

Amide-linked Heterobi- and Heterotermetalloenes with Very Low HOMO-LUMO Gaps

Hannah Huesmann,^a Christoph Förster,^a Daniel Siebler,^a Teuta Gasi,^b and Katja Heinze^{a,}*

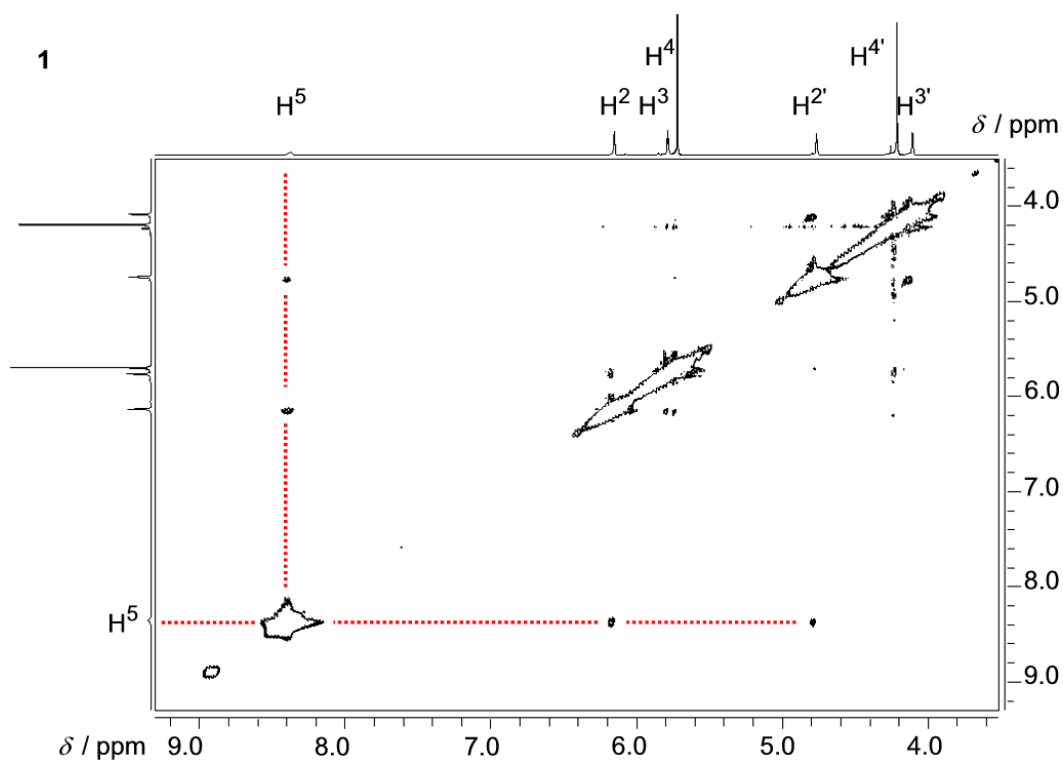
^a Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg-University of Mainz,
Duesbergweg 10-14, 55128 Mainz, Germany

^b Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg-University of Mainz,
Staudingerweg 9, 55128 Mainz, Germany

* Corresponding authors. Fax. int + 49-6131-3927277. E-mail: katja.heinze@uni-mainz.de.

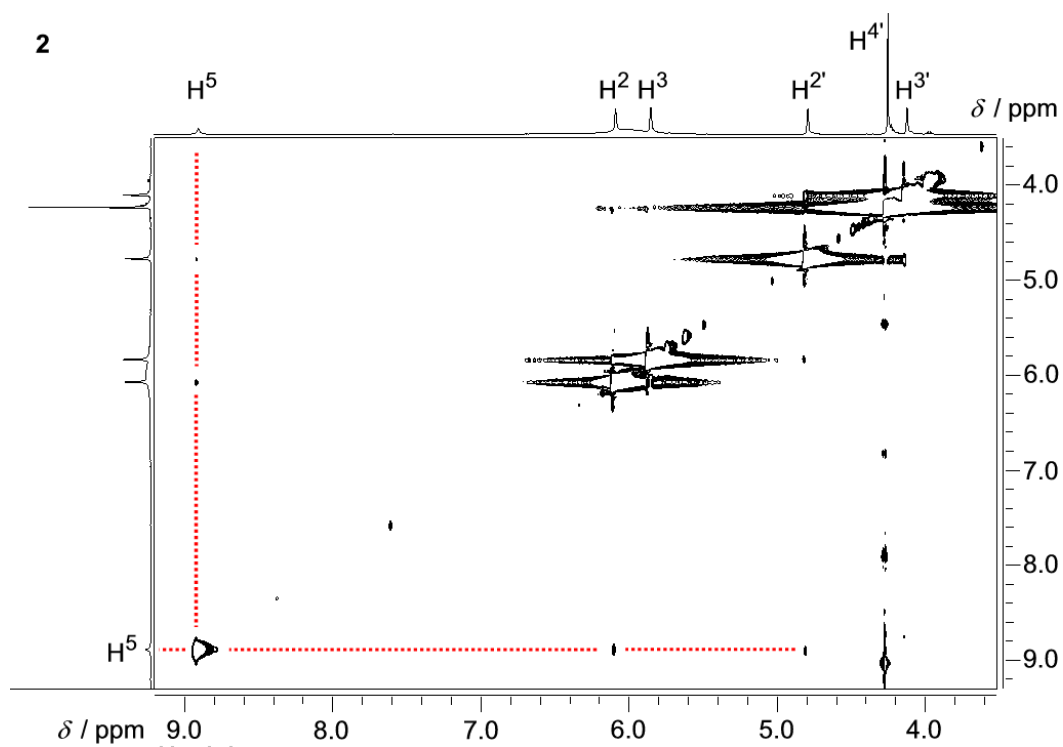
Supporting Information

Fig. S1 NOESY of **1** in CD₃CN.



The red dotted lines indicate correlations between H⁵ and H², H^{2'}.

Fig. S2 NOESY of **2** in CD₃CN.



The red dotted lines indicate correlations between H⁵ and H², H^{2'}.

Fig. S3 Molecular structure of **1-ox** in the crystal showing the supramolecular arrangement.

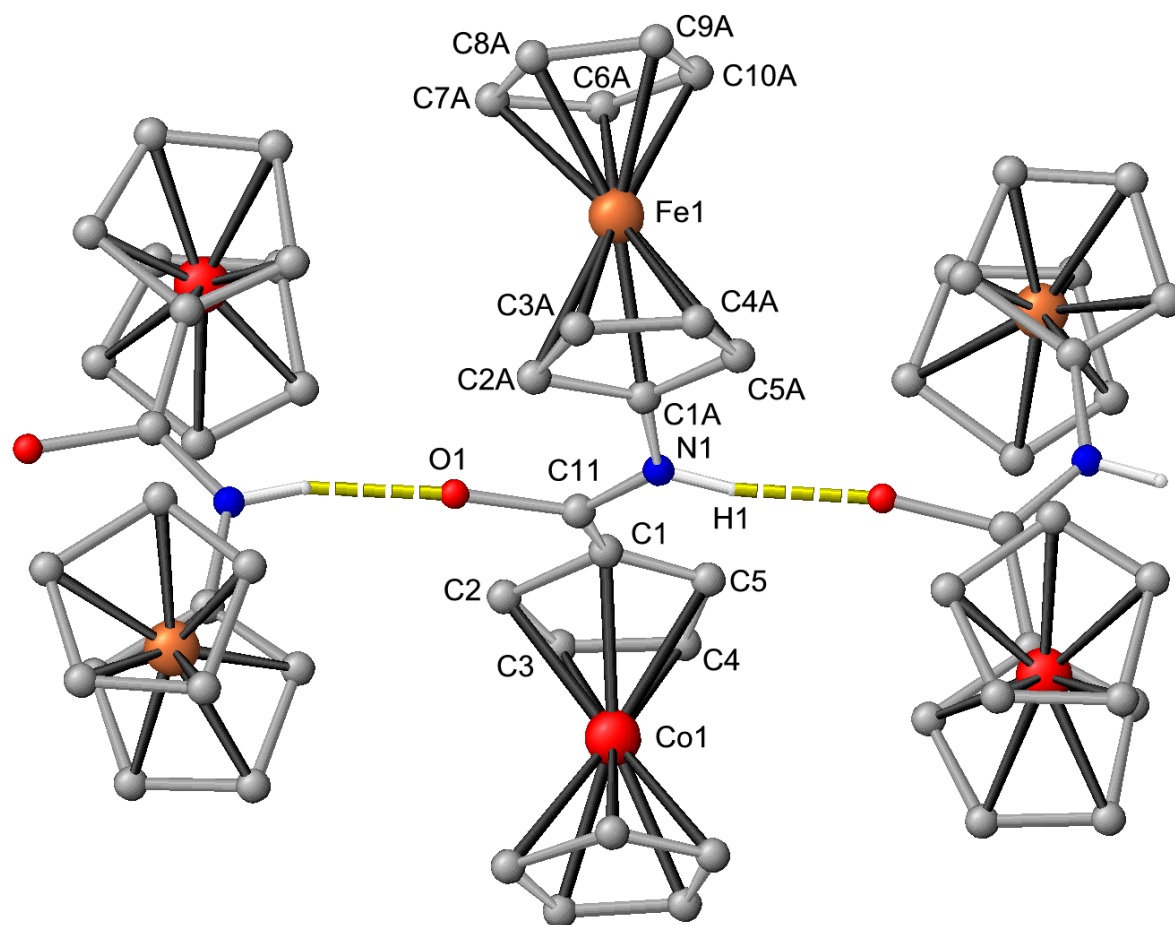


Fig. S4 Kamlet-Taft correlation for **1**.

