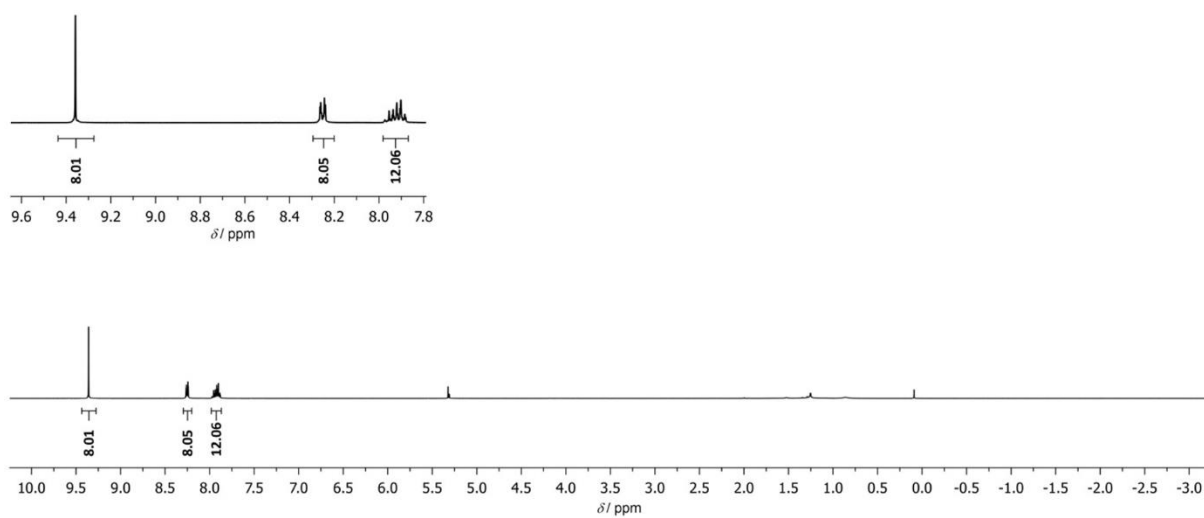


## Gold(III) tetraarylporphyrin amino acid derivatives: ligand or metal centred redox chemistry?

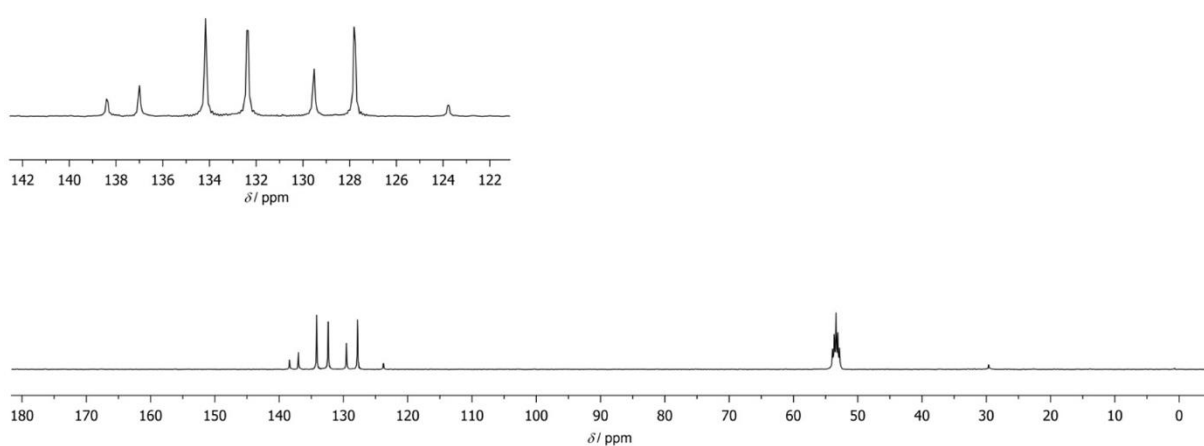
Sebastian Preiß, Jascha Melomedov, Anica Wünsche von Leupoldt and Katja Heinze\*

### Supporting Information

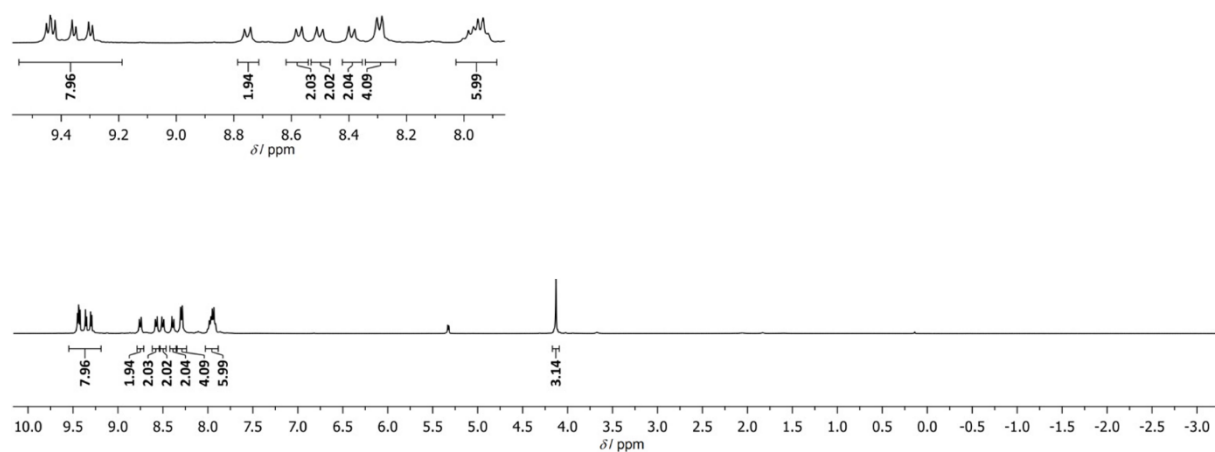
**Fig. S01**  $^1\text{H}$  NMR spectrum of  $[\text{Au}(\text{TPP})](\text{PF}_6)$  in  $\text{CD}_2\text{Cl}_2$ .



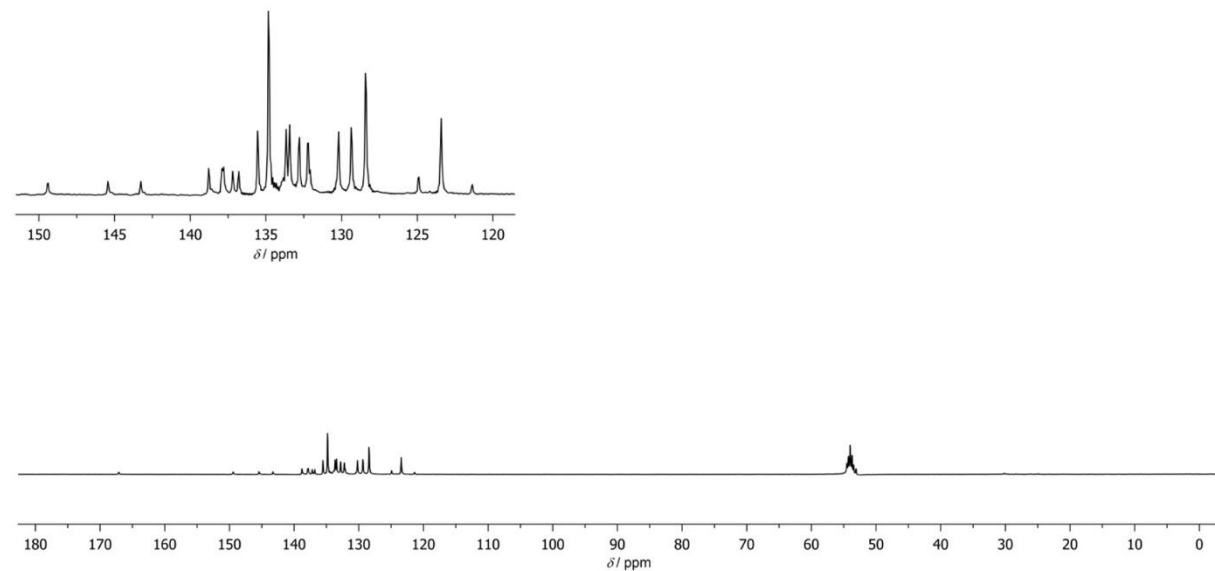
**Fig. S02**  $^{13}\text{C}$  NMR spectrum of  $[\text{Au}(\text{TPP})](\text{PF}_6)$  in  $\text{CD}_2\text{Cl}_2$ .



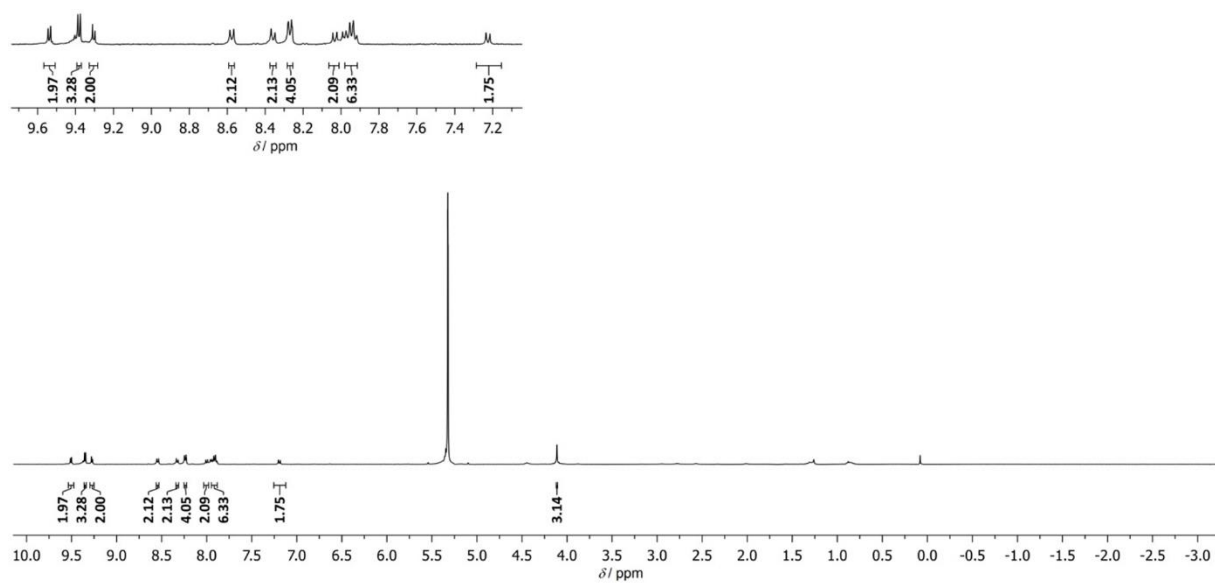
**Fig. S03**  $^1\text{H}$  NMR spectrum of **[1a](PF<sub>6</sub>)** in  $\text{CD}_2\text{Cl}_2$ .



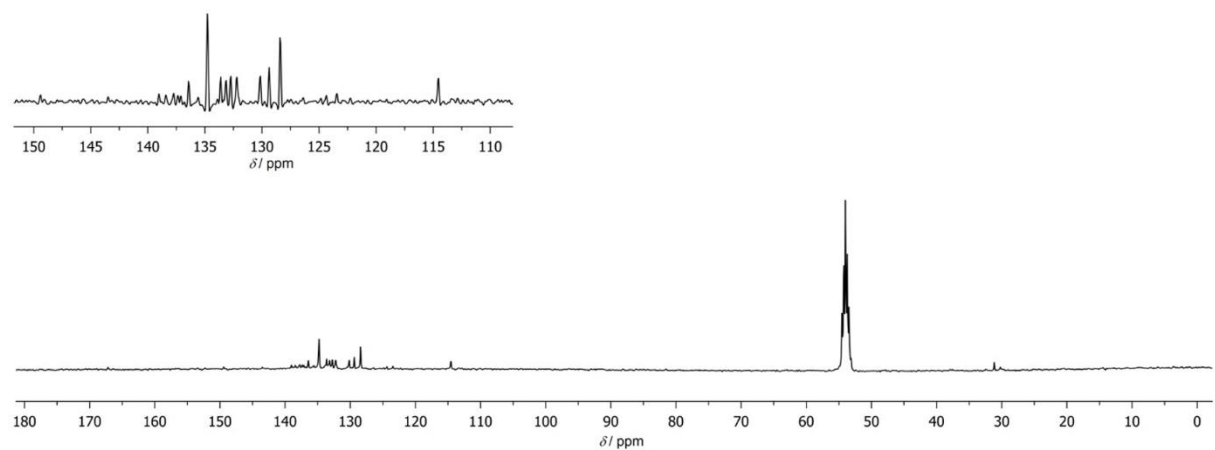
**Fig. S04**  $^{13}\text{C}$  NMR spectrum of **[1a](PF<sub>6</sub>)** in  $\text{CD}_2\text{Cl}_2$ .



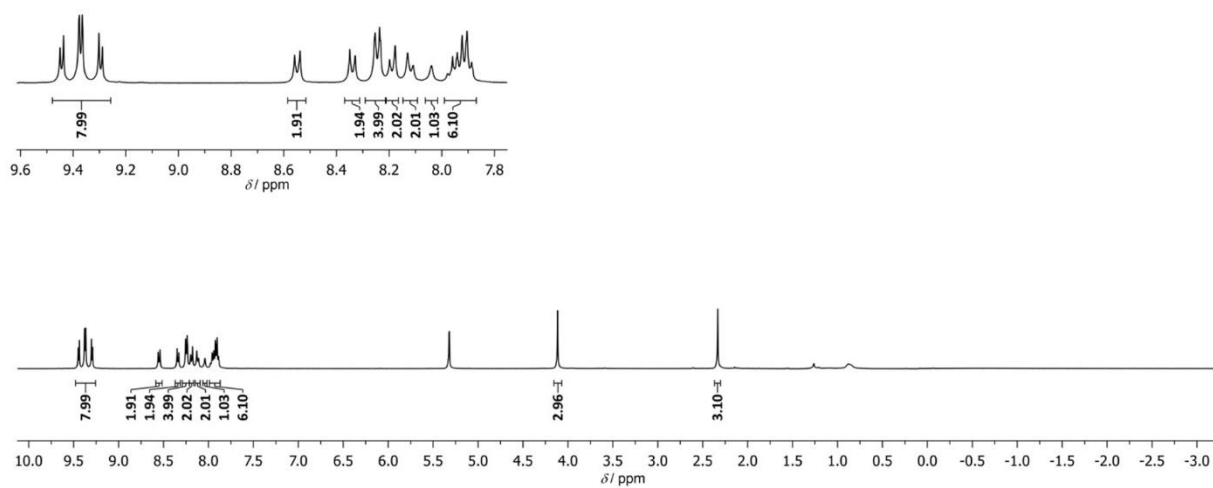
**Fig. S05**  $^1\text{H}$  NMR spectrum of **[2a](PF<sub>6</sub>)** in  $\text{CD}_2\text{Cl}_2$ .



