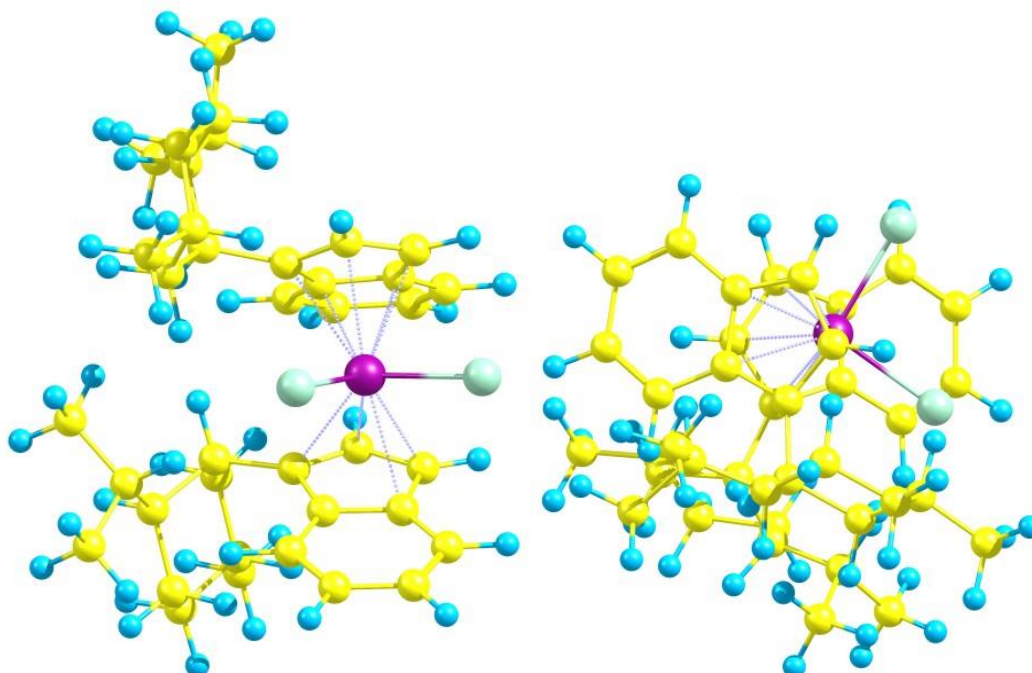
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6	-4.121472000	-2.301398000	-0.977427000	1	5.674531000	-2.391462000	-2.050807000
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6	2.560796000	-2.634493000	-0.575206000
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6	1.792908000	-3.146424000	2.146717000
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6	4.559634000	0.732613000	-0.932224000
6	4.869352000	1.747322000	0.199609000
6	4.368578000	3.152132000	-0.211148000

6	-6.174769000	2.420970000	0.514737000
1	-6.195682000	3.476931000	0.806934000
1	-7.000841000	2.241641000	-0.182599000
1	-6.334768000	1.814263000	1.411439000
6	-4.546527000	3.131202000	-1.273219000
1	-3.647061000	2.880451000	-1.843325000
1	-5.393368000	3.157023000	-1.968261000
1	-4.419994000	4.132101000	-0.846003000
6	-4.197956000	-3.582734000	-1.841904000
1	-4.770734000	-4.361136000	-1.325399000
1	-4.686116000	-3.369695000	-2.799660000
1	-3.189643000	-3.963514000	-2.039657000

3F



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ZPE= 0.880897 Hartree

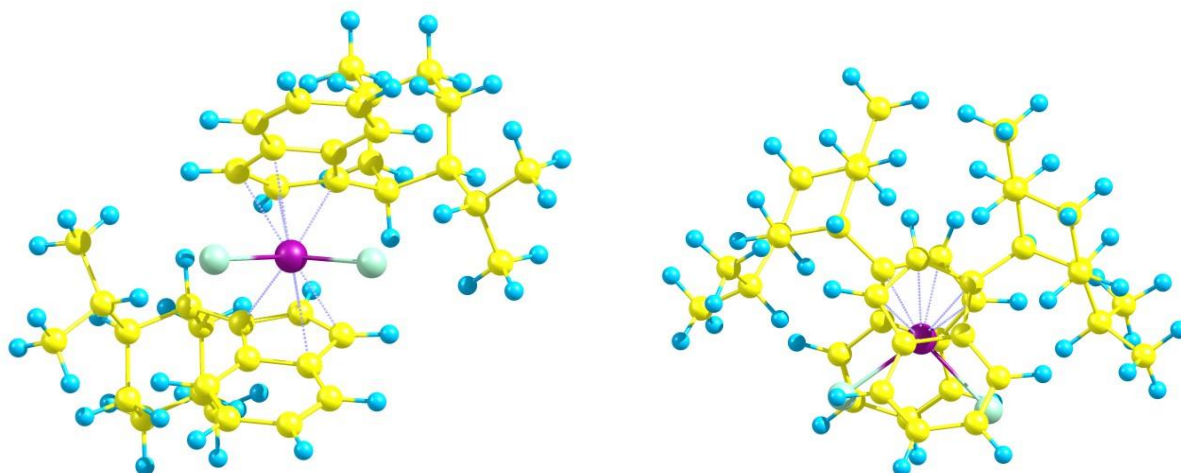
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6	1.961223000	0.153410000	0.332853000
6	2.471058000	-0.843122000	-0.724012000
6	1.898038000	2.004309000	1.773734000
1	2.032105000	3.012739000	2.163441000
6	1.377121000	-0.258982000	1.595592000
6	1.034765000	-1.560226000	2.124068000
6	1.313492000	0.892673000	2.477972000
6	0.845577000	0.738078000	3.837075000
17	-0.013314000	1.886536000	-1.778320000
6	0.533617000	-0.511834000	4.289098000
6	0.645936000	-1.669994000	3.429693000
1	0.786644000	1.616295000	4.486972000
1	1.121840000	-2.444359000	1.489299000
1	0.411671000	-2.652851000	3.848713000
1	0.204561000	-0.658292000	5.321482000
1	1.912527000	-1.776389000	-0.556511000
6	4.000279000	-1.170739000	-0.523592000
6	4.864753000	0.060396000	-0.904043000
6	4.622560000	0.467719000	-2.378625000