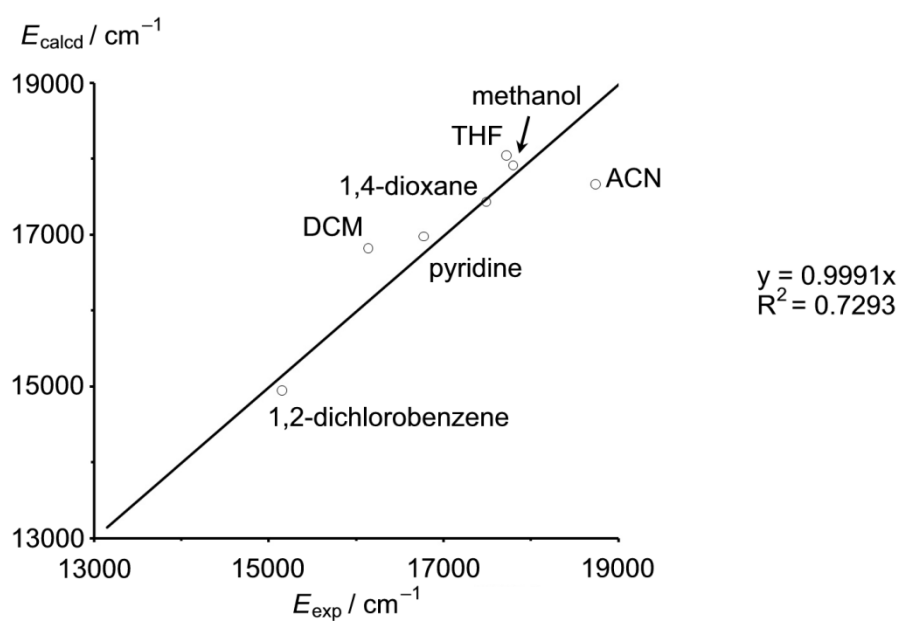


Fig. S5 Kamlet-Taft correlation for **2**.

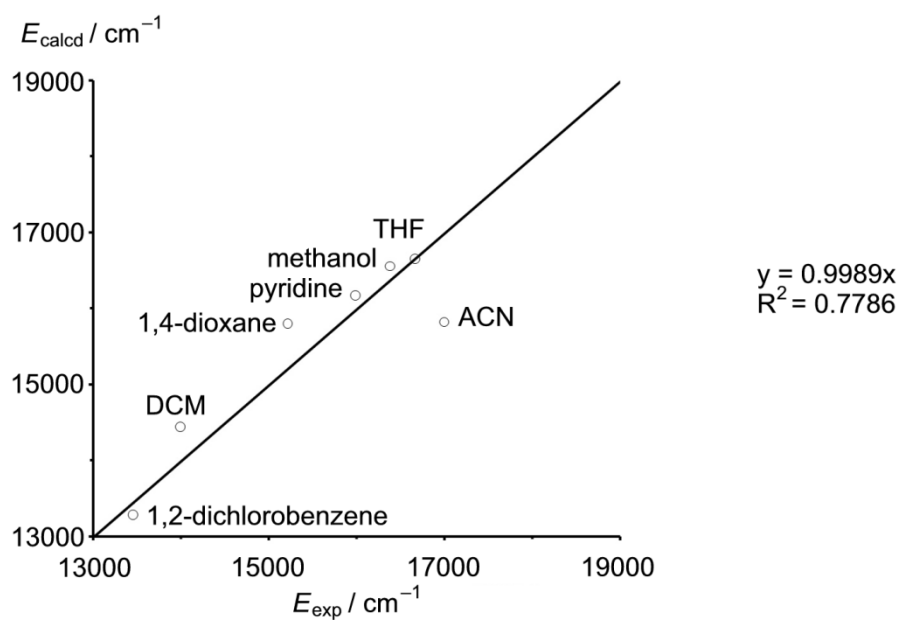


Fig. S6

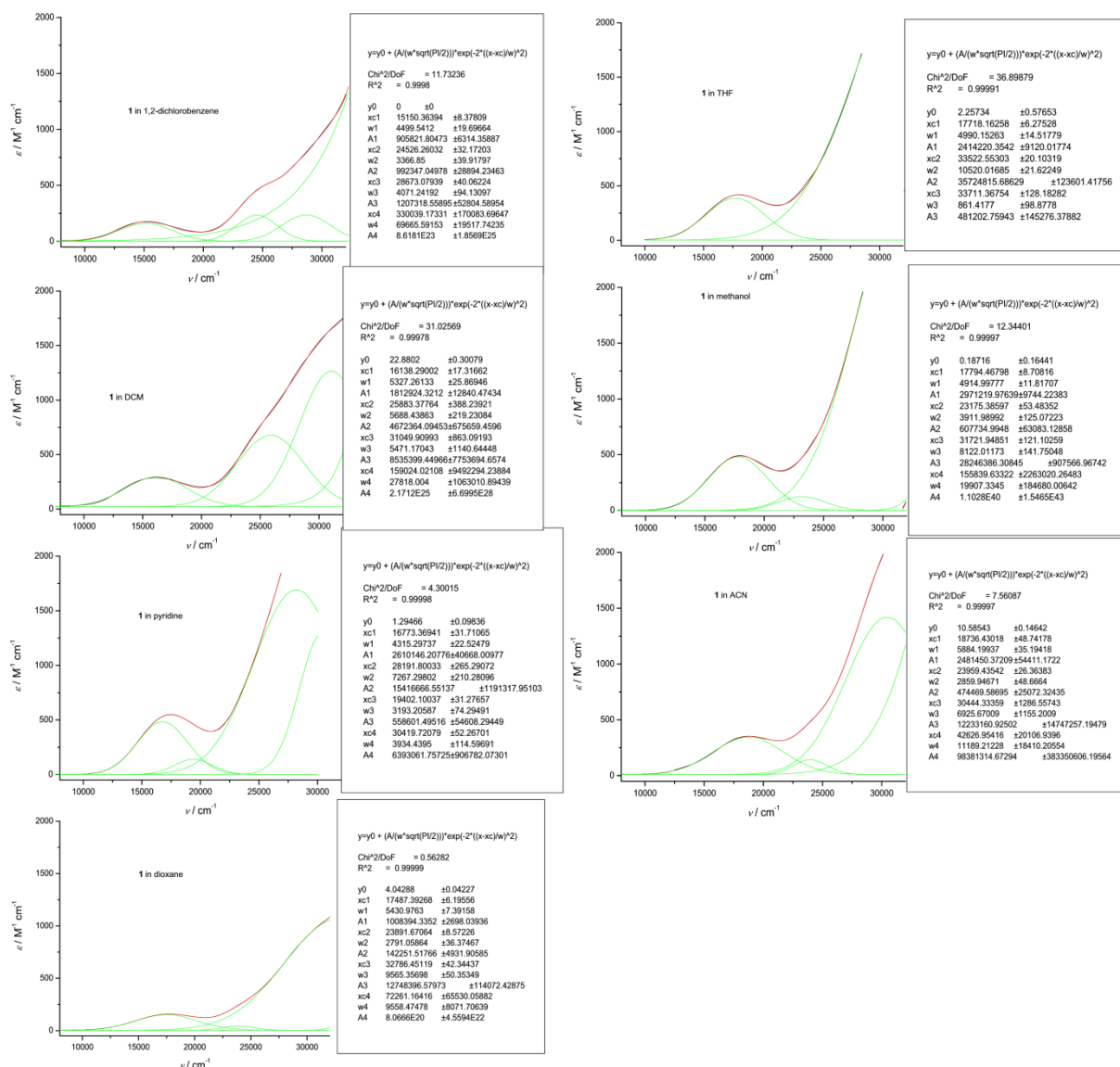
Gaussian deconvolution of the MM'CT bands of **1** in different solvents.

Fig. S7 Gaussian deconvolution of the MM'CT bands of **2** in different solvents.