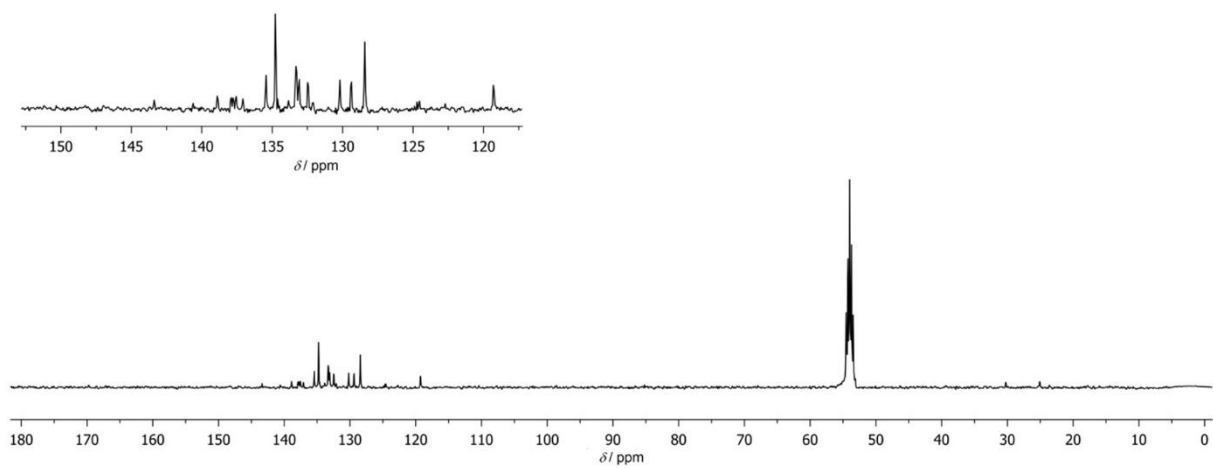
**Fig. S06**  $^{13}\text{C}$  NMR spectrum of **[2a](PF<sub>6</sub>)** in  $\text{CD}_2\text{Cl}_2$ .



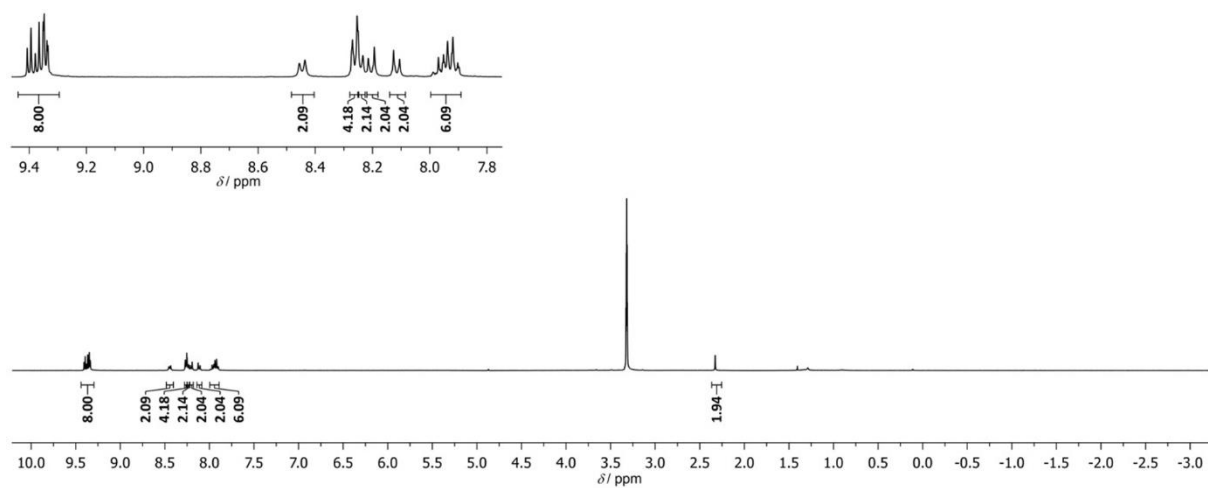
**Fig. S07**  $^1\text{H}$  NMR spectrum of **[3a](PF<sub>6</sub>)** in  $\text{CD}_2\text{Cl}_2$ .



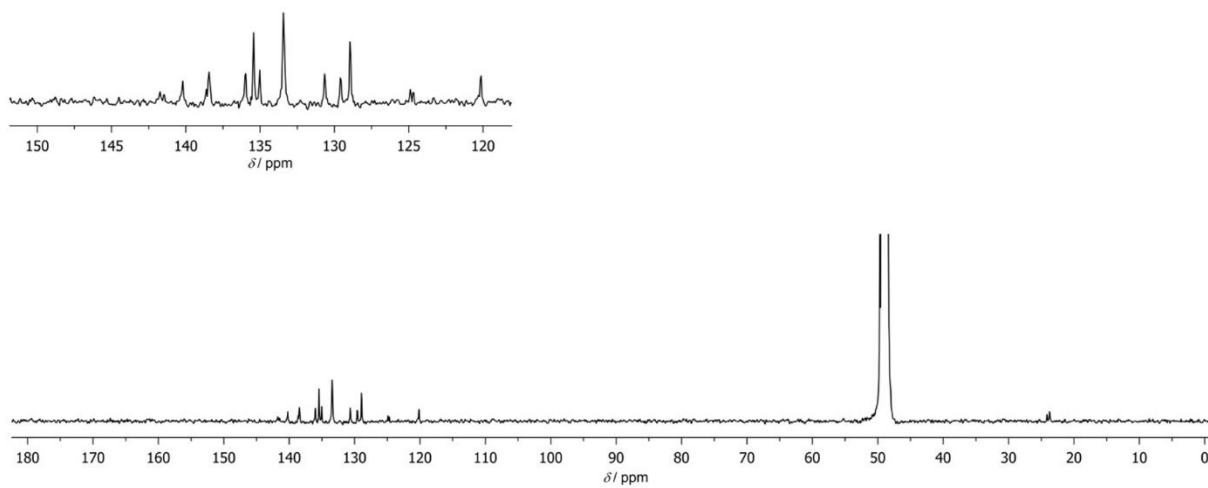
**Fig. S08**  $^{13}\text{C}$  NMR spectrum of **[3a](PF<sub>6</sub>)** in  $\text{CD}_2\text{Cl}_2$ .



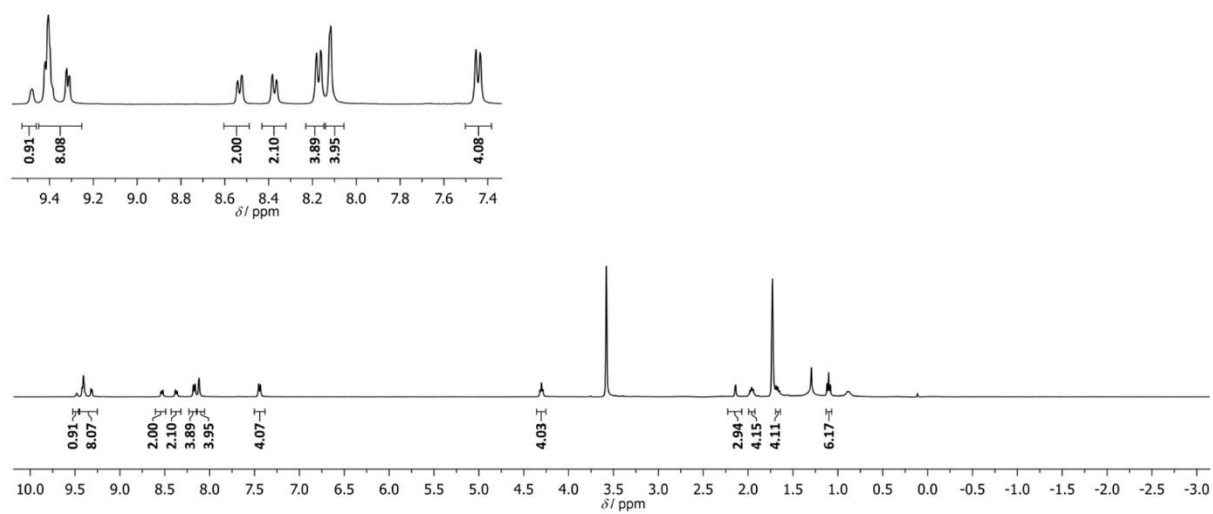
**Fig. S09**  $^1\text{H}$  NMR spectrum of **[4a](PF<sub>6</sub>)** in CD<sub>3</sub>OD.



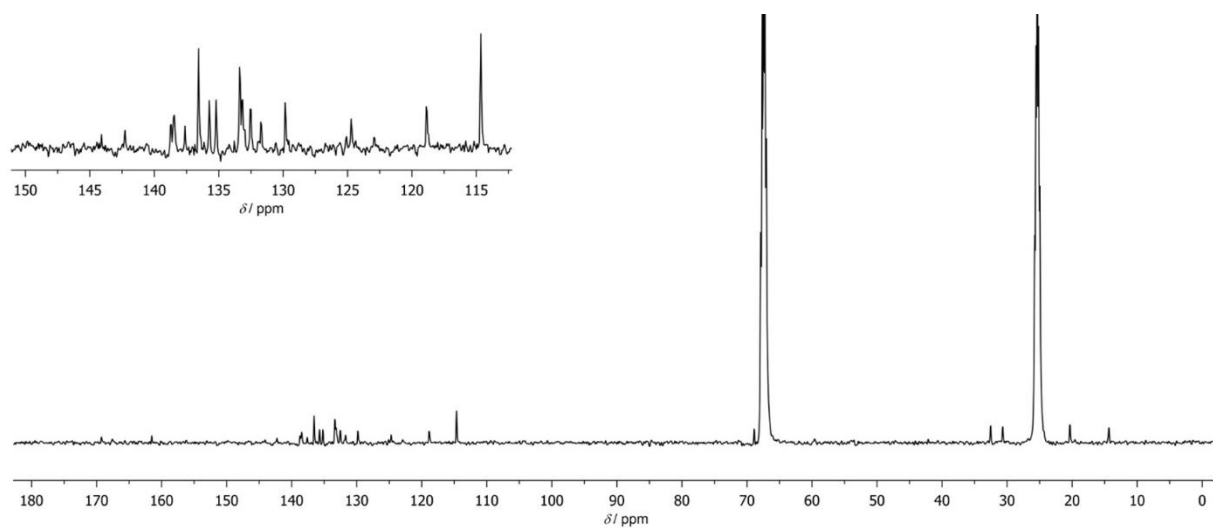
**Fig. S10**  $^{13}\text{C}$  NMR spectrum of **[4a](PF<sub>6</sub>)** in CD<sub>3</sub>OD.



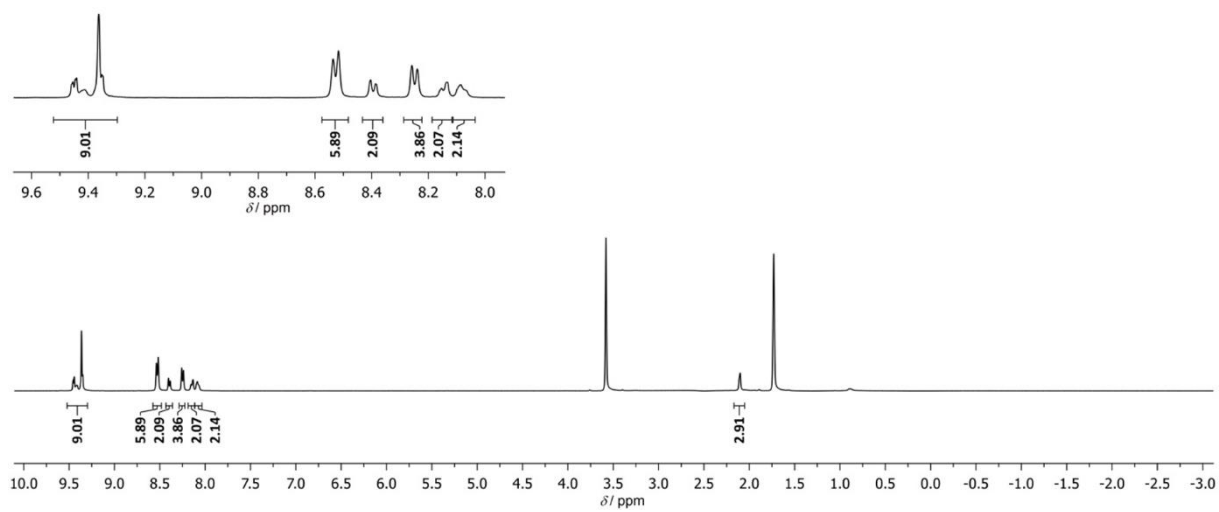
**Fig. S11**  $^1\text{H}$  NMR spectrum of **[4b](PF<sub>6</sub>)** in  $d_8$ -THF.



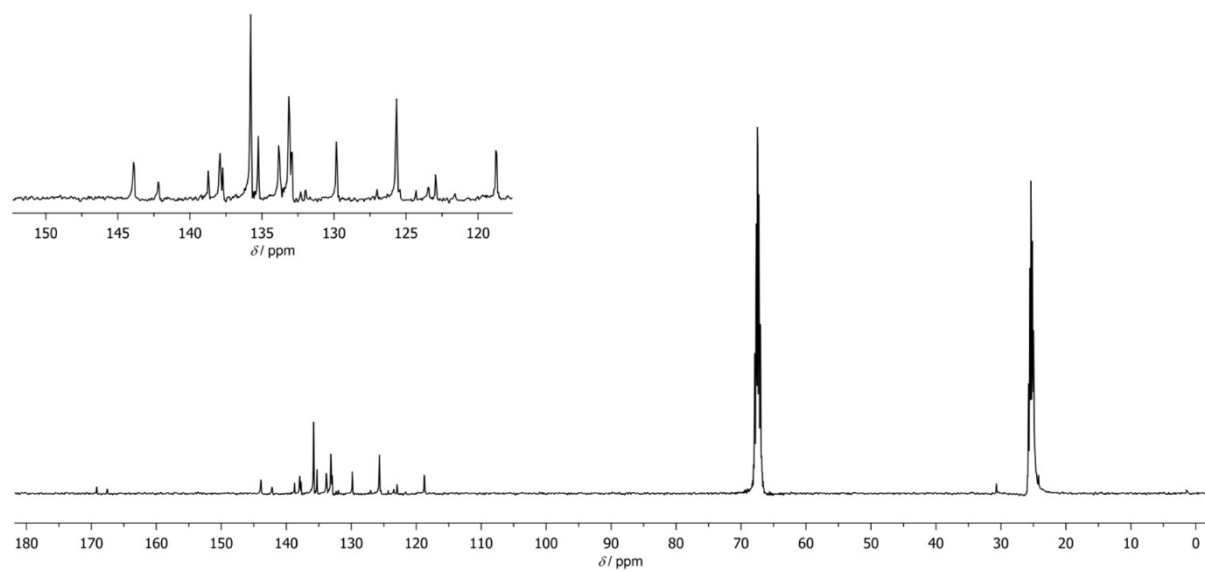
**Fig. S12**  $^{13}\text{C}$  NMR spectrum of **[4b](PF<sub>6</sub>)** in  $d_8$ -THF.