6	-2.001420000	-2.836524000	0.945529000
6	-3.541205000	-2.786716000	1.126850000
1	-1.708388000	-3.845713000	0.625743000
1	-4.052553000	-1.140933000	-1.149298000
1	-1.996116000	-3.361640000	-1.536774000
1	-4.040712000	-4.143151000	-0.492735000
1	-5.330359000	-2.990740000	-0.100867000
1	-3.814800000	-1.765985000	1.433636000
1	-4.093557000	2.406993000	-2.835237000
1	-4.387845000	4.140518000	-1.071837000
1	-3.492225000	3.763219000	1.231186000
1	-2.926463000	0.303027000	-2.385558000
17	-0.384583000	3.800883000	1.139375000
1	1.196567000	-0.190194000	-2.373576000
1	5.925511000	-0.187084000	-0.781120000
1	-4.220204000	-2.479067000	-2.301332000
1	-1.504618000	-2.638273000	1.901686000
6	4.300456000	-1.749584000	0.899921000
1	3.717680000	-1.179133000	1.636668000
6	3.868615000	-3.238194000	0.963712000
1	2.853078000	-3.378324000	0.581166000
1	4.546592000	-3.848203000	0.356067000

S24

6	2.250569000	-0.438879000	-2.210117000	1	3.905041000	-3.605469000	1.995267000
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1	2.495727000	-1.315667000	-2.824524000	1	5.957923000	-2.162352000	2.250189000
1	4.639544000	0.897269000	-0.232182000	1	6.428374000	-2.124875000	0.538250000
1	4.233943000	-1.961592000	-1.253972000	1	6.107352000	-0.606337000	1.409746000
1	4.964692000	-0.349053000	-3.029315000	6	2.906629000	0.999698000	-4.189889000
1	5.220581000	1.356295000	-2.621783000	1	3.177172000	0.110150000	-4.770119000
1	2.811308000	1.650622000	-2.142939000	1	1.853771000	1.236586000	-4.380101000
6	-1.700705000	-0.036289000	1.742540000	1	3.521520000	1.838857000	-4.533824000
1	-1.277599000	-0.686453000	2.505160000	6	-3.997349000	-3.775940000	2.225563000
6	-1.828200000	-0.374366000	0.347764000	1	-3.519772000	-3.537366000	3.182501000
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6	-2.154882000	1.285164000	1.983063000	1	-3.727242000	-4.801621000	1.949750000
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6	-3.046680000	1.032066000	-1.588502000	6	-0.262980000	-2.514153000	-3.097508000
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6	-3.866397000	3.213309000	-0.818854000	1	0.402588000	-2.598544000	-2.232626000
6	-3.695121000	2.211133000	-1.835638000	6	-2.447209000	-1.653921000	-3.996028000
1	-0.442006000	-1.925634000	-0.263396000	1	-3.333059000	-1.030106000	-3.839390000
6	-2.202477000	-2.281591000	-1.482572000	1	-1.899580000	-1.262152000	-4.860429000
6	-3.747923000	-2.171196000	-1.360952000	1	-2.780819000	-2.670640000	-4.232270000
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3G



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ZPE= 0.880836 Hartree

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6	-1.896865000	0.584275000	-0.517900000	1	4.731294000	0.402708000	0.908991000
6	-2.577626000	1.540993000	0.499181000	1	4.302363000	2.000478000	-1.661334000
6	-0.347399000	0.042901000	-2.203557000	1	5.462695000	3.270984000	0.095501000
1	0.481826000	0.109030000	-2.906616000	1	5.777327000	2.511849000	1.667742000
6	-2.297912000	-0.688035000	-1.127951000	1	3.327232000	2.285737000	2.068669000
6	-3.391291000	-1.612811000	-0.925632000	1	4.321259000	-3.425284000	1.547817000
6	-1.328946000	-1.015516000	-2.151856000	1	2.634384000	-3.963282000	3.298724000
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17	1.321068000	-2.520906000	-1.214562000	1	4.133714000	-1.426822000	0.151640000
6	-2.512286000	-3.046928000	-2.714119000	17	-1.321246000	-2.520972000	1.214545000
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1	-4.133468000	-1.426919000	-0.152617000	1	6.012722000	0.875271000	-0.222165000
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6	1.329657000	-1.016494000	2.151697000	1	4.228177000	0.959763000	-3.859409000
6	1.448024000	-2.222028000	2.932021000	1	3.293369000	-0.546981000	-3.996852000
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