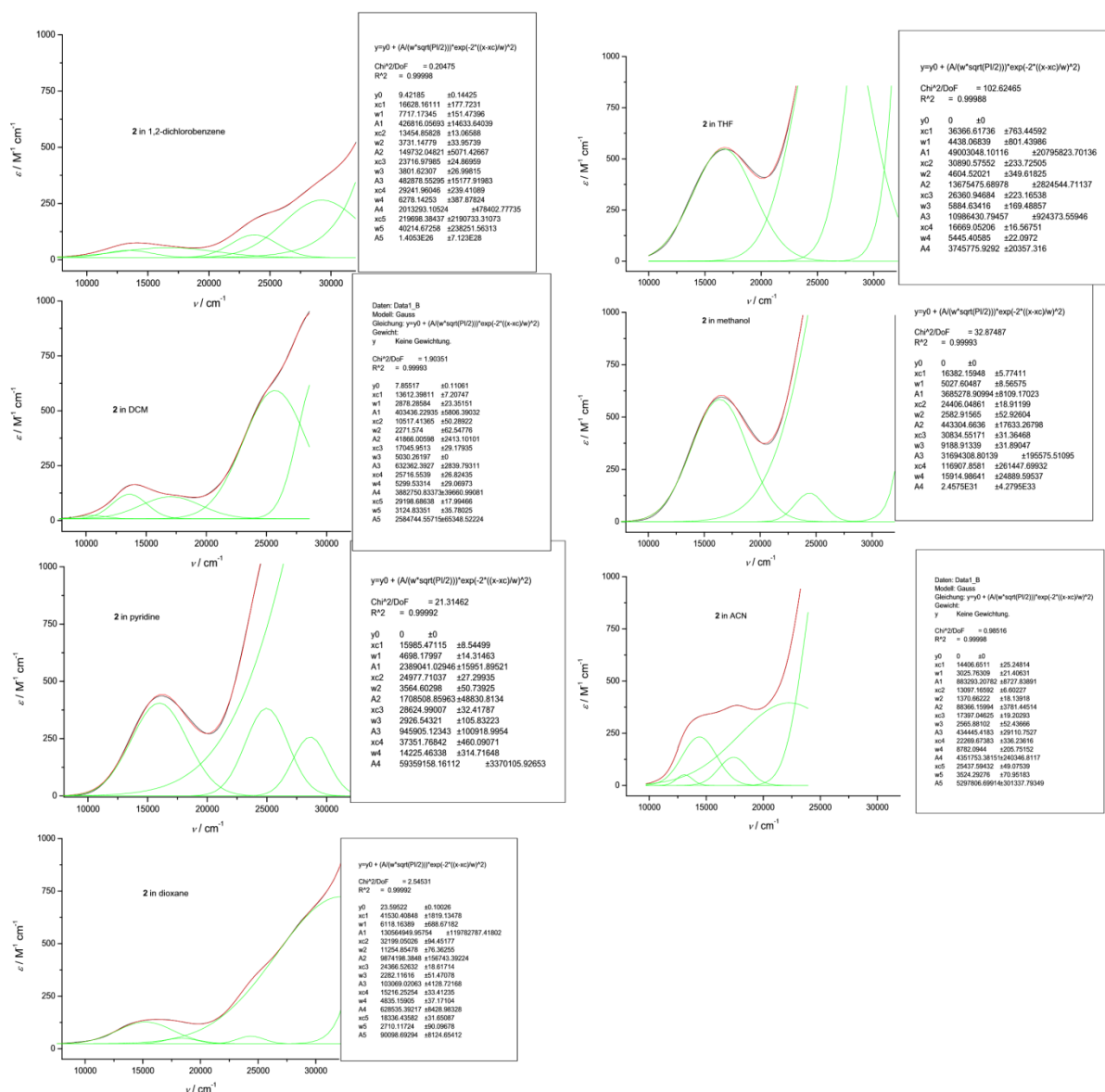


Fig. S8 Plot of absorption maxima of **1** and **2** vs. solvent function $1/\eta^2 - 1/D_S$.

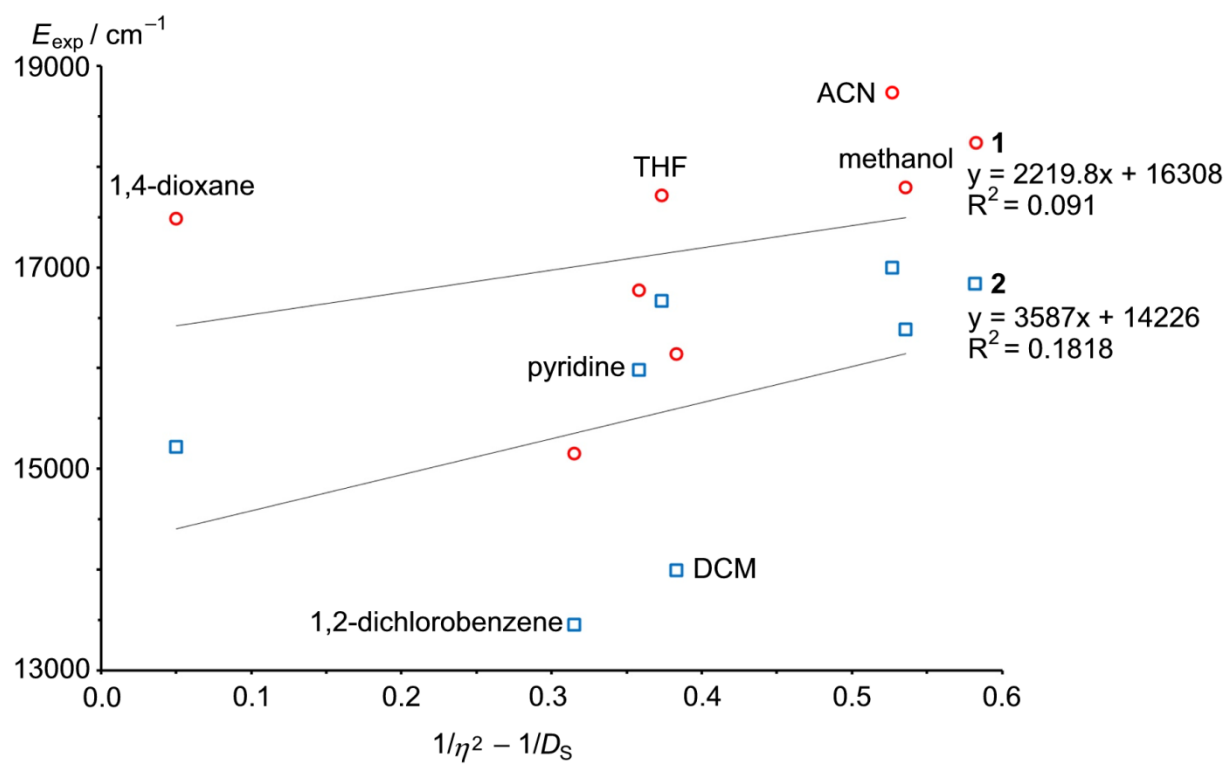
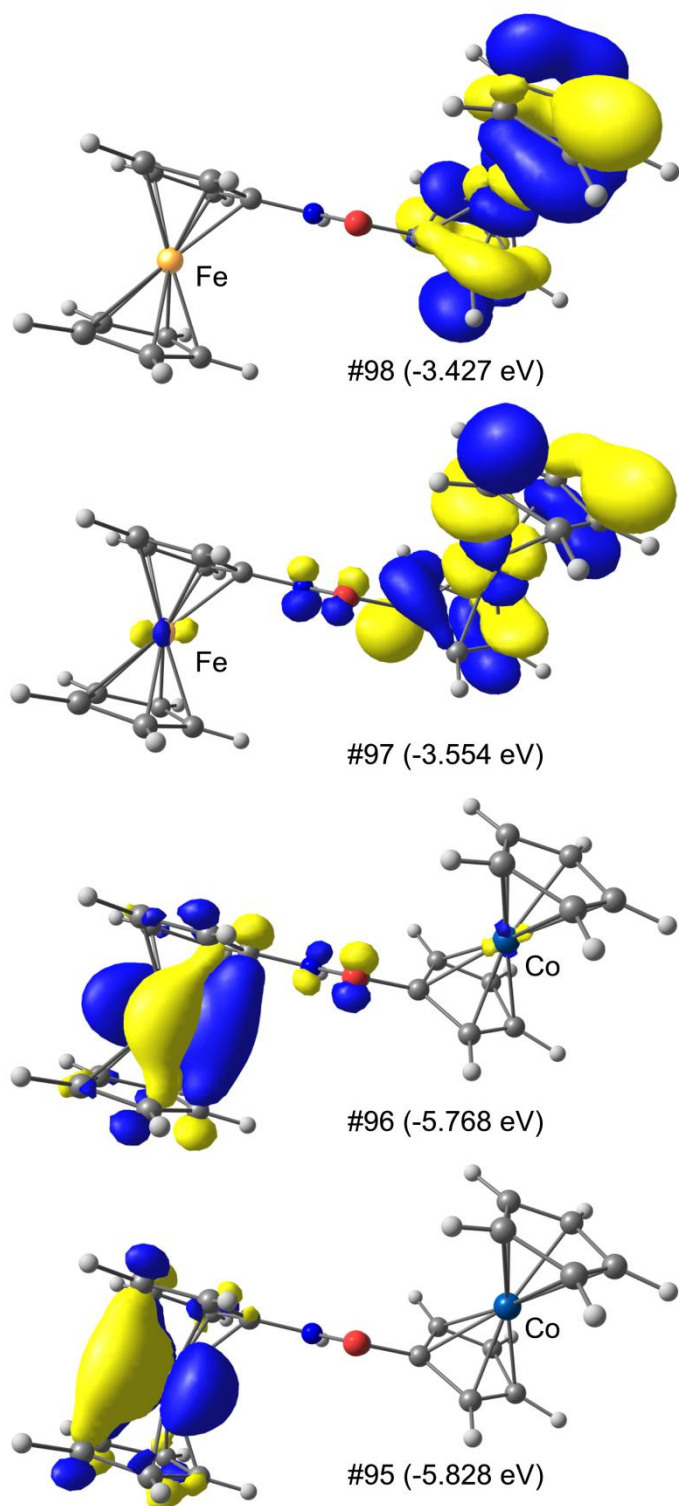


Fig. S9 HOMO and LUMO of **1** with contour value 0.03 a.u..