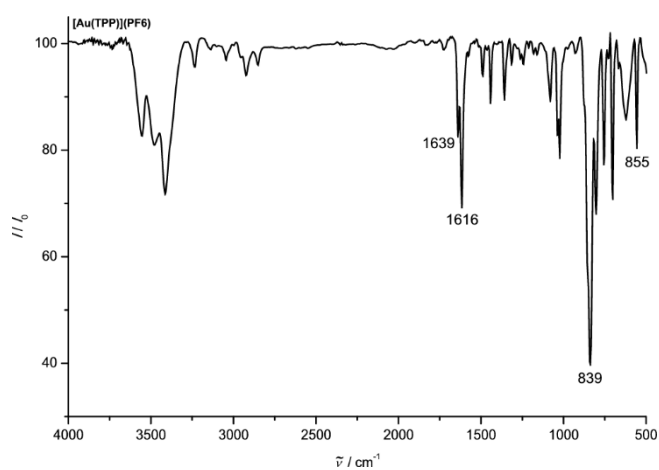
**Fig. S13**  $^1\text{H}$  NMR spectrum of **[4c](PF<sub>6</sub>)** in  $\text{d}_8\text{-THF}$ .



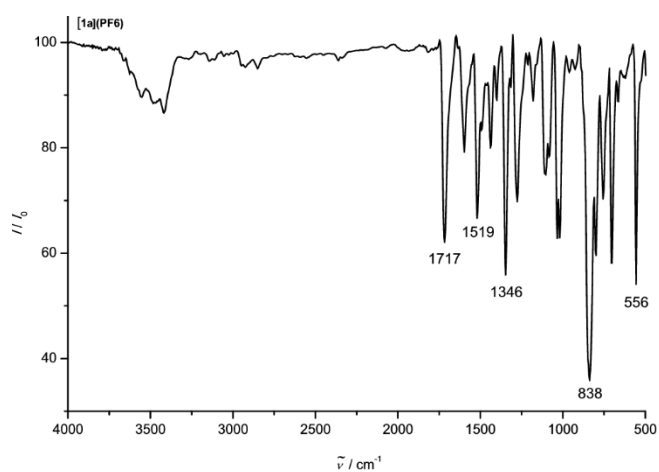
**Fig. S14**  $^{13}\text{C}$  NMR spectrum of **[4c](PF<sub>6</sub>)** in  $\text{d}_8\text{-THF}$ .



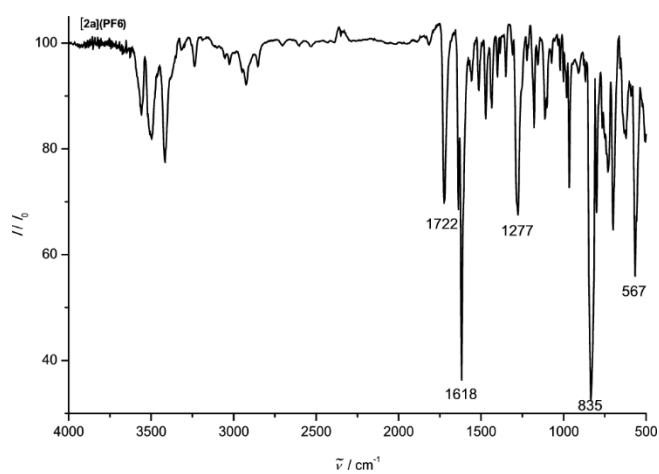
**Fig. S15** IR spectrum of [Au(TPP)](PF<sub>6</sub>) as KBr disk.



**Fig. S16** IR spectrum of [1a](PF<sub>6</sub>) as KBr disk.

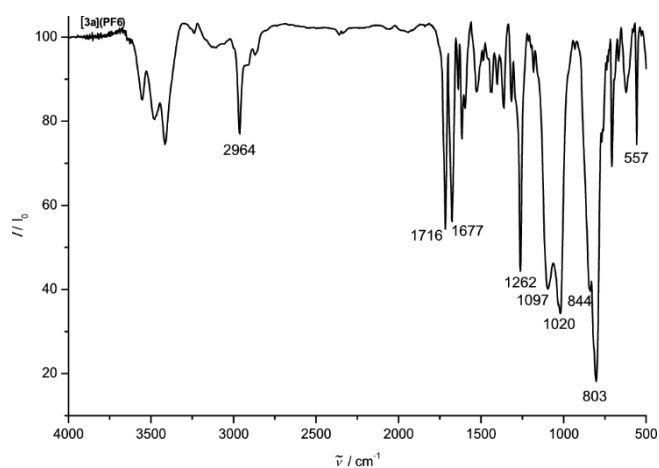


**Fig. S17** IR spectrum of [2a](PF<sub>6</sub>) as KBr disk.

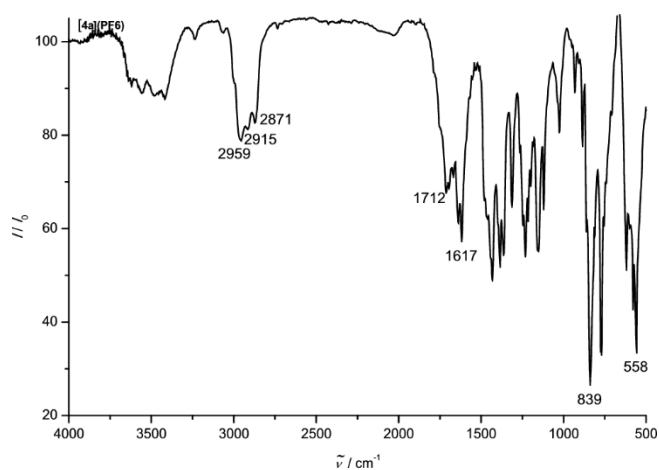




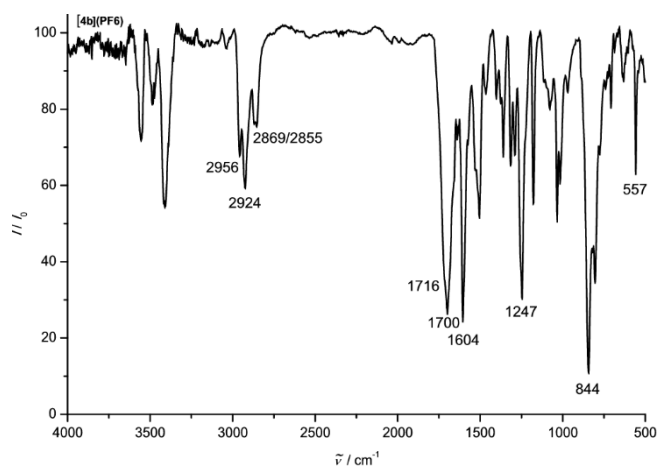
**Fig. S18** IR spectrum of **[3a](PF<sub>6</sub>)** as KBr disk.



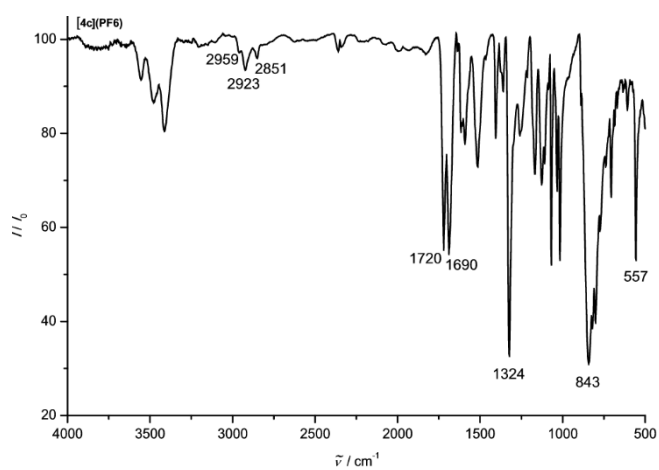
**Fig. S19** IR spectrum of **[4a](PF<sub>6</sub>)** as KBr disk.



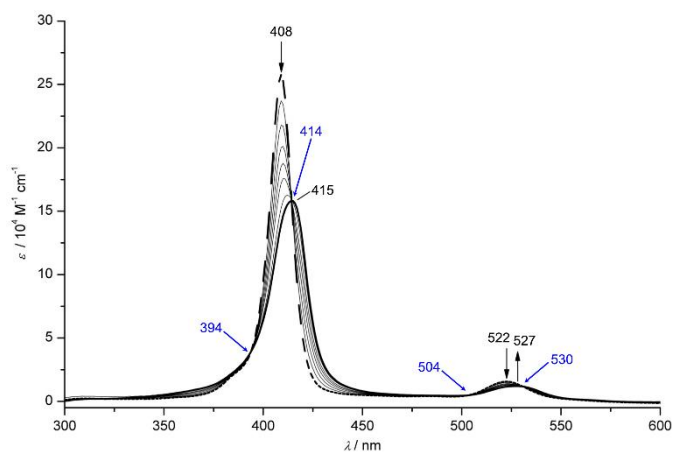
**Fig. S20** IR spectrum of **[4b](PF<sub>6</sub>)** as KBr disk.



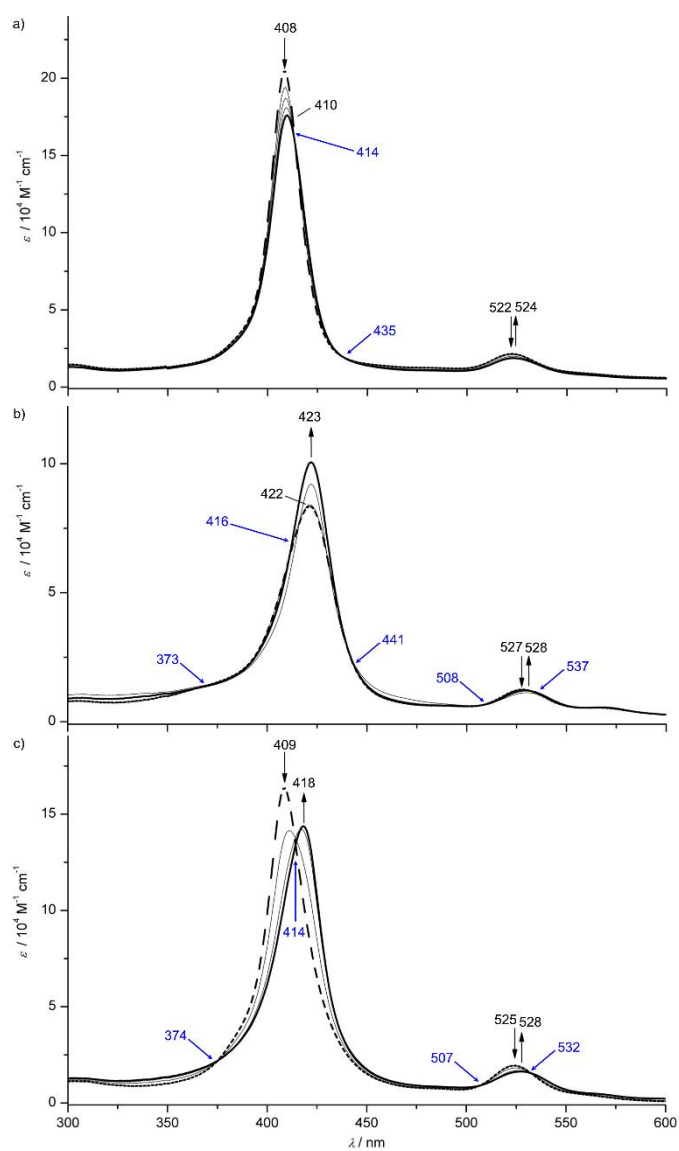
**Fig. S21** IR spectrum of **[4c](PF<sub>6</sub>)** as KBr disk.



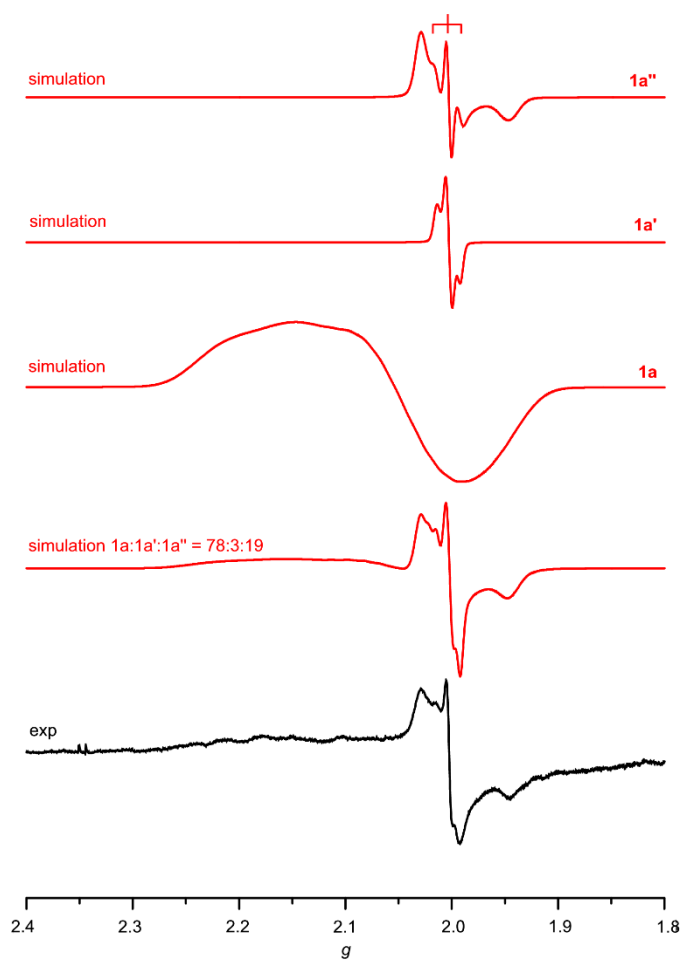
**Fig. S22** UV/Vis spectral changes upon the first electroreduction of  $[\text{Au}(\text{TPP})]^+ 10^{-5} \text{ M}$  in  $0.1 \text{ M } [{}^n\text{Bu}_4\text{N}](\text{PF}_6)/\text{THF}$  solution (isosbestic points indicated in blue).