Cartesian coordinates of a model of 1 (gas phase)

1	5.919867000	-1.093708000	1.196528000
1	3.614557000	-2.525645000	1.056904000
6	5.240124000	-1.125196000	0.356220000
6	4.014604000	-1.888287000	0.280348000
6	5.400292000	-0.416522000	-0.891368000
6	3.417450000	-1.651808000	-1.012954000
1	6.219661000	0.240483000	-1.148544000
1	4.236762000	1.864886000	2.296022000
6	4.271661000	-0.739701000	-1.735249000
1	2.079463000	0.237133000	2.477770000
27	3.594969000	0.171220000	0.041079000
1	-2.697483000	-0.373781000	2.747060000
1	-0.424458000	0.450669000	1.755978000
6	3.507192000	1.691248000	1.517328000
6	2.350382000	0.834932000	1.617713000
1	4.090579000	-0.363323000	-2.732370000
6	-2.729799000	-0.873486000	1.787985000
7	-0.531763000	-0.051741000	0.880604000
6	3.512968000	2.280947000	0.199407000
1	-4.628085000	-2.071761000	1.898372000
6	1.632846000	0.899691000	0.360504000
1	4.244729000	2.980183000	-0.180060000
6	-1.735409000	-0.788593000	0.740716000
6	-3.748666000	-1.786651000	1.339694000
6	0.435435000	0.107064000	-0.074911000
6	2.366555000	1.783100000	-0.518589000
1	-4.454889000	2.314507000	1.311176000
6	-2.151588000	-1.622230000	-0.364710000
6	-3.394040000	-2.242328000	0.019139000
1	2.081529000	2.016806000	-1.534685000
26	-3.618707000	-0.133388000	0.018533000
8	0.375883000	-0.359584000	-1.247021000
1	-1.617841000	-1.746950000	-1.292124000
1	-3.965199000	-2.927710000	-0.590294000
6	-4.481102000	1.771511000	0.376657000
1	-2.631842000	2.488477000	-0.699314000
1	-6.367636000	0.549020000	0.552543000
6	-3.513441000	1.862086000	-0.690412000
6	-5.503126000	0.837296000	-0.028864000
6	-3.936846000	0.983650000	-1.754037000
6	-5.167187000	0.352018000	-1.344939000
1	-5.733520000	-0.367218000	-1.919763000
1	-3.422714000	0.825259000	-2.691552000
1	2.464183000	-2.025794000	-1.360749000

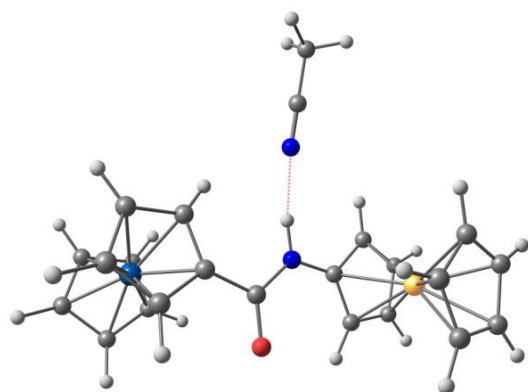
Cartesian coordinates of a model of 1 (ACN)

1	-5.909594000	-0.539659000	-1.564312000
1	-3.718142000	-2.129096000	-1.772155000
6	-5.280423000	-0.864267000	-0.747967000
6	-4.113527000	-1.708654000	-0.858634000
6	-5.442592000	-0.507324000	0.642836000
6	-3.555639000	-1.873748000	0.463240000
1	-6.214505000	0.130863000	1.048356000
1	-3.987055000	2.202124000	-2.060623000
6	-4.374919000	-1.129798000	1.390990000
1	-1.800854000	0.648201000	-2.255238000
27	-3.578003000	0.173443000	-0.064572000
1	2.375654000	-1.020697000	-2.510567000
1	0.272672000	0.112525000	-1.494456000
6	-3.345404000	1.916315000	-1.239725000
6	-2.170486000	1.089421000	-1.340206000
1	-4.210219000	-1.042994000	2.455290000
6	2.526201000	-1.283175000	-1.472465000
7	0.466378000	-0.187094000	-0.544818000
6	-3.523559000	2.278273000	0.147036000
1	4.402021000	-2.523984000	-1.515631000
6	-1.611574000	0.944561000	-0.009953000
1	-4.321740000	2.886304000	0.547075000
6	1.661039000	-0.924097000	-0.372118000
6	3.595953000	-2.090249000	-0.941378000
6	-0.407617000	0.182277000	0.442372000
6	-2.458859000	1.676859000	0.905098000
1	4.293911000	1.816124000	-2.023759000
6	2.209511000	-1.480597000	0.843805000
6	3.402342000	-2.208250000	0.482910000
1	-2.302234000	1.746485000	1.971323000
26	3.630768000	-0.172824000	-0.048147000
8	-0.231273000	-0.069293000	1.671173000
1	1.784835000	-1.374043000	1.827710000
1	4.040460000	-2.745212000	1.170364000
6	4.430317000	1.552168000	-0.984096000
1	2.677570000	2.544072000	0.032821000
1	6.302735000	0.293286000	-1.014735000
6	3.571269000	1.940038000	0.110013000
6	5.500223000	0.743798000	-0.447161000
6	4.110049000	1.370989000	1.323455000
6	5.302584000	0.632941000	0.979361000
1	5.930746000	0.083941000	1.667195000
1	3.691430000	1.475032000	2.314891000
1	-2.665352000	-2.433700000	0.711602000

Cartesian coordinates of a model of 1 (DCM)

1	-5.918412000	-0.565814000	-1.551137000
1	-3.719807000	-2.146527000	-1.752726000
6	-5.283012000	-0.877836000	-0.734629000
6	-4.112119000	-1.717125000	-0.841992000
6	-5.442383000	-0.510321000	0.653575000
6	-3.548723000	-1.867963000	0.479238000
1	-6.218095000	0.124683000	1.057012000
1	-3.999266000	2.201901000	-2.065931000
6	-4.368757000	-1.120639000	1.403259000
1	-1.812509000	0.645975000	-2.264490000
27	-3.582613000	0.174961000	-0.065281000
1	2.385199000	-0.993594000	-2.525265000
1	0.284446000	0.151539000	-1.500715000
6	-3.355769000	1.915488000	-1.246561000
6	-2.180619000	1.088688000	-1.349431000
1	-4.200773000	-1.025327000	2.466376000
6	2.529848000	-1.264173000	-1.488251000
7	0.468520000	-0.170392000	-0.556557000
6	-3.528122000	2.280854000	0.140033000
1	4.401283000	-2.511361000	-1.534168000
6	-1.616091000	0.947692000	-0.021330000
1	-4.323211000	2.892224000	0.541360000
6	1.662262000	-0.911129000	-0.387384000
6	3.594206000	-2.079863000	-0.959751000
6	-0.414282000	0.180222000	0.430443000
6	-2.460114000	1.681356000	0.895293000
1	4.326093000	1.842250000	-1.994764000
6	2.203548000	-1.480402000	0.825673000
6	3.394451000	-2.209336000	0.462521000
1	-2.297301000	1.752422000	1.960563000
26	3.632462000	-0.170296000	-0.050020000
8	-0.251871000	-0.092273000	1.655432000
1	1.775949000	-1.379282000	1.808929000
1	4.028927000	-2.753316000	1.147702000
6	4.452430000	1.560420000	-0.958513000
1	2.706233000	2.557977000	0.064599000
1	6.313061000	0.284857000	-0.996967000
6	3.591658000	1.941234000	0.136586000
6	5.511664000	0.734817000	-0.427492000
6	4.118562000	1.350485000	1.344501000
6	5.305546000	0.606191000	0.996007000
1	5.924808000	0.041533000	1.679118000
1	3.695047000	1.443724000	2.334846000
1	-2.654921000	-2.421114000	0.730435000

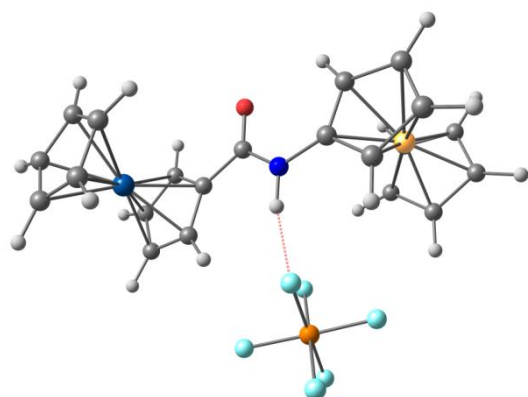
Cartesian coordinates of a model of 1*ACN (ACN)



1	-5.941007000	0.954698000	-1.035673000
1	-3.739879000	0.551749000	-2.574405000
6	-5.327933000	0.064957000	-1.047565000
6	-4.155937000	-0.148739000	-1.864631000
6	-5.521222000	-1.109810000	-0.228743000
6	-3.626010000	-1.455253000	-1.550973000
1	-6.303805000	-1.251771000	0.502727000
1	-4.041289000	2.315343000	1.415025000
6	-4.468021000	-2.048627000	-0.539125000
1	-1.835893000	1.966755000	-0.105133000
27	-3.642527000	-0.245509000	0.181033000
1	2.417363000	1.569992000	-1.680491000
1	0.303474000	1.079976000	-0.293408000
6	-3.400654000	1.445309000	1.422077000
6	-2.225513000	1.258380000	0.610192000
1	-4.326407000	-3.018089000	-0.083644000
6	2.515009000	0.496144000	-1.618570000
7	0.425662000	0.059307000	-0.299121000
6	-3.582863000	0.262000000	2.230548000
1	4.377378000	0.065795000	-2.804892000
6	-1.671153000	-0.043434000	0.921461000
1	-4.381288000	0.092683000	2.938177000
6	1.598288000	-0.396224000	-0.944444000
6	3.547890000	-0.307913000	-2.221639000
6	-0.478978000	-0.737084000	0.342595000
6	-2.521610000	-0.658208000	1.917129000
1	4.263304000	1.865821000	1.229846000
6	2.082707000	-1.750067000	-1.102654000
6	3.283441000	-1.689219000	-1.900910000
1	-2.369303000	-1.641038000	2.337710000
26	3.564564000	-0.578305000	-0.125268000
8	-0.351519000	-1.993181000	0.480580000
1	1.613204000	-2.631945000	-0.700937000
1	3.881426000	-2.538883000	-2.199169000
6	4.386838000	0.792299000	1.266925000