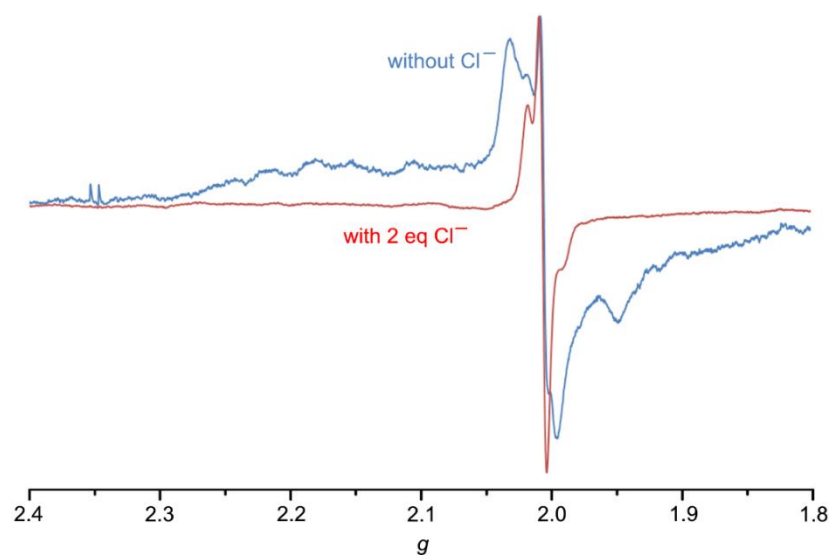
**Fig. S23** UV/Vis spectral changes upon the first electroreduction of a)  $[\mathbf{4a}]^+$  (in MeOH), b)  $[\mathbf{4b}]^+$  and c)  $[\mathbf{4c}]^+$   $10^{-5} \text{ M}$  in  $0.1 \text{ M } [{}^n\text{Bu}_4\text{N}](\text{PF}_6)$  THF solution (isosbestic points indicated in blue).



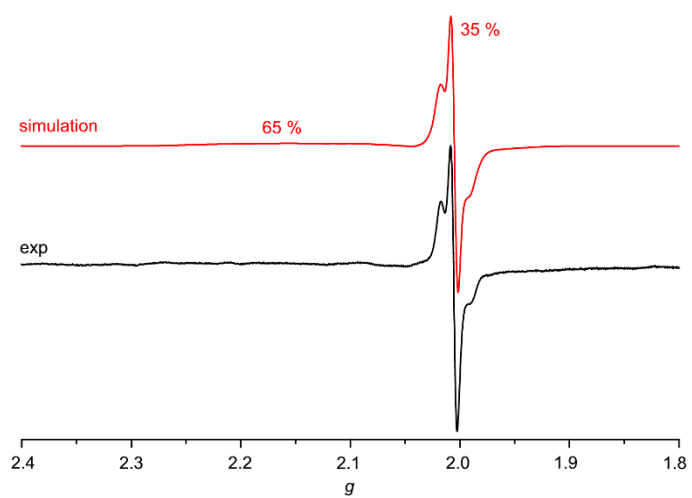
**Fig. S24** X-band EPR spectrum of **1a** /**1a'**/**1a''** in frozen CH<sub>2</sub>Cl<sub>2</sub> solution (77 K, 9.4 GHz) and deconvolution in the respective component spectra.



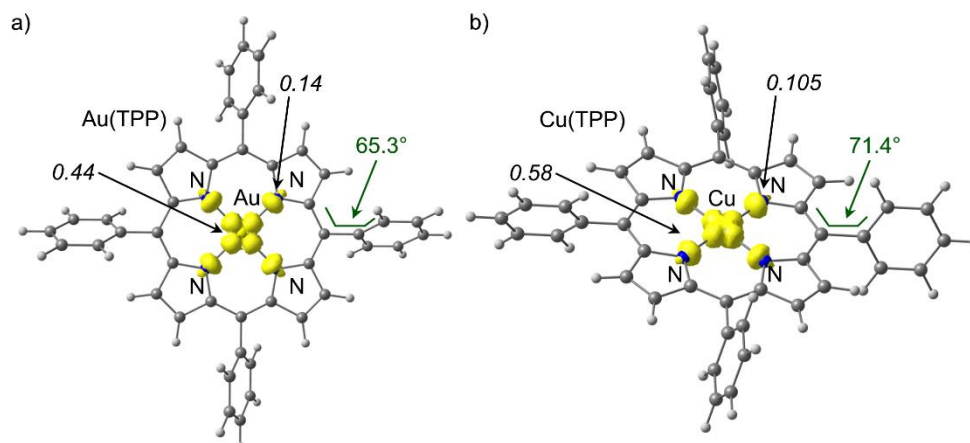
**Fig. S25** X-band EPR spectrum of **1a** in frozen CH<sub>2</sub>Cl<sub>2</sub> solution (77 K, 9.4 GHz) in the absence and in the presence of two equivalents [<sup>n</sup>Bu<sub>4</sub>N]Cl.



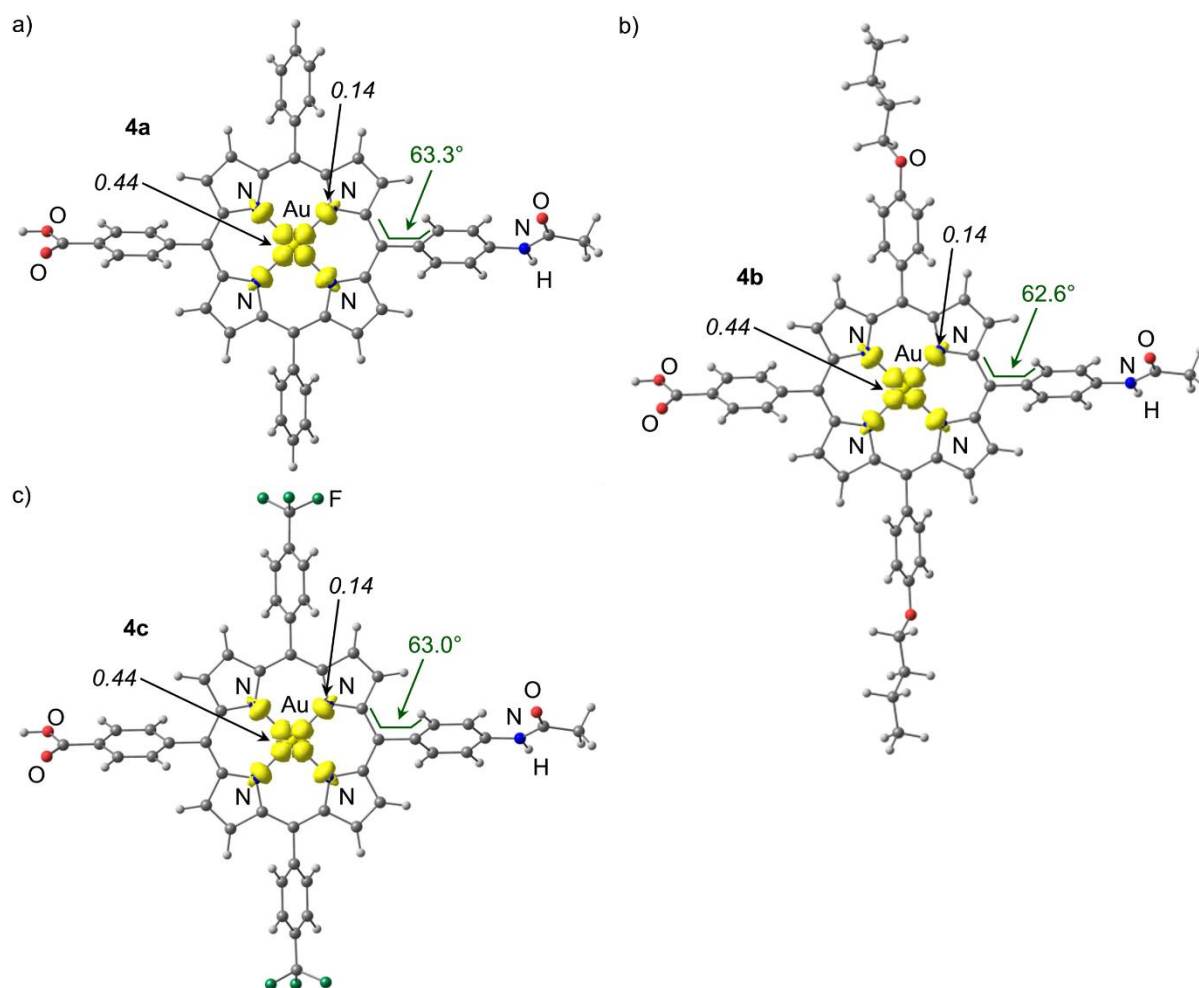
**Fig. S26** X-band EPR spectrum of **1a** in frozen CH<sub>2</sub>Cl<sub>2</sub> solution (77 K, 9.4 GHz) in the presence of two equivalents [<sup>n</sup>Bu<sub>4</sub>N]Cl and corresponding simulation.



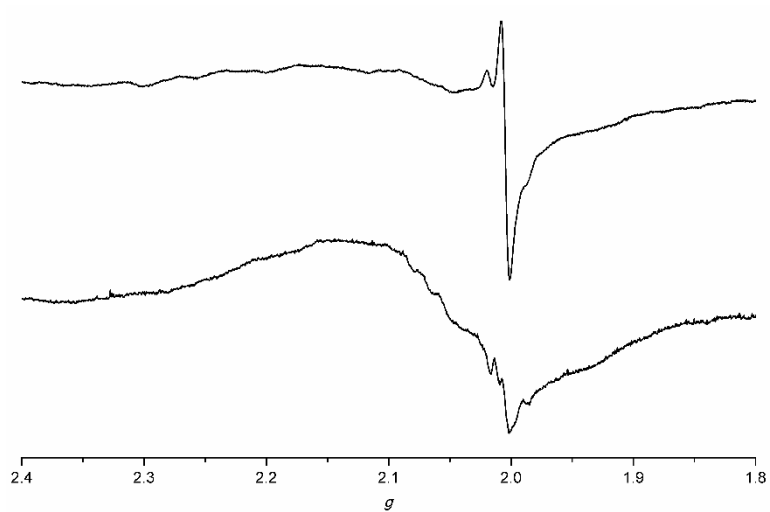
**Fig. S27** Spin densities of DFT optimized geometries of Au(TPP) and Cu(TPP) (isosurface value 0.01 a.u.; UB3LYP, LANL2DZ, IEFPCM CH<sub>2</sub>Cl<sub>2</sub>; Mulliken spin densities in italics).



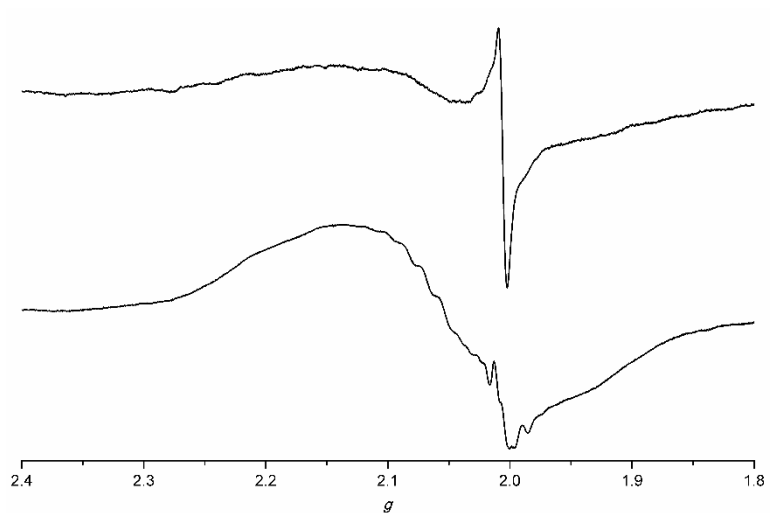
**Fig. S28** Spin densities of DFT optimized geometries of **4a**, **4b** and **4c** (isosurface value 0.01 a.u.; UB3LYP, LANL2DZ, IEFPCM CH<sub>2</sub>Cl<sub>2</sub>; Mulliken spin densities in italics).



**Fig. S29** X-band EPR spectrum of **2a** / **2a'** in frozen CH<sub>2</sub>Cl<sub>2</sub> (top) and THF (bottom) solution (77 K, 9.4 GHz).



**Fig. S30** X-band EPR spectrum of **3a** / **3a'** in frozen CH<sub>2</sub>Cl<sub>2</sub> (top) and THF (bottom) solution (77 K, 9.4 GHz).



## Cartesian coordinates of DFT optimised geometries (B3LYP, LANL2DZ, IEFPCM CH<sub>2</sub>Cl<sub>2</sub>)

```

[Au(TPP)]+
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7      1.401502000      1.497628000      0.007722000
7      -1.401410000     -1.497574000      0.007417000
7      1.498342000     -1.401185000     -0.009973000
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6      -3.567765000      2.397553000      0.219138000
6      -2.629510000      3.400467000      0.211938000
6      -1.327784000      2.788967000      0.058771000
1      -4.636175000      2.494941000      0.332148000
1      -2.797515000      4.460639000      0.318660000
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6      -3.498186000     -0.116641000      0.007945000
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6      3.400577000      2.629800000     -0.211839000
6      2.789229000      1.327730000     -0.058905000
6      1.139245000      2.870961000     -0.068668000
1      2.494361000      4.636273000     -0.331481000
1      4.460731000      2.797840000     -0.318598000
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6      2.629812000     -3.400494000      0.210591000
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1	0.738975000	7.702289000	1.889060000
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79	-0.000167000	0.000124000	-0.000678000

**Au(TPP)**

7	-1.998141000	0.719501000	-0.028358000
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7	1.998107000	-0.719513000	-0.028799000
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**Cu(TPP)**

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7	2.029437000	-0.013103000	0.000276000
7	0.013525000	2.029512000	0.000516000
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6	-2.482139000	-2.449562000	-0.000995000
6	2.449075000	-2.481671000	-0.000146000
6	-4.262823000	-0.658102000	0.003663000
6	-4.253570000	0.714328000	0.002450000
6	-2.861968000	1.136654000	0.005724000
6	-2.877109000	-1.099071000	-0.003569000
1	-5.120995000	-1.313276000	0.008725000
1	-5.102687000	1.381022000	-0.002632000
6	-2.449120000	2.481627000	-0.000169000
6	2.877009000	1.099039000	-0.003310000
6	4.262721000	0.658093000	0.003737000
6	4.253486000	-0.714335000	0.002186000
6	2.861893000	-1.136686000	0.005822000
1	5.120891000	1.313271000	0.008746000
1	5.102627000	-1.380995000	-0.003341000
6	-0.658161000	4.262620000	-0.005186000
6	0.714276000	4.253709000	-0.007330000
6	1.136946000	2.862218000	0.002236000
6	-1.098803000	2.876836000	-0.006277000
1	-1.313613000	5.120592000	-0.003634000
1	1.380680000	5.103026000	-0.016868000
6	2.482047000	2.449529000	-0.000755000
6	-3.552802000	-3.505480000	-0.000896000
6	-4.336373000	-3.736451000	-1.154554000
6	-5.338724000	-4.725525000	-1.155949000
6	-5.576055000	-5.495298000	0.000403000
6	-4.800673000	-5.270954000	1.155834000
6	-3.795175000	-4.285182000	1.153147000
1	-4.155236000	-3.148049000	-2.050758000
1	-5.928746000	-4.893551000	-2.053608000
1	-6.351757000	-6.257061000	0.001075000
1	-4.977698000	-5.857718000	2.053816000
1	-3.204318000	-4.114064000	2.049827000
6	3.505394000	-3.552190000	0.000488000
6	4.275397000	-3.802934000	1.159182000
6	5.262144000	-4.807531000	1.162267000
6	5.496881000	-5.573586000	0.002705000
6	4.736563000	-5.327940000	-1.158186000
6	3.746647000	-4.326398000	-1.157293000
1	4.096212000	-3.219053000	2.058861000
1	5.841546000	-4.991114000	2.063711000
1	4.912720000	-5.910830000	-2.058949000
1	3.165776000	-4.138547000	-2.057032000
6	3.552731000	3.505425000	-0.000768000
6	3.795304000	4.285020000	1.153303000
6	4.800812000	5.270790000	1.155902000
6	5.576040000	5.495189000	0.000380000
6	5.338574000	4.725447000	-1.155967000
6	4.336212000	3.736392000	-1.154488000
1	3.204573000	4.113869000	2.050060000
1	4.977951000	5.857513000	2.053888000
1	6.351763000	6.256930000	0.000992000
1	5.928505000	4.893486000	-2.053684000
1	4.154969000	3.148015000	-2.050690000
6	-3.505407000	3.552208000	0.000473000
6	-4.275696000	3.802690000	1.159024000
6	-5.262314000	4.807420000	1.162140000

6	-5.496531000	5.573924000	0.002766000
6	-4.735872000	5.328572000	-1.157963000
6	-3.746086000	4.326884000	-1.157094000
1	-4.096815000	3.218494000	2.058558000
1	-5.841936000	4.990811000	2.063483000
1	-4.911571000	5.911873000	-2.058555000
1	-3.164831000	4.139377000	-2.056663000
1	-6.258820000	6.349112000	0.003796000
1	6.259309000	-6.348636000	0.003699000

**[1a]<sup>+</sup>**

7	1.683508000	1.439232000	-0.000039000
7	-1.213988000	1.482679000	-0.073677000
7	1.639341000	-1.461160000	-0.023365000
7	-1.257984000	-1.416413000	-0.066483000
6	3.062011000	1.203284000	-0.024498000
6	3.741699000	2.473832000	-0.156165000
6	2.785845000	3.458205000	-0.198458000
6	1.490720000	2.823558000	-0.088157000
1	4.811258000	2.595374000	-0.228950000
1	2.938852000	4.520270000	-0.308443000
6	0.266435000	3.510795000	-0.065341000
6	3.704082000	-0.042540000	0.053467000
6	-2.250830000	3.537132000	0.108604000
6	-3.236366000	2.581166000	0.113103000
6	-2.599041000	1.288890000	-0.013028000
6	-0.978421000	2.861022000	-0.016629000
1	-2.368785000	4.605480000	0.199286000
1	-4.300095000	2.733759000	0.207876000
6	-3.282536000	0.064060000	-0.070821000
6	1.401323000	-2.840126000	0.019125000
6	2.668683000	-3.517023000	0.185853000
6	3.653823000	-2.561817000	0.225888000
6	3.021064000	-1.268433000	0.083259000
1	2.783177000	-4.585703000	0.277154000
1	4.713215000	-2.717992000	0.357309000
6	-3.309608000	-2.449443000	-0.298221000
6	-2.352905000	-3.434262000	-0.309532000
6	-1.062863000	-2.800156000	-0.149869000
6	-2.635218000	-1.179990000	-0.137275000
1	-4.376356000	-2.567366000	-0.407771000
1	-2.501496000	-4.496002000	-0.428255000
6	0.159787000	-3.488600000	-0.079628000
6	0.286647000	5.010879000	-0.090514000
6	0.831176000	5.740409000	0.991196000
6	0.842652000	7.147310000	0.967971000
6	0.320557000	7.841879000	-0.141460000
6	-0.218752000	7.120701000	-1.225392000
6	5.203676000	-0.063581000	0.100022000
6	5.945196000	-0.616017000	-0.970469000
6	7.346239000	-0.631325000	-0.938995000
6	7.999663000	-0.094868000	0.184952000
6	7.291485000	0.456117000	1.267976000
6	5.891098000	0.472264000	1.214253000
1	5.426536000	-1.018167000	-1.835181000
1	7.921189000	-1.043645000	-1.759750000
1	5.329700000	0.887578000	2.045412000
6	0.138731000	-4.988733000	-0.106150000
6	0.702586000	-5.692733000	-1.194937000
6	0.679417000	-7.099432000	-1.222837000
6	0.103219000	-7.819606000	-0.157416000
6	-0.455238000	-7.124091000	0.933591000
6	-0.442998000	-5.717196000	0.956756000
6	-4.782867000	0.082689000	-0.061395000
6	-5.503333000	0.633311000	-1.146195000
6	-6.905672000	0.641906000	-1.136487000
6	-7.611638000	0.108902000	-0.035900000
6	-6.898292000	-0.437150000	1.053413000
6	-5.495351000	-0.453656000	1.035723000
1	-4.967817000	1.038221000	-2.000189000
1	-7.460723000	1.056088000	-1.972497000
1	-7.440040000	-0.841900000	1.900893000
1	-4.952013000	-0.869359000	1.879624000
6	-0.241276000	5.714053000	-1.197815000
6	-9.101465000	0.141273000	-0.063151000
8	-9.784499000	0.618213000	-0.994951000
1	7.824741000	0.856679000	2.122032000

7	9.469680000	-0.109513000	0.228786000
8	-9.665892000	-0.416984000	1.059602000
6	-11.142408000	-0.440602000	1.143534000
1	-11.555733000	-1.006730000	0.304062000
1	-11.360642000	-0.931749000	2.091819000
1	-11.533755000	0.580627000	1.131969000
1	1.142724000	-5.142915000	-2.023061000
1	1.107751000	-7.628204000	-2.070124000
1	-0.896856000	-7.672287000	1.761495000
1	-0.869187000	-5.187027000	1.804740000
1	-0.652975000	5.163557000	-2.040008000
1	1.228413000	5.211101000	1.853635000
1	-0.619187000	7.648683000	-2.086695000
1	1.255444000	7.696216000	1.810146000
1	0.333446000	8.928447000	-0.160921000
1	0.089731000	-8.906165000	-0.176973000
79	0.212761000	0.011064000	-0.040851000
8	10.057143000	0.386905000	1.253527000
8	10.107381000	-0.617910000	-0.759386000

**1a**

7	1.732986000	1.494319000	0.029183000
7	-1.269620000	1.530035000	-0.071475000
7	1.697942000	-1.509762000	-0.035824000
7	-1.306166000	-1.473598000	-0.016306000
6	3.098003000	1.246144000	-0.000968000
6	3.781350000	2.534807000	-0.098252000
6	2.818395000	3.518418000	-0.113443000
6	1.514506000	2.865902000	-0.026139000
1	4.849851000	2.674595000	-0.169425000
1	2.977314000	4.583311000	-0.195435000
6	0.255219000	3.524220000	-0.020773000
6	3.722563000	-0.031745000	0.024095000
6	-2.308647000	3.577922000	0.073794000
6	-3.294165000	2.616444000	0.059172000
6	-2.641026000	1.313138000	-0.038940000
6	-1.020437000	2.895151000	-0.015063000
1	-2.442534000	4.646313000	0.155092000
1	-4.359793000	2.777406000	0.128257000
6	-3.296935000	0.052161000	-0.068765000
6	1.445397000	-2.875762000	0.011198000
6	2.730471000	-3.559421000	0.132040000
6	3.716739000	-2.599143000	0.144431000
6	3.067211000	-1.294350000	0.031116000
1	2.861647000	-4.627948000	0.215907000
1	4.779305000	-2.764616000	0.243644000
6	-3.352010000	-2.511438000	-0.199021000
6	-2.389609000	-3.496145000	-0.189658000
6	-1.088213000	-2.844267000	-0.067434000
6	-2.670707000	-1.224095000	-0.083283000
1	-4.419063000	-2.646935000	-0.295495000
1	-2.546606000	-4.561023000	-0.275544000
6	0.171375000	-3.503670000	-0.028716000
6	0.272576000	5.028264000	-0.020700000
6	0.796662000	5.743219000	1.081377000
6	0.809086000	7.150802000	1.083919000
6	0.306083000	7.866014000	-0.021355000
6	-0.213871000	7.162316000	-1.126212000
6	5.223196000	-0.049741000	0.044869000
6	5.952313000	-0.637269000	-1.018331000
6	7.352758000	-0.654352000	-1.011076000
6	8.028829000	-0.084129000	0.084117000
6	7.336613000	0.502910000	1.160159000
6	5.936470000	0.520236000	1.128182000
1	5.417902000	-1.063497000	-1.861526000
1	7.912791000	-1.092391000	-1.828952000
1	5.389288000	0.959833000	1.956202000
6	0.152619000	-5.007724000	-0.030417000
6	0.684628000	-5.734245000	-1.121027000
6	0.662540000	-7.141736000	-1.125344000
6	0.116576000	-7.845378000	-0.033114000
6	-0.411400000	-7.130166000	1.060489000
6	-0.397734000	-5.722609000	1.058838000
6	-4.799646000	0.069857000	-0.085940000
6	-5.503127000	0.622666000	-1.182431000
6	-6.905121000	0.635209000	-1.200979000
6	-7.635393000	0.102229000	-0.115575000

6	-6.942321000	-0.447121000	0.985955000
6	-5.539458000	-0.465652000	0.994755000
1	-4.949510000	1.027131000	-2.024980000
1	-7.442180000	1.052026000	-2.047614000
1	-7.500550000	-0.851664000	1.823028000
1	-5.013012000	-0.882047000	1.848873000
6	-0.234871000	5.754866000	-1.122960000
6	-9.121860000	0.138496000	-0.171227000
8	-9.789959000	0.617746000	-1.113901000
1	7.884012000	0.927459000	1.993556000
7	9.494453000	-0.102042000	0.104510000
8	-9.711807000	-0.419864000	0.941059000
6	-11.188738000	-0.436500000	0.994262000
1	-11.588405000	-1.003120000	0.148331000
1	-11.429297000	-0.923893000	1.939246000
1	-11.576255000	0.586136000	0.971698000
1	1.100879000	-5.197791000	-1.970065000
1	1.067951000	-7.684103000	-1.975816000
1	-0.830504000	-7.663685000	1.909926000
1	-0.800519000	-5.177416000	1.908803000
1	-0.631123000	5.218500000	-1.981553000
1	1.179713000	5.198040000	1.940422000
1	-0.600048000	7.704650000	-1.985605000
1	1.207851000	7.684298000	1.943102000
1	0.318919000	8.953059000	-0.021661000
1	0.102789000	-8.932412000	-0.034165000
79	0.213766000	0.010246000	-0.023415000
8	10.103792000	0.422237000	1.104791000
8	10.118365000	-0.641454000	-0.878558000

### 1a'' (constrained)

7	1.692306000	1.442567000	0.011539000
7	-1.224019000	1.485671000	-0.058579000
7	1.649212000	-1.459449000	-0.027216000
7	-1.267361000	-1.414976000	-0.043608000
6	3.067527000	1.208831000	-0.083154000
6	3.724118000	2.470858000	-0.323256000
6	2.761528000	3.457120000	-0.329564000
6	1.485974000	2.828891000	-0.113039000
1	4.782416000	2.591699000	-0.490241000
1	2.905296000	4.513546000	-0.494754000
6	0.257793000	3.512683000	-0.034192000
6	3.731291000	-0.039524000	0.030213000
6	-2.249886000	3.532136000	0.250507000
6	-3.236964000	2.575014000	0.238456000
6	-2.605668000	1.289403000	0.033512000
6	-0.983420000	2.867579000	0.052796000
1	-2.366589000	4.595044000	0.395074000
1	-4.296886000	2.722305000	0.376101000
6	-3.292770000	0.065727000	-0.066865000
6	1.397808000	-2.839583000	0.079338000