1	2.630654000	0.114513000	2.511053000
1	6.251230000	0.446238000	0.043352000
6	3.519110000	-0.138859000	1.948902000
6	5.445298000	0.037548000	0.637143000
6	4.040605000	-1.469562000	1.739489000
6	5.231208000	-1.360398000	0.929808000
1	5.848713000	-2.181958000	0.593598000
1	3.612385000	-2.387167000	2.118834000
1	-2.737753000	-1.899683000	-1.976709000
7	0.406415000	2.997825000	-0.383935000
6	0.589650000	4.158117000	-0.416347000
6	0.821378000	5.601239000	-0.453959000
1	1.895823000	5.809442000	-0.494716000
1	0.344384000	6.038164000	-1.337536000
1	0.405286000	6.073984000	0.441965000

Cartesian coordinates of a model of 1*PF₆ (ACN)



1	-5.845863000	0.890567000	-1.253688000
1	-3.679479000	0.022718000	-2.640859000
6	-5.376777000	-0.078226000	-1.158393000
6	-4.222463000	-0.539137000	-1.894604000
6	-5.777447000	-1.129789000	-0.251930000
6	-3.911377000	-1.875771000	-1.444122000
1	-6.598062000	-1.084626000	0.449570000
1	-3.862598000	2.170616000	1.172361000
6	-4.870383000	-2.240292000	-0.427799000
1	-1.705005000	1.388722000	-0.221354000
27	-3.803912000	-0.522179000	0.173887000
1	2.095552000	0.104725000	-2.183677000
1	0.115999000	0.113812000	-0.533846000
6	-3.357712000	1.221458000	1.278951000
6	-2.199982000	0.799384000	0.534642000
1	-4.896315000	-3.174263000	0.114784000
6	2.199463000	-0.899188000	-1.798248000
7	0.187219000	-0.876032000	-0.300892000

6	-3.733514000	0.153052000	2.175528000
1	4.010103000	-1.696730000	-2.868622000
6	-1.851040000	-0.536932000	0.975041000
1	-4.569072000	0.161486000	2.860151000
6	1.317954000	-1.530016000	-0.841574000
6	3.208156000	-1.861868000	-2.163305000
6	-0.742842000	-1.436569000	0.527895000
6	-2.806914000	-0.930980000	1.986935000
1	4.128737000	1.259204000	0.293973000
6	1.797085000	-2.870632000	-0.591200000
6	2.962857000	-3.072480000	-1.417911000
1	-2.807028000	-1.882354000	2.497702000
26	3.312028000	-1.462337000	-0.089655000
8	-0.699731000	-2.638361000	0.934032000
1	1.343130000	-3.581340000	0.078577000
1	3.548213000	-3.979897000	-1.465305000
6	4.227561000	0.269492000	0.715623000
1	2.475186000	0.155369000	2.128115000
1	6.041313000	-0.572583000	-0.329289000
6	3.342638000	-0.320709000	1.692454000
6	5.237660000	-0.706911000	0.381755000
6	3.806052000	-1.662225000	1.962227000
6	4.977257000	-1.901477000	1.151381000
1	5.553011000	-2.816352000	1.120535000
1	3.352163000	-2.366673000	2.645671000
1	-3.088306000	-2.485847000	-1.787805000
9	0.413436000	1.896847000	-1.143285000
15	0.875474000	3.257708000	-0.228887000
9	2.478807000	2.850503000	-0.461616000
9	0.833615000	2.300141000	1.147615000
9	0.899181000	4.167639000	-1.623687000
9	-0.744068000	3.625356000	-0.014496000
9	1.316700000	4.577892000	0.680613000

Cartesian coordinates of a model of 1*PF₆ (DCM)

1	5.400266000	0.553900000	-0.145391000
1	3.087770000	1.250014000	1.102487000
6	4.817953000	-0.076157000	0.511708000
6	3.594210000	0.299648000	1.180992000
6	5.112794000	-1.449276000	0.852186000
6	3.135205000	-0.841857000	1.937619000
1	5.954706000	-2.025976000	0.496421000
1	3.716054000	-0.586705000	-2.850973000
6	4.070078000	-1.923277000	1.733294000
1	1.445459000	0.265246000	-1.681186000

27	3.244218000	-1.327755000	-0.116324000
1	-2.036220000	1.654343000	0.822839000
1	-0.233636000	0.121864000	-0.195491000
6	3.075674000	-1.181411000	-2.215617000
6	1.861110000	-0.727407000	-1.589303000
1	3.996243000	-2.915499000	2.154972000
6	-2.403672000	0.704294000	1.182548000
7	-0.601226000	-0.740492000	0.205132000
6	3.293258000	-2.558431000	-1.836051000
1	-4.226119000	1.265690000	2.373025000
6	1.317381000	-1.831648000	-0.821770000
1	4.126793000	-3.176649000	-2.136430000
6	-1.794974000	-0.585435000	0.947447000
6	-3.561328000	0.493111000	2.013778000
6	0.068489000	-1.912889000	0.000479000
6	2.209538000	-2.958569000	-0.979375000
1	-4.027913000	1.311017000	-1.983290000
6	-2.588929000	-1.596883000	1.608401000
6	-3.677072000	-0.921318000	2.273403000
1	2.065494000	-3.924939000	-0.519550000
26	-3.789902000	-0.558788000	0.194143000
8	-0.307817000	-3.036168000	0.455317000
1	-2.380405000	-2.653504000	1.608120000
1	-4.446246000	-1.400726000	2.862399000
6	-4.377465000	0.351695000	-1.627510000
1	-2.868828000	-1.094828000	-2.477908000
1	-6.206097000	0.887217000	-0.419680000
6	-3.761871000	-0.927638000	-1.891427000
6	-5.536822000	0.126024000	-0.796349000
6	-4.540091000	-1.944027000	-1.222402000
6	-5.637651000	-1.292938000	-0.546572000
1	-6.395206000	-1.780708000	0.051236000
1	-4.332781000	-3.005175000	-1.221706000
1	2.233746000	-0.885962000	2.532198000
9	0.129384000	1.833277000	-0.903582000
15	0.795811000	3.219230000	-0.165716000
9	2.303076000	2.756694000	-0.737845000
9	1.064563000	2.302506000	1.217701000
9	0.520177000	4.075379000	-1.563134000
9	-0.723001000	3.616043000	0.399376000
9	1.455750000	4.552758000	0.569190000

Cartesian coordinates of a model of 2-open (gas phase)

1	2.136546000	-3.277156000	0.318765000
1	-0.118179000	-3.813492000	-1.124249000

6	1.574103000	-2.582927000	-0.289546000
6	0.377363000	-2.855941000	-1.046016000
6	1.915785000	-1.190018000	-0.477363000
6	-0.037922000	-1.631054000	-1.688858000
1	0.146469000	-2.569659000	3.021973000
6	0.904734000	-0.600365000	-1.333789000
1	-2.130971000	-2.876278000	1.576622000
27	0.007793000	-1.366780000	0.412936000
1	-6.803102000	-2.031876000	0.782974000
1	-4.288627000	-1.441790000	1.216500000
6	-0.351975000	-1.800296000	2.449080000
6	-1.569306000	-1.958301000	1.687228000
1	0.837485000	0.436629000	-1.634063000
6	-6.605925000	-1.431708000	-0.095399000
7	-4.179886000	-0.926538000	0.348950000
6	0.090208000	-0.433865000	2.311105000
1	-8.554634000	-1.503929000	-1.213297000
6	-1.881560000	-0.683707000	1.073999000
1	0.997370000	-0.023943000	2.732880000
6	-5.352540000	-0.795970000	-0.438046000
6	-7.531703000	-1.160311000	-1.164673000
6	-2.963932000	-0.352714000	0.090381000
6	-0.841815000	0.250400000	1.451234000
1	-7.970990000	0.861020000	2.398388000
6	-5.509075000	-0.109580000	-1.700117000
6	-6.858330000	-0.347165000	-2.145857000
1	-0.796289000	1.281203000	1.129051000
26	-6.891643000	0.654427000	-0.276923000
8	-2.717149000	0.408205000	-0.887206000
1	-4.745611000	0.462140000	-2.200897000
1	-7.290222000	0.030709000	-3.061320000
6	-7.718507000	1.432479000	1.515942000
1	-5.582277000	2.053181000	1.889460000
1	-9.621745000	1.370585000	0.309162000
6	-6.449975000	2.064547000	1.243936000
6	-8.599731000	1.708681000	0.407705000
6	-6.547017000	2.730330000	-0.032929000
6	-7.876211000	2.510755000	-0.548308000
1	-8.260283000	2.875505000	-1.490614000
1	-5.761948000	3.291960000	-0.519307000
1	-0.921895000	-1.485547000	-2.294041000
6	3.045949000	-0.517841000	0.242905000
8	3.338059000	-0.860551000	1.422954000
1	3.431076000	0.580811000	-1.446786000
7	3.696272000	0.449384000	-0.475967000
6	4.784616000	1.238685000	-0.026063000