6	2.645738000	-3.507133000	0.335613000
6	3.636703000	-2.550051000	0.371262000
6	3.026825000	-1.267503000	0.116456000
1	2.751736000	-4.568426000	0.498200000
1	4.684190000	-2.703630000	0.575345000
6	-3.305100000	-2.442188000	-0.387528000
6	-2.346482000	-3.427970000	-0.389296000
6	-1.065433000	-2.802824000	-0.159933000
6	-2.640226000	-1.177382000	-0.160579000
1	-4.365988000	-2.556577000	-0.547316000
1	-2.491400000	-4.485780000	-0.545250000
6	0.153103000	-3.485555000	-0.044609000
6	0.281340000	5.012871000	-0.040723000
6	0.916263000	5.726618000	1.002232000
6	0.932571000	7.133623000	0.998961000
6	0.325356000	7.846915000	-0.054041000
6	-0.303557000	7.143182000	-1.100519000
6	5.210689000	-0.061261000	0.057614000
6	5.953293000	-0.916168000	-0.807900000
6	7.347476000	-0.932172000	-0.800014000
6	8.052963000	-0.104125000	0.112615000
6	7.338037000	0.746374000	0.996819000
6	5.944762000	0.772461000	0.950632000
1	5.422966000	-1.539313000	-1.522280000
1	7.905608000	-1.560379000	-1.483994000
1	5.406281000	1.412548000	1.643615000

6	0.133203000	-4.985832000	-0.052589000
6	0.776586000	-5.707159000	-1.085088000
6	0.753444000	-7.114044000	-1.095980000
6	0.097809000	-7.819960000	-0.067327000
6	-0.539722000	-7.108817000	0.968878000
6	-0.527190000	-5.701625000	0.972889000
6	-4.791357000	0.085777000	-0.074157000
6	-5.501225000	0.736558000	-1.111416000
6	-6.903177000	0.749360000	-1.120551000
6	-7.626698000	0.118414000	-0.084318000
6	-6.927405000	-0.528948000	0.958404000
6	-5.524742000	-0.547316000	0.957455000
1	-4.953339000	1.216839000	-1.917221000
1	-7.445372000	1.240505000	-1.922855000
1	-7.481071000	-1.008049000	1.758268000
1	-4.993839000	-1.040133000	1.767102000
6	-0.330648000	5.736241000	-1.090684000
6	-9.113958000	0.157256000	-0.127913000
8	-9.787182000	0.712089000	-1.024096000
1	7.887927000	1.358560000	1.701672000
7	9.469817000	-0.126577000	0.141075000
8	-9.695921000	-0.491653000	0.937894000
6	-11.172710000	-0.515885000	0.999223000
1	-11.576533000	-1.015653000	0.114078000
1	-11.405913000	-1.076469000	1.904593000
1	-11.562218000	0.504454000	1.059216000
1	1.279788000	-5.168626000	-1.884102000
1	1.243785000	-7.654411000	-1.901521000
1	-1.042292000	-7.645179000	1.769578000
1	-1.014328000	-5.159094000	1.779169000
1	-0.811148000	5.199158000	-1.904557000
1	1.381820000	5.182646000	1.820148000
1	-0.769113000	7.685019000	-1.919683000
1	1.415687000	7.668383000	1.812569000
1	0.342536000	8.933749000	-0.059253000
1	0.084739000	-8.906851000	-0.072819000
79	0.212468000	0.013429000	-0.029464000
8	10.128775000	0.657460000	1.019062000
8	10.138507000	-0.931973000	-0.709803000

### [1a<sup>+</sup>PF<sub>6</sub>]

7	-1.429033000	-1.124024000	-0.853684000
7	1.457642000	-1.286153000	-0.689884000
7	-1.290145000	1.752916000	-0.525890000
7	1.600518000	1.593804000	-0.373952000
6	-2.791782000	-0.833456000	-0.928504000
6	-3.506243000	-2.058290000	-1.219189000
6	-2.585329000	-3.073229000	-1.282336000
6	-1.280420000	-2.500998000	-1.030997000
1	-4.573387000	-2.128733000	-1.361571000
1	-2.765558000	-4.117671000	-1.482823000
6	-0.091507000	-3.241025000	-0.951364000
6	-3.396995000	0.417658000	-0.741201000
6	2.406416000	-3.389406000	-0.628355000
6	3.424230000	-2.478575000	-0.488611000
6	2.841509000	-1.155019000	-0.531863000
6	1.169390000	-2.652917000	-0.766346000
1	2.478783000	-4.465625000	-0.623300000
1	4.474562000	-2.681523000	-0.348876000
6	3.568519000	0.040878000	-0.424689000
6	-1.010319000	3.106599000	-0.310038000
6	-2.263715000	3.812754000	-0.155513000
6	-3.279588000	2.899109000	-0.288078000
6	-2.679927000	1.604863000	-0.531765000
1	-2.348964000	4.868653000	0.047912000
1	-4.340171000	3.080765000	-0.209520000
6	3.696203000	2.561297000	-0.357822000
6	2.775751000	3.579264000	-0.311557000
6	1.457422000	2.984167000	-0.308881000
6	2.970187000	1.310368000	-0.387538000
1	4.771326000	2.647099000	-0.385092000
1	2.966997000	4.640720000	-0.293622000
6	0.256021000	3.709240000	-0.244165000
6	-0.181516000	-4.737021000	-1.018340000
6	-0.805921000	-5.446320000	0.033944000
6	-0.888453000	-6.850493000	-0.008693000
6	-0.357735000	-7.559548000	-1.105197000

6	0.261838000	-6.856531000	-2.157821000
6	-4.895775000	0.479493000	-0.728054000
6	-5.601943000	1.148724000	-1.754147000
6	-7.002323000	1.201702000	-1.741242000
6	-7.688220000	0.584085000	-0.679353000
6	-7.012655000	-0.082901000	0.359269000
6	-5.612340000	-0.135583000	0.326381000
1	-5.056646000	1.613518000	-2.569906000
1	-7.552891000	1.703530000	-2.528154000
1	-5.066656000	-0.635706000	1.120796000
6	0.329393000	5.200439000	-0.091303000
6	-0.118693000	6.050041000	-1.128643000
6	-0.046151000	7.448374000	-0.987299000
6	0.465207000	8.014808000	0.197430000
6	0.908104000	7.173711000	1.237797000
6	0.845690000	5.775341000	1.092530000
6	5.064361000	-0.041218000	-0.339268000
6	5.823042000	-0.499428000	-1.441010000
6	7.221379000	-0.569812000	-1.361964000
6	7.885372000	-0.192465000	-0.174113000
6	7.133511000	0.259874000	0.932379000
6	5.735157000	0.338671000	0.845794000
1	5.319987000	-0.785465000	-2.360411000
1	7.805476000	-0.913325000	-2.210192000
1	7.642016000	0.543908000	1.846923000
1	5.161366000	0.680236000	1.702601000
6	0.354756000	-5.452650000	-2.112062000
6	9.371551000	-0.285631000	-0.129979000
8	10.088318000	-0.676634000	-1.076865000
1	-7.571160000	-0.542483000	1.166368000
7	-9.156529000	0.637746000	-0.655901000
8	9.894360000	0.109379000	1.079485000
6	11.363468000	0.056786000	1.238896000
1	11.842957000	0.714391000	0.508165000
1	11.546806000	0.403301000	2.255974000
1	11.718034000	-0.969075000	1.104291000
1	-0.508788000	5.619151000	-2.047414000
1	-0.386340000	8.089708000	-1.796127000
1	1.298106000	7.602225000	2.157250000
1	1.180977000	5.131830000	1.901937000
1	0.828810000	-4.914518000	-2.929328000
1	-1.207131000	-4.898304000	0.882743000
1	0.669917000	-7.396174000	-3.008495000
1	-1.362638000	-7.386349000	0.809416000
1	-0.425510000	-8.643936000	-1.138705000
1	0.516818000	9.094786000	0.308634000
79	0.082210000	0.232152000	-0.597942000
8	-9.777169000	0.073522000	0.313067000
8	-9.764491000	1.247106000	-1.606401000
9	-1.183600000	-0.218353000	2.246133000
9	-2.419394000	-0.215968000	4.356402000
9	-0.401018000	-1.590865000	4.114978000
15	-1.894714000	-1.441917000	3.256625000
9	-3.385273000	-1.286127000	2.377259000
9	-2.608373000	-2.659244000	4.252813000
9	-1.371438000	-2.663624000	2.139832000

**[1a<sup>III</sup>PF<sub>6</sub>]<sup>-</sup>**

7	-1.408606000	-0.958248000	-0.936870000
7	1.574280000	-1.249423000	-0.769617000
7	-1.153856000	1.999993000	-0.484018000
7	1.824006000	1.695934000	-0.225105000
6	-2.742490000	-0.592425000	-1.028221000
6	-3.506112000	-1.784512000	-1.392432000
6	-2.622532000	-2.834509000	-1.481651000
6	-1.289410000	-2.320312000	-1.178519000
1	-4.571570000	-1.817779000	-1.564711000
1	-2.851355000	-3.858522000	-1.735796000
6	-0.094486000	-3.086710000	-1.139420000
6	-3.275552000	0.708867000	-0.819199000
6	2.434496000	-3.382754000	-0.811491000
6	3.486907000	-2.518684000	-0.606073000
6	2.947035000	-1.161329000	-0.580521000
6	1.218155000	-2.582303000	-0.925074000
1	2.476994000	-4.460472000	-0.861141000
1	4.524192000	-2.781205000	-0.459428000
6	3.694122000	0.029077000	-0.366560000

6	-0.808228000	3.311685000	-0.181952000
6	-2.046110000	4.072096000	-0.031036000
6	-3.096702000	3.209686000	-0.250060000
6	-2.535473000	1.892929000	-0.546618000
1	-2.106360000	5.117623000	0.232186000
1	-4.149188000	3.443909000	-0.190236000
6	3.949223000	2.569488000	-0.098375000
6	3.064718000	3.620991000	-0.003806000
6	1.713269000	3.072521000	-0.077109000
6	3.167318000	1.342939000	-0.232380000
1	5.027746000	2.625612000	-0.096680000
1	3.306729000	4.669266000	0.089401000
6	0.507059000	3.824647000	-0.022483000
6	-0.238612000	-4.574091000	-1.303900000
6	-0.957517000	-5.325732000	-0.343708000
6	-1.089867000	-6.720179000	-0.484135000
6	-0.515771000	-7.382219000	-1.588320000
6	0.196756000	-6.639352000	-2.551069000
6	-4.769688000	0.837027000	-0.858678000
6	-5.403748000	1.659811000	-1.821994000
6	-6.798308000	1.779117000	-1.863164000
6	-7.563651000	1.071365000	-0.916272000
6	-6.964478000	0.250126000	0.058565000
6	-5.568591000	0.133873000	0.078283000
1	-4.800864000	2.190311000	-2.552582000
1	-7.287546000	2.397679000	-2.606451000
1	-5.087544000	-0.484323000	0.830422000
6	0.636648000	5.301347000	0.231583000
6	0.242339000	6.240810000	-0.749518000
6	0.366279000	7.622892000	-0.512436000
6	0.878410000	8.088274000	0.715354000
6	1.269559000	7.160122000	1.701225000
6	1.153869000	5.778403000	1.458690000
6	5.186425000	-0.116900000	-0.269895000
6	5.939605000	-0.574932000	-1.377349000
6	7.332635000	-0.708195000	-1.291470000
6	8.004094000	-0.395629000	-0.088309000
6	7.260819000	0.056780000	1.024837000
6	5.868204000	0.198278000	0.929394000
1	5.432031000	-0.811143000	-2.308256000
1	7.907590000	-1.051018000	-2.146449000
1	7.772280000	0.290625000	1.952101000
1	5.301927000	0.537488000	1.792041000
6	0.338265000	-5.246145000	-2.406191000
6	9.481793000	-0.556410000	-0.035283000
8	10.192995000	-0.952328000	-0.985528000
1	-7.579287000	-0.275369000	0.780153000
7	-9.022527000	1.193889000	-0.947751000
8	10.013390000	-0.220593000	1.190650000
6	11.476108000	-0.348532000	1.356876000
1	11.992974000	0.305716000	0.648806000
1	11.668973000	-0.040887000	2.384799000
1	11.782946000	-1.385845000	1.194532000
1	-0.147514000	5.888702000	-1.701368000
1	0.065470000	8.330363000	-1.281226000
1	1.660298000	7.508494000	2.654081000
1	1.449464000	5.068153000	2.226764000
1	0.883065000	-4.677511000	-3.155989000
1	-1.397596000	-4.817379000	0.510691000
1	0.638723000	-7.139726000	-3.409298000
1	-1.637836000	-7.285616000	0.265657000
1	-0.622285000	-8.458856000	-1.697081000
1	0.970333000	9.155556000	0.901030000
79	0.206409000	0.368825000	-0.589991000
8	-9.560272000	1.955248000	-1.831592000
8	-9.717608000	0.536739000	-0.091726000
9	-1.482015000	-1.162928000	2.789164000
9	-3.165693000	-1.156573000	4.568230000
15	-2.702366000	-2.268633000	3.325707000
9	-2.243984000	-3.382349000	2.076669000
9	-3.927729000	-3.372634000	3.852162000
9	-1.566141000	-3.008003000	4.400927000
9	-3.845045000	-1.529389000	2.245735000

**[1a''...PF<sub>6</sub>]<sup>-</sup>**

7	-1.602519000	-1.173078000	-0.710296000
7	1.315052000	-1.242623000	-0.715067000



7	-1.534413000	1.706021000	-0.397275000
7	1.381780000	1.632807000	-0.355534000
6	-2.969046000	-0.919118000	-0.851882000
6	-3.622058000	-2.157429000	-1.204589000
6	-2.669025000	-3.152969000	-1.211188000
6	-1.401255000	-2.549985000	-0.901642000
1	-4.670965000	-2.258914000	-1.431513000
1	-2.811859000	-4.199055000	-1.434224000
6	-0.183298000	-3.249333000	-0.827401000
6	-3.626351000	0.323637000	-0.664737000
6	-2.326988000	-3.315216000	-0.592979000
6	3.322983000	-2.367459000	-0.560105000
6	2.697604000	-1.064519000	-0.636501000
6	1.063966000	-2.626810000	-0.706047000
1	2.435793000	-4.387199000	-0.534459000
1	4.384739000	-2.532240000	-0.461539000
6	3.393951000	0.159234000	-0.615237000
6	-1.279742000	3.050625000	-0.067907000
6	-2.536203000	3.692774000	0.207881000
6	-3.534894000	2.760020000	0.026711000
6	-2.918278000	1.518543000	-0.373412000
1	-2.645417000	4.718338000	0.524661000
1	-4.592867000	2.898233000	0.182443000
6	3.423837000	2.688534000	-0.550163000
6	2.473834000	3.667375000	-0.375213000
6	1.189393000	3.021899000	-0.243762000
6	2.751183000	1.407352000	-0.520203000
1	4.483976000	2.821431000	-0.699989000
1	2.625913000	4.735563000	-0.354333000
6	-0.025844000	3.688948000	-0.039146000
6	-0.234558000	-4.748330000	-0.867875000
6	-0.826884000	-5.458610000	0.202006000
6	-0.878775000	-6.864851000	0.179055000
6	-0.349150000	-7.577280000	-0.915978000
6	0.239347000	-6.874414000	-1.986409000
6	-5.102148000	0.381448000	-0.757760000
6	-5.745364000	1.354220000	-1.577963000
6	-7.133786000	1.412398000	-1.693916000
6	-7.935257000	0.501442000	-0.958519000
6	-7.324050000	-0.464201000	-0.117750000
6	-5.932962000	-0.523637000	-0.035070000
1	-5.137937000	2.041480000	-2.159938000
1	-7.611702000	2.135316000	-2.344487000
1	-5.474579000	-1.247415000	0.631980000
6	0.011644000	5.168685000	0.208683000
6	-0.576217000	6.070481000	-0.708375000