6	5.390633000	1.261130000	1.285792000
6	5.430488000	2.233712000	-0.854204000
6	6.395552000	2.293123000	1.269199000
1	5.120694000	0.622867000	2.110598000
6	6.419477000	2.892743000	-0.041152000
1	5.191252000	2.467265000	-1.883176000
1	7.027728000	2.564110000	2.102510000
26	6.858408000	0.824085000	-0.189261000
1	7.068530000	3.692989000	-0.365487000
6	7.829693000	-0.062817000	-1.854434000
6	7.181476000	-1.080438000	-1.062607000
1	7.634155000	0.158019000	-2.894592000
6	8.749366000	-0.005301000	0.290379000
6	7.749068000	-1.044201000	0.263866000
1	6.411908000	-1.758875000	-1.404895000
1	9.350079000	0.276009000	1.143983000
1	7.471505000	-1.679602000	1.093070000
6	8.798423000	0.601793000	-1.017113000
1	9.445248000	1.414612000	-1.316237000

Cartesian coordinates of a model of 2-open (ACN)

1	1.891334000	-3.140823000	1.081437000
1	-0.353906000	-3.715504000	-0.345575000
6	1.443805000	-2.531950000	0.309818000
6	0.256757000	-2.830245000	-0.447018000
6	1.951445000	-1.251876000	-0.133859000
6	0.019376000	-1.734073000	-1.356633000
1	0.029941000	-1.589206000	3.460073000
6	1.057023000	-0.754607000	-1.161476000
1	-2.188368000	-2.190828000	2.057991000
27	0.000630000	-1.032880000	0.641357000
1	-6.540834000	-2.201186000	0.680704000
1	-4.125988000	-1.350015000	1.102298000
6	-0.428692000	-0.961379000	2.710007000
6	-1.620732000	-1.275503000	1.964112000
1	1.125204000	0.188171000	-1.685966000
6	-6.420307000	-1.590229000	-0.203409000
7	-4.093074000	-0.774551000	0.267372000
6	0.052775000	0.325566000	2.266404000
1	-8.338993000	-1.916669000	-1.331031000
6	-1.882417000	-0.174637000	1.056929000
1	0.938964000	0.828959000	2.624679000
6	-5.254172000	-0.805551000	-0.539369000
6	-7.368125000	-1.445197000	-1.279559000
6	-2.979322000	-0.008160000	0.054234000

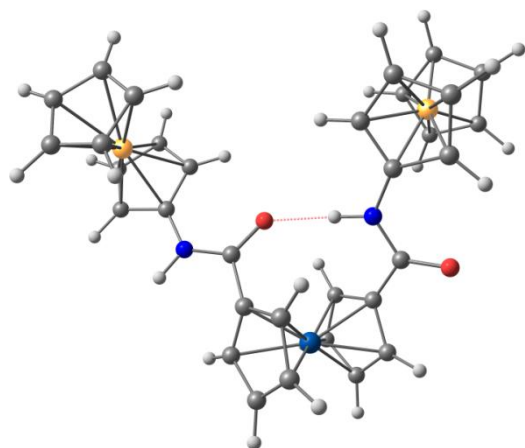
6	-0.836998000	0.807441000	1.243523000
1	-7.987415000	0.507085000	2.290956000
6	-5.489665000	-0.151071000	-1.806475000
6	-6.796697000	-0.557916000	-2.262636000
1	-0.756125000	1.736770000	0.699264000
26	-6.976600000	0.442983000	-0.406508000
8	-2.859015000	0.814526000	-0.900919000
1	-4.801525000	0.507632000	-2.308964000
1	-7.264464000	-0.242723000	-3.184573000
6	-7.847734000	1.112733000	1.406202000
1	-5.794858000	1.999869000	1.707160000
1	-9.759891000	0.786815000	0.253308000
6	-6.682504000	1.907621000	1.096424000
6	-8.791604000	1.262911000	0.323207000
6	-6.906253000	2.549107000	-0.178266000
6	-8.209861000	2.151546000	-0.655441000
1	-8.665637000	2.456207000	-1.587406000
1	-6.216239000	3.206645000	-0.688601000
1	-0.807557000	-1.645302000	-2.046354000
6	3.171003000	-0.620123000	0.457659000
8	3.626931000	-1.021573000	1.568925000
1	3.348735000	0.578524000	-1.200410000
7	3.742746000	0.374969000	-0.287906000
6	4.882847000	1.133621000	0.065374000
6	5.629696000	1.116123000	1.302936000
6	5.459722000	2.132207000	-0.805378000
6	6.653035000	2.128106000	1.200379000
1	5.437240000	0.468168000	2.141407000
6	6.547387000	2.755373000	-0.094030000
1	5.113025000	2.385260000	-1.797908000
1	7.376823000	2.366856000	1.966705000
26	6.930612000	0.686130000	-0.324182000
1	7.174633000	3.549284000	-0.473210000
6	7.652722000	-0.197827000	-2.110917000
6	7.083618000	-1.212074000	-1.254803000
1	7.319221000	0.052570000	-3.108527000
6	8.846070000	-0.199355000	-0.101851000
6	7.820854000	-1.212300000	-0.012684000
1	6.247547000	-1.853502000	-1.497667000
1	9.558971000	0.053128000	0.670884000
1	7.634374000	-1.854325000	0.836998000
6	8.741864000	0.428418000	-1.398318000
1	9.363927000	1.232228000	-1.767173000

Cartesian coordinates of a model of 2-open (DCM)

1	1.891334000	-3.140823000	1.081437000
1	-0.353906000	-3.715504000	-0.345575000
6	1.443805000	-2.531950000	0.309818000
6	0.256757000	-2.830245000	-0.447018000
6	1.951445000	-1.251876000	-0.133859000
6	0.019376000	-1.734073000	-1.356633000
1	0.029941000	-1.589206000	3.460073000
6	1.057023000	-0.754607000	-1.161476000
1	-2.188368000	-2.190828000	2.057991000
27	0.000630000	-1.032880000	0.641357000
1	-6.540834000	-2.201186000	0.680704000
1	-4.125988000	-1.350015000	1.102298000
6	-0.428692000	-0.961379000	2.710007000
6	-1.620732000	-1.275503000	1.964112000
1	1.125204000	0.188171000	-1.685966000
6	-6.420307000	-1.590229000	-0.203409000
7	-4.093074000	-0.774551000	0.267372000
6	0.052775000	0.325566000	2.266404000
1	-8.338993000	-1.916669000	-1.331031000
6	-1.882417000	-0.174637000	1.056929000
1	0.938964000	0.828959000	2.624679000
6	-5.254172000	-0.805551000	-0.539369000
6	-7.368125000	-1.445197000	-1.279559000
6	-2.979322000	-0.008160000	0.054234000
6	-0.836998000	0.807441000	1.243523000
1	-7.987415000	0.507085000	2.290956000
6	-5.489665000	-0.151071000	-1.806475000
6	-6.796697000	-0.557916000	-2.262636000
1	-0.756125000	1.736770000	0.699264000
26	-6.976600000	0.442983000	-0.406508000
8	-2.859015000	0.814526000	-0.900919000
1	-4.801525000	0.507632000	-2.308964000
1	-7.264464000	-0.242723000	-3.184573000
6	-7.847734000	1.112733000	1.406202000
1	-5.794858000	1.999869000	1.707160000
1	-9.759891000	0.786815000	0.253308000
6	-6.682504000	1.907621000	1.096424000
6	-8.791604000	1.262911000	0.323207000
6	-6.906253000	2.549107000	-0.178266000
6	-8.209861000	2.151546000	-0.655441000
1	-8.665637000	2.456207000	-1.587406000
1	-6.216239000	3.206645000	-0.688601000
1	-0.807557000	-1.645302000	-2.046354000
6	3.171003000	-0.620123000	0.457659000
8	3.626931000	-1.021573000	1.568925000
1	3.348735000	0.578524000	-1.200410000

7	3.742746000	0.374969000	-0.287906000
6	4.882847000	1.133621000	0.065374000
6	5.629696000	1.116123000	1.302936000
6	5.459722000	2.132207000	-0.805378000
6	6.653035000	2.128106000	1.200379000
1	5.437240000	0.468168000	2.141407000
6	6.547387000	2.755373000	-0.094030000
1	5.113025000	2.385260000	-1.797908000
1	7.376823000	2.366856000	1.966705000
26	6.930612000	0.686130000	-0.324182000
1	7.174633000	3.549284000	-0.473210000
6	7.652722000	-0.197827000	-2.110917000
6	7.083618000	-1.212074000	-1.254803000
1	7.319221000	0.052570000	-3.108527000
6	8.846070000	-0.199355000	-0.101851000
6	7.820854000	-1.212300000	-0.012684000
1	6.247547000	-1.853502000	-1.497667000
1	9.558971000	0.053128000	0.670884000
1	7.634374000	-1.854325000	0.836998000
6	8.741864000	0.428418000	-1.398318000
1	9.363927000	1.232228000	-1.767173000

Cartesian coordinates of a model of 2-ring (gas phase)



1	3.310739000	4.280723000	-0.572908000
1	1.946690000	5.900760000	1.154732000
6	2.623017000	3.974975000	0.203202000
6	1.906154000	4.820902000	1.120212000
6	2.291332000	2.598068000	0.496786000
6	1.128279000	3.970588000	1.993393000
1	-0.932253000	5.958590000	-1.011808000
6	1.360319000	2.600582000	1.606029000
1	-2.221973000	4.215350000	0.610615000
27	0.531358000	3.664048000	-0.004295000
1	-5.580779000	0.866757000	1.301784000