6	-0.533605000	7.457698000	-0.475379000
6	0.087712000	7.962671000	0.684567000
6	0.671216000	7.070486000	1.606241000
6	0.638509000	5.683958000	1.366819000
6	4.890573000	0.126861000	-0.672737000
6	5.556728000	-0.406164000	-1.802739000
6	6.956961000	-0.432695000	-1.863645000
6	7.725067000	0.065873000	-0.787753000
6	7.070346000	0.592122000	0.348277000
6	5.668968000	0.624248000	0.399790000
1	4.974316000	-0.784214000	-2.638303000
1	7.464246000	-0.833174000	-2.736170000
1	7.657329000	0.966615000	1.179638000
1	5.172964000	1.019285000	1.281722000
6	0.301044000	-5.468159000	-1.959592000
6	9.208094000	0.018497000	-0.889734000
8	9.843397000	-0.431987000	-1.869032000
1	-7.947980000	-1.136472000	0.459436000
7	-9.356217000	0.558010000	-1.063732000
8	9.837224000	0.530976000	0.223503000
6	11.314881000	0.529865000	0.232661000
1	11.695630000	1.140067000	-0.591561000
1	11.589178000	0.960358000	1.195912000
1	11.689809000	-0.493464000	0.139880000
1	-1.052648000	5.687805000	-1.607429000
1	-0.982465000	8.138539000	-1.194124000
1	1.147238000	7.450031000	2.506726000
1	1.083239000	4.999941000	2.085071000
1	0.750522000	-4.929713000	-2.790463000
1	-1.222799000	-4.907731000	1.050812000
1	0.646868000	-7.415924000	-2.836438000
1	-1.327777000	-7.400122000	1.011880000

1	-0.393697000	-8.663428000	-0.934527000
1	0.115713000	9.033880000	0.867608000
79	-0.110109000	0.228086000	-0.531249000
8	-10.086340000	-0.308020000	-0.395438000
8	-9.908558000	1.475070000	-1.828487000
9	0.402646000	-0.783384000	2.512901000
9	-0.508358000	-0.303760000	4.734133000
9	0.686725000	-2.404189000	4.324921000
15	-0.669873000	-1.605949000	3.605933000
9	-2.022804000	-0.805203000	2.875550000
9	-1.737916000	-2.425590000	4.691842000
9	-0.829858000	-2.906311000	2.467771000

**[2a]<sup>+</sup>**

7	2.015073000	1.424382000	0.010459000
7	-0.887364000	1.484436000	-0.067041000
7	1.956993000	-1.472878000	-0.031519000
7	-0.946329000	-1.413735000	-0.080577000
6	3.392851000	1.178818000	-0.046114000
6	4.069520000	2.438967000	-0.248810000
6	3.117227000	3.429668000	-0.284852000
6	1.826059000	2.806872000	-0.111166000
1	5.135404000	2.546446000	-0.372208000
1	3.271512000	4.486366000	-0.437117000
6	0.603902000	3.502406000	-0.063687000
6	4.042051000	-0.067080000	0.074791000
6	-1.908731000	3.540520000	0.178057000
6	-2.899302000	2.589626000	0.181159000
6	-2.272013000	1.296609000	0.013390000
6	-0.642194000	2.861579000	0.011839000
1	-2.019347000	4.607237000	0.294775000
1	-3.960077000	2.745609000	0.300981000
6	-2.962872000	0.076985000	-0.071525000
6	1.705173000	-2.848489000	0.035158000
6	2.955209000	-3.529700000	0.276922000
6	3.945655000	-2.578886000	0.343988000
6	3.336592000	-1.286578000	0.129151000
1	3.055374000	-4.595998000	0.405744000
1	4.994155000	-2.734938000	0.541443000
6	-2.997983000	-2.430014000	-0.375237000
6	-2.046082000	-3.419483000	-0.395421000
6	-0.755650000	-2.797586000	-0.193401000
6	-2.320681000	-1.168302000	-0.168233000
1	-4.063107000	-2.538925000	-0.508037000
1	-2.198119000	-4.476867000	-0.545442000
6	0.460434000	-3.490925000	-0.098596000
6	0.634584000	5.001872000	-0.092048000
6	1.239235000	5.728755000	0.959569000
6	1.260821000	7.135407000	0.934503000
6	0.689143000	7.833732000	-0.147926000
6	0.090234000	7.116070000	-1.202467000
6	5.530267000	-0.092720000	0.146591000
6	6.302019000	-0.844296000	-0.775606000
6	7.699420000	-0.865265000	-0.713826000
6	8.390529000	-0.143232000	0.299985000
6	7.621292000	0.608110000	1.232709000
6	6.225703000	0.636181000	1.144788000
1	5.802633000	-1.394890000	-1.569154000
1	8.265108000	-1.434762000	-1.447640000
1	5.664125000	1.207569000	1.879935000
6	0.434999000	-4.990528000	-0.129025000
6	1.057035000	-5.695297000	-1.185595000
6	1.030299000	-7.101712000	-1.218609000
6	0.392661000	-7.822483000	-0.189084000
6	-0.223188000	-7.127227000	0.870741000
6	-0.207257000	-5.720446000	0.897835000
6	-4.462831000	0.102852000	-0.060171000
6	-5.182580000	0.706534000	-1.117300000
6	-6.584800000	0.723235000	-1.105354000
6	-7.292963000	0.144788000	-0.029251000
6	-6.581227000	-0.455171000	1.032533000
6	-5.178528000	-0.479132000	1.011733000
1	-4.645689000	1.146908000	-1.952695000
1	-7.138221000	1.178356000	-1.920969000
1	-7.124393000	-0.894730000	1.861600000
1	-4.636756000	-0.936245000	1.834959000
6	0.057663000	5.709680000	-1.171958000

6	-8.782167000	0.187863000	-0.051901000
8	-9.464606000	0.708977000	-0.960397000
1	8.124597000	1.161518000	2.021978000
7	9.771884000	-0.170642000	0.376806000
1	10.265081000	0.339615000	1.095686000
8	-9.348481000	-0.414746000	1.047261000
6	-10.824758000	-0.431612000	1.133516000
1	-11.244011000	-0.959224000	0.272149000
1	-11.044565000	-0.960573000	2.060899000
1	-11.209192000	0.591829000	1.165639000
1	1.545438000	-5.145229000	-1.986004000
1	1.503361000	-7.630067000	-2.042109000
1	-0.711816000	-7.675621000	1.671747000
1	-0.677273000	-5.190820000	1.722670000
1	-0.399692000	5.161999000	-1.992105000
1	1.675638000	5.196773000	1.801159000
1	-0.348320000	7.646628000	-2.043450000
1	1.719727000	7.681507000	1.754424000
1	0.709894000	8.920196000	-0.169217000
1	0.376363000	-8.908988000	-0.212138000
79	0.534380000	0.005435000	-0.042188000
1	10.320414000	-0.710638000	-0.277185000

## 2a

7	2.061948000	1.481007000	0.052744000
7	-0.943937000	1.530363000	-0.055741000
7	2.015401000	-1.519083000	-0.056993000
7	-0.992526000	-1.471061000	-0.038295000
6	3.427688000	1.225894000	-0.003776000
6	4.110726000	2.509121000	-0.135007000
6	3.151086000	3.497880000	-0.141945000
6	1.848266000	2.851990000	-0.018929000
1	5.177990000	2.636982000	-0.236077000
1	3.311746000	4.560930000	-0.243598000
6	0.589513000	3.517162000	-0.006442000
6	4.057792000	-0.051755000	0.033857000
6	-1.973429000	3.583390000	0.088693000
6	-2.963155000	2.626295000	0.069578000
6	-2.315952000	1.319730000	-0.030737000
6	-0.687373000	2.895841000	0.001992000
1	-2.103284000	4.652216000	0.172200000
1	-4.028403000	2.792221000	0.133887000
6	-2.978023000	0.062068000	-0.072442000
6	1.755173000	-2.882454000	0.004457000
6	3.031479000	-3.570561000	0.168722000
6	4.022307000	-2.613489000	0.197431000
6	3.386014000	-1.308494000	0.046623000
1	3.154021000	-4.638491000	0.272357000
1	5.080734000	-2.776360000	0.334218000
6	-3.041893000	-2.501026000	-0.220016000
6	-2.083374000	-3.489575000	-0.215614000
6	-0.778678000	-2.844061000	-0.092328000
6	-2.355811000	-1.216228000	-0.099275000
1	-4.109843000	-2.632326000	-0.313275000
1	-2.245124000	-4.553482000	-0.305864000
6	0.476588000	-3.506397000	-0.048434000
6	0.616587000	5.021073000	-0.010685000
6	1.159873000	5.734888000	1.083056000
6	1.182314000	7.142341000	1.083290000
6	0.670249000	7.859612000	-0.016586000
6	0.131703000	7.157646000	-1.113592000
6	5.555222000	-0.075711000	0.065643000
6	6.303435000	-0.729849000	-0.943742000
6	7.704514000	-0.752444000	-0.922684000
6	8.421636000	-0.127450000	0.134021000
6	7.678022000	0.525741000	1.154735000
6	6.277709000	0.553470000	1.109165000
1	5.780832000	-1.208494000	-1.768606000
1	8.250610000	-1.250003000	-1.721391000
1	5.733973000	1.051385000	1.908570000
6	0.454944000	-5.010409000	-0.047908000
6	1.004956000	-5.739090000	-1.128369000
6	0.981156000	-7.146546000	-1.132502000
6	0.415467000	-7.849124000	-0.049549000
6	-0.129893000	-7.132407000	1.034480000
6	-0.114033000	-5.724787000	1.032239000
6	-4.480603000	0.085736000	-0.088248000

6	-5.184397000	0.650535000	-1.178732000
6	-6.586348000	0.669152000	-1.195427000
6	-7.317772000	0.129214000	-0.114058000
6	-6.625042000	-0.432696000	0.981521000
6	-5.222293000	-0.456118000	0.988360000
1	-4.630164000	1.060032000	-2.018477000
1	-7.122711000	1.095577000	-2.037771000
1	-7.183689000	-0.842546000	1.815785000
1	-4.696271000	-0.881770000	1.838199000
6	0.101171000	5.750285000	-1.107669000
6	-8.803666000	0.171539000	-0.167358000
8	-9.472043000	0.661861000	-1.104375000
1	8.202848000	1.004682000	1.978564000
7	9.809663000	-0.154379000	0.168333000
1	10.320439000	0.289694000	0.917664000
8	-9.394675000	-0.395056000	0.940760000
6	-10.871392000	-0.406424000	0.995511000
1	-11.274484000	-0.963449000	0.144814000
1	-11.112848000	-0.901810000	1.936136000
1	-11.255195000	0.617815000	0.983135000
1	1.437194000	-5.203456000	-1.969898000
1	1.400515000	-7.689873000	-1.975655000
1	-0.563913000	-7.664828000	1.877178000
1	-0.529834000	-5.178504000	1.875202000
1	-0.308939000	5.215256000	-1.960561000
1	1.550663000	5.188177000	1.937622000
1	-0.261302000	7.701252000	-1.969162000
1	1.595815000	7.674307000	1.936523000
1	0.690639000	8.946597000	-0.018829000
1	0.400213000	-8.936196000	-0.050293000
79	0.534984000	0.005262000	-0.024437000
1	10.339110000	-0.624635000	-0.551409000

**[3a]<sup>+</sup>**

7	-1.424907000	1.507089000	-0.092426000
7	1.474077000	1.472725000	0.029136000
7	-1.460503000	-1.391005000	-0.072655000
7	1.439224000	-1.426345000	0.016984000
6	-2.810605000	1.308016000	-0.059309000
6	-3.452297000	2.596129000	0.081059000
6	-2.469574000	3.555169000	0.110634000
6	-1.193848000	2.885277000	-0.007256000
1	-4.517568000	2.742369000	0.166087000
1	-2.592362000	4.621096000	0.221550000
6	0.049960000	3.539156000	-0.030353000
6	-3.493088000	0.082344000	-0.150070000
6	2.570261000	3.495898000	-0.158063000
6	3.529193000	2.513924000	-0.120436000
6	2.853941000	1.240962000	0.007545000
6	1.276889000	2.856759000	-0.052939000
1	2.719901000	4.559071000	-0.262418000
1	4.598837000	2.636322000	-0.189708000
6	3.501810000	-0.001383000	0.096762000
6	-1.256984000	-2.774418000	-0.143248000
6	-2.537244000	-3.413748000	-0.349139000
6	-3.496844000	-2.431730000	-0.383488000
6	-2.835580000	-1.159262000	-0.197730000
1	-2.677304000	-4.476537000	-0.469121000
1	-4.557421000	-2.552830000	-0.538127000
6	3.452917000	-2.516264000	0.312824000
6	2.470585000	-3.475003000	0.279632000
6	1.203866000	-2.805228000	0.081670000
6	2.819206000	-1.227562000	0.138274000
1	4.511511000	-2.663991000	0.459455000
1	2.586430000	-4.541362000	0.393722000
6	-0.034075000	-3.458025000	-0.031973000
6	0.066866000	5.039551000	-0.028244000
6	-0.455823000	5.763925000	-1.124276000
6	-0.434963000	7.170901000	-1.124400000
6	0.097657000	7.871604000	-0.023808000
6	0.614726000	7.156069000	1.074602000
6	-4.989793000	0.099072000	-0.193849000
6	-5.752132000	-0.502262000	0.831825000
6	-7.155959000	-0.488753000	0.810859000
6	-7.834127000	0.128092000	-0.267394000
6	-7.078565000	0.727181000	-1.304880000
6	-5.678944000	0.718145000	-1.262810000

1	-5.245977000	-0.972014000	1.671309000
1	-7.723990000	-0.943286000	1.610639000
1	-5.120102000	1.177249000	-2.073756000
6	-0.052491000	-4.958429000	-0.035536000
6	-0.669814000	-5.670248000	1.018719000
6	-0.681748000	-7.077341000	1.018108000
6	-0.087238000	-7.790419000	-0.042079000
6	0.524551000	-7.087327000	-1.099074000
6	0.547111000	-5.680356000	-1.093162000
6	5.001295000	-0.019372000	0.149423000
6	5.687102000	0.524748000	1.259954000
6	7.088405000	0.505218000	1.309980000
6	7.829371000	-0.049847000	0.243798000
6	7.151333000	-0.590816000	-0.870416000
6	5.748789000	-0.579148000	-0.912046000
1	5.124112000	0.947851000	2.087032000
1	7.615790000	0.914993000	2.165849000
1	7.720027000	-1.012679000	-1.691506000
1	5.233475000	-0.990364000	-1.775465000
6	0.604807000	5.748966000	1.070183000
6	9.316917000	-0.044250000	0.332739000
8	9.969726000	0.425286000	1.289793000
1	-7.585870000	1.198556000	-2.143861000
6	-10.206802000	-0.321613000	0.487361000
8	-9.922778000	-0.944246000	1.549344000
7	-9.248927000	0.185899000	-0.374100000
1	-9.601157000	0.665506000	-1.196227000
8	9.917452000	-0.617668000	-0.763583000
6	11.395473000	-0.665494000	-0.787178000
1	11.765150000	-1.237317000	0.068640000
1	11.644180000	-1.161225000	-1.725533000
1	11.802820000	0.349171000	-0.760083000
6	-11.648073000	-0.086630000	0.065176000
1	-12.189871000	0.385884000	0.891435000
1	-11.744991000	0.540273000	-0.826398000
1	-12.126244000	-1.053419000	-0.131146000
1	-1.124504000	-5.126445000	1.842925000
1	-1.151187000	-7.612059000	1.839530000
1	0.980726000	-7.629661000	-1.922994000
1	1.014791000	-5.144012000	-1.915021000
1	0.998570000	5.203189000	1.923924000
1	-0.862023000	5.229387000	-1.979334000
1	1.022574000	7.688830000	1.929498000
1	-0.831203000	7.715162000	-1.977528000