1	-3.499952000	1.935130000	0.134132000
6	-0.864535000	4.880604000	-1.058684000
6	-1.560143000	3.952469000	-0.203832000
1	0.909993000	1.727164000	2.056836000
6	-4.861535000	0.073350000	1.456049000
7	-2.866696000	1.187634000	0.401317000
6	-0.064819000	4.119108000	-1.989954000
1	-6.038841000	-1.471683000	2.585519000
6	-1.189455000	2.609130000	-0.607763000
1	0.566657000	4.526153000	-2.767149000
6	-3.472676000	0.079258000	1.049866000
6	-5.098776000	-1.164545000	2.151138000
6	-1.559717000	1.311078000	0.043321000
6	-0.259866000	2.720307000	-1.711133000
1	-6.555921000	-0.698079000	-1.672135000
6	-2.859251000	-1.160208000	1.469682000
6	-3.871888000	-1.920593000	2.155612000
1	0.209388000	1.888616000	-2.218265000
26	-4.485424000	-1.549722000	0.156659000
8	-0.679936000	0.412929000	0.228085000
1	-1.831982000	-1.439089000	1.306742000
1	-3.731285000	-2.897995000	2.594068000
6	-5.803312000	-1.455718000	-1.503196000
1	-3.980506000	-0.622737000	-2.538703000
1	-6.916205000	-3.021579000	-0.323904000
6	-4.434893000	-1.415194000	-1.959674000
6	-5.997732000	-2.694800000	-0.790809000
6	-3.783771000	-2.628706000	-1.528379000
6	-4.750754000	-3.419174000	-0.806823000
1	-4.571566000	-4.383331000	-0.352126000
1	-2.755108000	-2.901355000	-1.717924000
1	0.492460000	4.300975000	2.803282000
6	2.909489000	1.448941000	-0.242841000
8	4.050126000	1.614316000	-0.760771000
1	1.199892000	0.313414000	0.039691000
7	2.169271000	0.301433000	-0.299135000
6	2.573737000	-0.895689000	-0.935304000
6	3.770100000	-1.147696000	-1.708793000
6	1.760611000	-2.091962000	-0.938996000
6	3.673648000	-2.493486000	-2.213475000
1	4.566335000	-0.441517000	-1.876433000
6	2.440194000	-3.074250000	-1.743903000
1	0.801567000	-2.205567000	-0.453367000
1	4.410872000	-2.983631000	-2.832967000
26	3.652809000	-2.527879000	-0.096483000
1	2.088028000	-4.074626000	-1.949999000

6	3.423454000	-3.328827000	1.855631000
6	4.213501000	-2.122610000	1.909939000
1	2.485063000	-3.500395000	2.364397000
6	5.330328000	-3.653216000	0.548579000
6	5.390642000	-2.321566000	1.099431000
1	3.971738000	-1.225425000	2.463330000
1	6.062415000	-4.102467000	-0.107735000
1	6.176146000	-1.598368000	0.931251000
6	4.114955000	-4.275214000	1.013797000
1	3.780318000	-5.274305000	0.771994000

Cartesian coordinates of a model of 2-ring (ACN)

1	3.742135000	4.004732000	-0.744068000
1	2.663037000	5.714742000	1.071022000
6	3.103395000	3.739203000	0.085794000
6	2.532854000	4.642358000	1.051627000
6	2.654140000	2.401110000	0.399246000
6	1.736727000	3.866007000	1.973990000
1	-0.253332000	6.135151000	-0.692683000
6	1.809662000	2.483712000	1.573212000
1	-1.622725000	4.421879000	0.886808000
27	0.989501000	3.635156000	0.015637000
1	-5.366499000	1.276911000	1.301623000
1	-3.184386000	2.339689000	0.365372000
6	-0.324205000	5.066457000	-0.834821000
6	-1.060828000	4.153756000	0.002935000
1	1.317725000	1.654848000	2.062036000
6	-4.691511000	0.447443000	1.461773000
7	-2.624995000	1.502079000	0.497795000
6	0.317125000	4.303197000	-1.879348000
1	-5.971878000	-1.074691000	2.510705000
6	-0.867722000	2.817805000	-0.522263000
1	0.942148000	4.700848000	-2.665467000
6	-3.294559000	0.404876000	1.094040000
6	-5.005454000	-0.797987000	2.114598000
6	-1.344966000	1.519559000	0.043917000
6	-0.009959000	2.915608000	-1.685584000
1	-6.364462000	-0.188038000	-1.688954000
6	-2.749103000	-0.872337000	1.494946000
6	-3.812575000	-1.608607000	2.132215000
1	0.316137000	2.087241000	-2.297777000
26	-4.353974000	-1.165564000	0.131664000
8	-0.574059000	0.506009000	0.067932000
1	-1.732384000	-1.195683000	1.347759000
1	-3.725355000	-2.603961000	2.544221000

6	-5.632511000	-0.971605000	-1.549320000
1	-3.770653000	-0.110431000	-2.487727000
1	-6.794550000	-2.571628000	-0.463159000
6	-4.253010000	-0.930713000	-1.973871000
6	-5.862193000	-2.240771000	-0.899359000
6	-3.629636000	-2.174416000	-1.585896000
6	-4.624341000	-2.984301000	-0.922593000
1	-4.467028000	-3.969503000	-0.505913000
1	-2.598111000	-2.448778000	-1.757474000
1	1.177428000	4.251133000	2.814312000
6	3.111884000	1.166763000	-0.318478000
8	4.308461000	1.104745000	-0.736977000
1	1.213205000	0.349737000	-0.165674000
7	2.189568000	0.171985000	-0.449446000
6	2.413920000	-1.090339000	-1.044226000
6	3.616989000	-1.612978000	-1.651692000
6	1.370889000	-2.083069000	-1.166369000
6	3.301865000	-2.921257000	-2.174431000
1	4.561531000	-1.098852000	-1.712841000
6	1.919488000	-3.209243000	-1.879018000
1	0.356049000	-1.973410000	-0.811373000
1	3.991493000	-3.571751000	-2.693706000
26	2.996158000	-2.909092000	-0.084105000
1	1.385480000	-4.112354000	-2.138112000
6	2.325444000	-3.531657000	1.829170000
6	3.378327000	-2.553627000	1.971991000
1	1.313361000	-3.435543000	2.197531000
6	4.243573000	-4.380069000	0.798397000
6	4.563236000	-3.077427000	1.333341000
1	3.293845000	-1.595366000	2.466151000
1	4.918068000	-5.026204000	0.253643000
1	5.520313000	-2.579101000	1.263640000
6	2.859972000	-4.660652000	1.103636000
1	2.317369000	-5.555025000	0.829939000

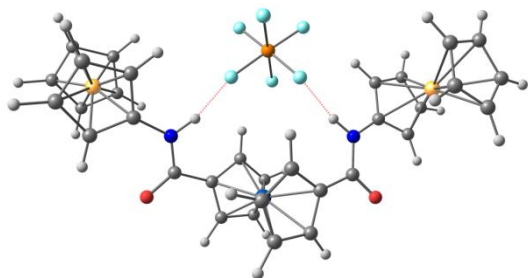
Cartesian coordinates of a model of 2-ring (DCM)

1	3.726380000	4.018863000	-0.738612000
1	2.638023000	5.730246000	1.072665000
6	3.083312000	3.755000000	0.088465000
6	2.508449000	4.657726000	1.052051000
6	2.639034000	2.415720000	0.403413000
6	1.713639000	3.879744000	1.974367000
1	-0.289369000	6.133150000	-0.717143000
6	1.792116000	2.497074000	1.575254000
1	-1.653592000	4.422852000	0.870671000

27	0.969040000	3.644280000	0.015677000
1	-5.384482000	1.258519000	1.289575000
1	-3.206241000	2.319374000	0.334249000
6	-0.351078000	5.062584000	-0.849890000
6	-1.085584000	4.151418000	-0.008567000
1	1.302869000	1.666342000	2.063770000
6	-4.706056000	0.432436000	1.453376000
7	-2.640288000	1.490042000	0.487932000
6	0.298562000	4.295504000	-1.886440000
1	-5.982040000	-1.090125000	2.506559000
6	-0.883180000	2.812673000	-0.523660000
1	0.922609000	4.691255000	-2.674409000
6	-3.308140000	0.392867000	1.087745000
6	-5.016076000	-0.811172000	2.111093000
6	-1.353761000	1.515371000	0.052444000
6	-0.021222000	2.907342000	-1.684011000
1	-6.380159000	-0.238429000	-1.697796000
6	-2.758450000	-0.880397000	1.495484000
6	-3.820417000	-1.617188000	2.134103000
1	0.312634000	2.076155000	-2.288370000
26	-4.359060000	-1.184190000	0.130524000
8	-0.571887000	0.512009000	0.101175000
1	-1.740731000	-1.201085000	1.349508000
1	-3.730985000	-2.610642000	2.549995000
6	-5.640005000	-1.012992000	-1.551495000
1	-3.786967000	-0.142971000	-2.499271000
1	-6.786964000	-2.616330000	-0.455076000
6	-4.261124000	-0.962401000	-1.976558000
6	-5.857732000	-2.279560000	-0.893243000
6	-3.626296000	-2.197487000	-1.580529000
6	-4.613420000	-3.011679000	-0.911804000
1	-4.447344000	-3.992619000	-0.488691000
1	-2.592438000	-2.463603000	-1.750941000
1	1.155018000	4.263831000	2.815768000
6	3.103950000	1.184360000	-0.316331000
8	4.295715000	1.138626000	-0.747156000
1	1.215993000	0.347570000	-0.142894000
7	2.190647000	0.179489000	-0.435869000
6	2.422346000	-1.079921000	-1.034973000
6	3.627433000	-1.589742000	-1.648914000
6	1.386537000	-2.080487000	-1.157049000
6	3.320941000	-2.898235000	-2.175246000
1	4.567557000	-1.067531000	-1.710140000
6	1.942209000	-3.199137000	-1.876017000
1	0.371662000	-1.980392000	-0.798894000
1	4.014175000	-3.541478000	-2.698592000

26	3.022353000	-2.896153000	-0.083745000
1	1.415495000	-4.106006000	-2.136778000
6	2.370134000	-3.534357000	1.831016000
6	3.416531000	-2.549233000	1.971728000
1	1.360542000	-3.449626000	2.208900000
6	4.286974000	-4.361839000	0.782030000
6	4.600585000	-3.060056000	1.321752000
1	3.329687000	-1.595090000	2.473295000
1	4.962374000	-4.999582000	0.228685000
1	5.552792000	-2.553377000	1.247031000
6	2.908097000	-4.654875000	1.095425000
1	2.370821000	-5.552087000	0.820702000

Cartesian coordinates of a model of 2*PF₆, chelate (ACN)



1	-0.813115000	0.644010000	1.546088000
1	0.963595000	2.366179000	2.608978000
6	-0.856760000	1.719702000	1.459302000
6	0.089854000	2.639616000	2.034695000
6	-1.861113000	2.495892000	0.757065000
6	-0.312769000	3.981487000	1.684689000
1	-0.881818000	2.134512000	-2.692773000
6	-1.516563000	3.893066000	0.900993000
1	0.862367000	0.488620000	-1.483361000
27	0.046773000	2.856601000	-0.070375000
1	3.402709000	-1.983313000	1.336935000
1	2.397544000	0.084698000	0.176236000
6	-0.003467000	2.445000000	-2.145263000
6	0.929432000	1.566597000	-1.487759000
1	-2.074960000	4.713804000	0.475766000
6	4.215952000	-1.292125000	1.504646000
7	3.200145000	0.687812000	0.345391000
6	0.422581000	3.806686000	-1.923145000
1	5.687722000	-2.486861000	2.715284000
6	1.946853000	2.388483000	-0.861344000
1	-0.078587000	4.695380000	-2.278161000
6	4.260702000	0.081625000	1.057327000
6	5.426527000	-1.550775000	2.242793000
6	3.166553000	1.979815000	-0.096754000

6	1.626355000	3.771634000	-1.135703000
1	4.995552000	-3.087725000	-1.535713000
6	5.510331000	0.664649000	1.491664000
6	6.223320000	-0.348478000	2.232073000
1	2.201036000	4.619281000	-0.792602000
26	5.902592000	-1.017862000	0.251950000
8	4.097666000	2.819825000	0.094316000
1	5.826425000	1.676956000	1.304414000
1	7.191421000	-0.221301000	2.695624000
6	5.784787000	-2.365003000	-1.381084000
1	5.017217000	-0.527816000	-2.442634000
1	7.294644000	-3.508376000	-0.154899000
6	5.797217000	-1.004427000	-1.864874000
6	7.008644000	-2.589355000	-0.647528000
6	7.028691000	-0.387402000	-1.429520000
6	7.777648000	-1.367168000	-0.677999000
1	8.740369000	-1.210382000	-0.211362000
1	7.333529000	0.631212000	-1.625960000
1	0.204795000	4.890959000	1.953080000
6	-3.083091000	2.039331000	0.022742000
8	-3.968798000	2.886218000	-0.305880000
1	-2.407148000	0.088502000	0.046452000
7	-3.168484000	0.701407000	-0.240815000
6	-4.237188000	0.052629000	-0.902113000
6	-4.206855000	-1.350404000	-1.249046000
6	-5.488818000	0.612510000	-1.360332000
6	-5.430326000	-1.651637000	-1.948933000
1	-3.399625000	-2.038502000	-1.044239000
6	-6.219439000	-0.446017000	-2.014733000
1	-5.793694000	1.638874000	-1.245278000
1	-5.705410000	-2.617740000	-2.347406000
26	-5.874123000	-0.972904000	0.003868000
1	-7.193168000	-0.345493000	-2.473015000
6	-6.940641000	-0.214633000	1.672666000
6	-5.715549000	-0.840283000	2.113219000
1	-7.213751000	0.821275000	1.819075000
6	-6.999387000	-2.457290000	1.018239000
6	-5.751722000	-2.226088000	1.708304000
1	-4.908499000	-0.354277000	2.644256000
1	-7.321740000	-3.394354000	0.585630000
1	-4.977766000	-2.960362000	1.884318000
6	-7.734158000	-1.213983000	0.996092000
1	-8.704075000	-1.057195000	0.544565000
9	1.148589000	-1.354713000	0.221296000
15	-0.129212000	-2.362816000	-0.243478000
9	-1.419456000	-3.310873000	-0.697073000

9	-0.300113000	-1.447396000	-1.637480000
9	0.937246000	-3.369937000	-1.018231000
9	0.040027000	-3.215298000	1.170488000
9	-1.196136000	-1.301943000	0.542105000

Cartesian coordinates of a model of 2*PF₆, chelate (DCM)

1	-0.798178000	0.622852000	1.542572000
1	0.991850000	2.335411000	2.600405000
6	-0.840745000	1.699238000	1.463884000
6	0.113221000	2.613898000	2.035801000
6	-1.850946000	2.481809000	0.777008000
6	-0.290674000	3.958792000	1.698717000
1	-0.903969000	2.119127000	-2.679967000
6	-1.502619000	3.877219000	0.926829000
1	0.852331000	0.476800000	-1.486045000
27	0.049828000	2.844721000	-0.066999000
1	3.419725000	-1.982836000	1.331122000
1	2.415994000	0.069418000	0.142145000
6	-0.021117000	2.431576000	-2.140666000
6	0.919565000	1.554757000	-1.492022000
1	-2.067843000	4.700055000	0.514787000
6	4.229646000	-1.287026000	1.496421000
7	3.211314000	0.680500000	0.318036000
6	0.405603000	3.794010000	-1.923721000
1	5.700647000	-2.465754000	2.722725000
6	1.942580000	2.378163000	-0.876803000
1	-0.099497000	4.681534000	-2.276327000
6	4.272049000	0.082988000	1.037424000
6	5.438107000	-1.534572000	2.241444000
6	3.166135000	1.975682000	-0.114038000
6	1.617932000	3.760629000	-1.149155000
1	5.020468000	-3.100726000	-1.527331000
6	5.517674000	0.674548000	1.471335000
6	6.230857000	-0.329598000	2.223256000
1	2.198499000	4.607528000	-0.814003000
26	5.919877000	-1.017868000	0.248099000
8	4.085158000	2.825806000	0.087419000
1	5.830087000	1.686504000	1.275990000
1	7.196799000	-0.195235000	2.689230000
6	5.810027000	-2.377992000	-1.374660000
1	5.051228000	-0.549008000	-2.455914000
1	7.310790000	-3.512621000	-0.129948000
6	5.826969000	-1.021521000	-1.869195000
6	7.029156000	-2.597501000	-0.632230000
6	7.056203000	-0.402019000	-1.431497000
6	7.799549000	-1.376461000	-0.667864000
1	8.759425000	-1.216775000	-0.196398000

1	7.362511000	0.615032000	-1.633466000
1	0.230141000	4.865513000	1.970445000
6	-3.077895000	2.035692000	0.043146000
8	-3.950631000	2.892972000	-0.291501000
1	-2.424675000	0.076400000	0.078561000
7	-3.176324000	0.697934000	-0.216007000
6	-4.245117000	0.060425000	-0.888577000
6	-4.218191000	-1.338448000	-1.252162000
6	-5.492015000	0.631482000	-1.345530000
6	-5.439555000	-1.625783000	-1.960881000
1	-3.414487000	-2.032280000	-1.052415000
6	-6.223589000	-0.416181000	-2.015729000
1	-5.792005000	1.658098000	-1.219771000
1	-5.716422000	-2.586004000	-2.372005000
26	-5.889353000	-0.968853000	-0.002400000
1	-7.194845000	-0.306476000	-2.477109000
6	-6.969367000	-0.231411000	1.666796000
6	-5.745732000	-0.858503000	2.109054000
1	-7.246003000	0.802294000	1.821692000
6	-7.016910000	-2.466929000	0.988148000
6	-5.774858000	-2.239828000	1.689137000
1	-4.944094000	-0.376209000	2.651469000
1	-7.333094000	-3.400139000	0.542968000
1	-4.999469000	-2.973450000	1.861293000
6	-7.755119000	-1.225681000	0.974167000
1	-8.722162000	-1.066755000	0.517302000
9	1.134158000	-1.326195000	0.226326000
15	-0.137443000	-2.348497000	-0.235766000
9	-1.422882000	-3.301029000	-0.685575000
9	-0.327447000	-1.420480000	-1.620484000
9	0.933689000	-3.335625000	-1.025438000
9	0.051359000	-3.203706000	1.171880000
9	-1.207455000	-1.298022000	0.565149000