1	0.109448000	8.958396000	-0.022095000
1	-0.100498000	-8.877192000	-0.044538000
79	0.007056000	0.040538000	-0.029716000

### 3a

7	-1.479178000	1.554161000	-0.109391000
7	1.521527000	1.527879000	0.049053000
7	-1.508091000	-1.448746000	-0.040464000
7	1.496512000	-1.475619000	0.001838000
6	-2.850786000	1.332273000	-0.094774000
6	-3.508125000	2.633045000	0.001711000
6	-2.525865000	3.598060000	0.032685000
6	-1.234584000	2.920033000	-0.042908000
1	-4.575058000	2.788392000	0.061777000
1	-2.664138000	4.665598000	0.118888000
6	0.039270000	3.553122000	-0.025441000
6	-3.505933000	0.070223000	-0.141150000
6	2.604887000	3.554581000	-0.067511000
6	3.569838000	2.572861000	-0.033885000
6	2.888281000	1.282729000	0.047370000
6	1.300757000	2.898903000	-0.008283000
1	2.762836000	4.620154000	-0.143381000
1	4.639863000	2.712283000	-0.078392000
6	3.517464000	0.008336000	0.091236000
6	-1.283794000	-2.818850000	-0.087962000
6	-2.579232000	-3.474701000	-0.244818000
6	-3.544426000	-2.492808000	-0.279406000
6	-2.871927000	-1.203253000	-0.143495000
1	-2.730434000	-4.540090000	-0.335472000
1	-4.608097000	-2.630360000	-0.404815000
6	3.516072000	-2.556665000	0.219323000
6	2.533684000	-3.521026000	0.189643000
6	1.248159000	-2.842367000	0.044727000

6	2.864295000	-1.254649000	0.093494000
1	4.578161000	-2.714948000	0.334590000
1	2.667073000	-4.589143000	0.276163000
6	-0.023004000	-3.474166000	-0.020932000
6	0.051343000	5.057292000	-0.021227000
6	-0.442895000	5.785409000	-1.128574000
6	-0.427547000	7.192989000	-1.127980000
6	0.073738000	7.895883000	-0.013996000
6	0.563576000	7.179514000	1.096449000
6	-5.006878000	0.084196000	-0.191497000
6	-5.778590000	-0.472611000	0.852244000
6	-7.183533000	-0.461795000	0.822896000
6	-7.854870000	0.110257000	-0.282917000
6	-7.093308000	0.666599000	-1.338670000
6	-5.693114000	0.657550000	-1.287789000
1	-5.276197000	-0.907549000	1.712501000
1	-7.755981000	-0.884459000	1.637167000
1	-5.128263000	1.083473000	-2.112585000
6	-0.037324000	-4.978336000	-0.022543000
6	-0.610153000	-5.694745000	1.054125000
6	-0.620275000	-7.102398000	1.056090000
6	-0.065643000	-7.816689000	-0.024857000
6	0.503098000	-7.111874000	-1.104665000
6	0.521030000	-5.704269000	-1.100405000
6	5.019558000	-0.005425000	0.139447000
6	5.712549000	0.534024000	1.249416000
6	7.113786000	0.516227000	1.297449000
6	7.855062000	-0.035085000	0.228691000
6	7.173098000	-0.571267000	-0.886292000
6	5.770701000	-0.558605000	-0.924611000
1	5.150359000	0.951949000	2.079645000
1	7.641864000	0.922955000	2.154616000
1	7.739763000	-0.989873000	-1.710730000
1	5.253277000	-0.964916000	-1.789047000
6	0.556495000	5.771872000	1.089990000
6	9.340125000	-0.032244000	0.315772000
8	9.999346000	0.432670000	1.271960000
1	-7.596100000	1.104438000	-2.198789000
6	-10.236815000	-0.314063000	0.462836000
8	-9.966922000	-0.900761000	1.549993000
7	-9.271671000	0.164480000	-0.402960000
1	-9.614613000	0.616494000	-1.244302000
8	9.940943000	-0.605155000	-0.783565000
6	11.417772000	-0.655752000	-0.805051000
1	11.786420000	-1.229234000	0.050305000
1	11.667268000	-1.150835000	-1.743718000
1	11.828194000	0.357755000	-0.776222000
6	-11.674397000	-0.094303000	0.017420000
1	-12.218854000	0.428222000	0.811465000
1	-11.761076000	0.481865000	-0.908913000
1	-12.157473000	-1.067655000	-0.127138000
1	-1.033881000	-5.150238000	1.894292000
1	-1.057323000	-7.636647000	1.896008000
1	0.929261000	-7.653432000	-1.945519000
1	0.955128000	-5.166905000	-1.939909000
1	0.929249000	5.225862000	1.953014000
1	-0.824754000	5.249653000	-1.994070000
1	0.947936000	7.712138000	1.962746000
1	-0.803447000	7.736096000	-1.991499000
1	0.082405000	8.983002000	-0.011244000
1	-0.076498000	-8.903791000	-0.025738000
79	0.007757000	0.039271000	-0.024855000

**[4a]<sup>+</sup>**

7	-1.200372000	1.512789000	-0.099938000
7	1.698137000	1.440906000	-0.002995000
7	-1.273383000	-1.385044000	-0.086832000
7	1.625571000	-1.458291000	-0.019646000
6	-2.588117000	1.331501000	-0.050257000
6	-3.211571000	2.627889000	0.095930000
6	-2.216377000	3.574378000	0.111134000
6	-0.950851000	2.887910000	-0.020581000
1	-4.273777000	2.787818000	0.193688000
1	-2.324025000	4.642023000	0.221334000
6	0.301012000	3.525672000	-0.058501000
6	-3.287362000	0.114809000	-0.134130000
6	2.819835000	3.449093000	-0.200608000

6	3.766010000	2.454859000	-0.162930000
6	3.074553000	1.191112000	-0.029256000
6	1.518653000	2.827262000	-0.087840000
1	2.982866000	4.509891000	-0.308986000
1	4.836879000	2.563374000	-0.236575000
6	3.706067000	-0.059745000	0.058176000
6	-1.088519000	-2.770556000	-0.167557000
6	-2.379066000	-3.392147000	-0.363221000
6	-3.326279000	-2.397719000	-0.380388000
6	-2.646567000	-1.134988000	-0.194818000
1	-2.534182000	-4.452286000	-0.488033000
1	-4.390018000	-2.504193000	-0.523617000
6	3.626384000	-2.574953000	0.264169000
6	2.632009000	-3.521051000	0.228604000
6	1.373137000	-2.834317000	0.038877000
6	3.008399000	-1.277454000	0.097954000
1	4.683392000	-2.737220000	0.406810000
1	2.734810000	-4.589394000	0.336495000
6	0.126375000	-3.470611000	-0.071023000
6	0.336479000	5.025681000	-0.064534000
6	-0.186953000	5.749965000	-1.160311000
6	-0.149490000	7.156573000	-1.168734000
6	0.400607000	7.857110000	-0.076674000
6	0.918444000	7.141736000	1.021479000
6	-4.784210000	0.149584000	-0.157379000
6	-5.538725000	-0.446026000	0.877440000
6	-6.942455000	-0.417800000	0.875806000
6	-7.628720000	0.208200000	-0.191976000
6	-6.881217000	0.801825000	-1.238399000
6	-5.481297000	0.778300000	-1.215491000
1	-5.025977000	-0.923191000	1.708713000
1	-7.504320000	-0.868345000	1.682169000
1	-4.928911000	1.233072000	-2.033278000
6	0.089310000	-4.970548000	-0.084715000
6	-0.529479000	-5.682365000	0.968675000
6	-0.558079000	-7.089174000	0.958374000
6	0.021052000	-7.801794000	-0.110602000
6	0.634225000	-7.098615000	-1.166728000
6	0.673490000	-5.692092000	-1.151223000
6	5.205307000	-0.096222000	0.110264000
6	5.896504000	0.440144000	1.221673000
6	7.296962000	0.403401000	1.273554000
6	8.030542000	-0.162289000	0.207405000
6	7.348064000	-0.695178000	-0.907962000
6	5.946016000	-0.665455000	-0.950910000
1	5.337667000	0.870402000	2.047741000
1	7.828343000	0.806895000	2.129919000
1	7.912391000	-1.124550000	-1.728219000
1	5.426115000	-1.069947000	-1.814605000
6	0.891910000	5.734840000	1.025290000
6	9.513330000	-0.177653000	0.295920000
8	10.182839000	0.281095000	1.243989000
1	-7.395162000	1.279895000	-2.069511000
6	-9.995439000	-0.222088000	0.591998000
8	-9.703267000	-0.851396000	1.647824000
7	-9.044125000	0.280377000	-0.279652000
1	-9.402122000	0.766331000	-1.095533000
8	10.115994000	-0.765240000	-0.801104000
1	11.096965000	-0.762894000	-0.719076000
6	-11.439940000	0.027009000	0.189422000
1	-11.966752000	0.501453000	1.024224000
1	-11.543092000	0.657586000	-0.698848000
1	-11.929036000	-0.934955000	-0.003679000
1	-0.972132000	-5.139082000	1.799744000
1	-1.028375000	-7.624047000	1.779202000
1	1.078682000	-7.640500000	-1.997315000
1	1.142247000	-5.155557000	-1.972335000
1	1.286145000	5.189353000	1.878985000
1	-0.606832000	5.215375000	-2.008719000
1	1.339576000	7.674495000	1.869910000
1	-0.546544000	7.700643000	-2.021605000
1	0.425086000	8.943675000	-0.081268000
1	-0.004956000	-8.888286000	-0.120435000
79	0.212607000	0.027510000	-0.052303000

#### 4a

7	-1.256263000	1.556853000	-0.114756000
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6	-2.630178000	1.350754000	-0.089034000
6	-3.271764000	2.658896000	0.013481000
6	-2.278264000	3.612535000	0.036960000
6	-0.995549000	2.919736000	-0.049312000
1	-4.336323000	2.826358000	0.082274000
1	-2.403506000	4.681542000	0.124782000
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6	-3.300121000	0.096339000	-0.130781000
6	2.850582000	3.510403000	-0.101913000
6	3.804445000	2.517740000	-0.075793000
6	3.108671000	1.235366000	0.009182000
6	1.539508000	2.869614000	-0.033918000
1	3.020056000	4.574169000	-0.178154000
1	4.875606000	2.645350000	-0.128025000
6	3.723128000	-0.046394000	0.046724000
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6	-2.415189000	-3.458767000	-0.247126000
6	-3.369258000	-2.465807000	-0.271991000
6	-2.680804000	-1.184311000	-0.140018000
1	-2.579321000	-4.522199000	-0.338166000
1	-4.435488000	-2.590777000	-0.388518000
6	3.693677000	-2.611667000	0.170516000
6	2.700090000	-3.564601000	0.146440000
6	1.421448000	-2.871026000	0.012048000
6	3.055932000	-1.302041000	0.051228000
1	4.754600000	-2.782672000	0.278097000
1	2.821875000	-4.634305000	0.230373000
6	0.142658000	-3.488027000	-0.044537000
6	0.314991000	5.042146000	-0.035966000
6	-0.177955000	5.776767000	-1.139571000
6	-0.145997000	7.184061000	-1.138135000
6	0.370835000	7.880215000	-0.027020000
6	0.859455000	7.157324000	1.079734000
6	-4.801181000	0.127560000	-0.167269000
6	-5.569297000	-0.421023000	0.883470000
6	-6.974217000	-0.393496000	0.867732000
6	-7.649318000	0.187352000	-0.231187000
6	-6.891463000	0.735267000	-1.293991000
6	-5.491049000	0.709639000	-1.256649000
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1	-4.929153000	1.129355000	-2.086629000
6	0.110943000	-4.991923000	-0.048382000
6	-0.462251000	-5.703368000	1.031387000
6	-0.488882000	-7.110783000	1.031148000
6	0.049289000	-7.829719000	-0.055038000
6	0.618245000	-7.129771000	-1.137898000
6	0.652764000	-5.722494000	-1.131528000
6	5.225114000	-0.077291000	0.085947000
6	5.929708000	0.454467000	1.192836000
6	7.330332000	0.420600000	1.234192000
6	8.058415000	-0.139584000	0.160402000
6	7.365696000	-0.668038000	-0.951718000
6	5.963630000	-0.639239000	-0.982473000
1	5.376144000	0.878482000	2.025624000
1	7.867255000	0.820911000	2.088867000
1	7.923414000	-1.092999000	-1.779049000
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8	-9.755469000	-0.801994000	1.619928000
7	-9.066410000	0.258912000	-0.337487000
1	-9.411631000	0.716566000	-1.174841000
8	10.137351000	-0.730946000	-0.870845000
1	11.118377000	-0.726638000	-0.790627000
6	-11.468043000	0.028381000	0.106025000
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1	1.207648000	5.198884000	1.932650000
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1	1.255699000	7.684776000	1.943842000
1	-0.521130000	7.732204000	-1.998806000
1	0.392307000	8.967154000	-0.023647000
1	0.025680000	-8.916617000	-0.057606000
79	0.213782000	0.024972000	-0.043371000

**[4b]<sup>+</sup>**

7	1.466667000	1.376593000	-0.209349000
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7	-1.370787000	-1.577899000	0.043103000
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6	2.496174000	3.435013000	-0.045971000
6	3.486645000	2.483335000	-0.077587000
6	2.854125000	1.189127000	-0.196252000
1	2.612369000	4.502605000	0.055442000
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6	3.546565000	-0.032139000	-0.295165000
6	-0.025677000	3.397099000	-0.167473000
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6	2.897181000	-1.278897000	-0.313086000
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6	-3.352930000	-2.674492000	0.485328000
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6	-1.118004000	-2.951167000	0.139148000
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1	-4.399072000	-2.824501000	0.700489000
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6	5.039866000	-0.002094000	-0.388086000
6	5.685931000	0.640064000	-1.474312000
6	7.081694000	0.660565000	-1.572714000
6	7.871254000	0.047493000	-0.573592000
6	7.245807000	-0.590009000	0.520383000
6	-0.056420000	4.893135000	-0.215539000
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6	-0.667130000	7.047079000	0.802018000
6	-0.114105000	7.736935000	-0.303153000
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6	-7.136562000	-0.899866000	-0.542935000
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6	-0.480138000	-5.842526000	-1.001615000
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1	1.346520000	-7.703034000	1.897514000
1	-0.924662000	-7.815769000	-1.770130000
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6	5.842277000	-0.614573000	0.598542000
6	0.271012000	-9.402665000	0.129034000
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1	5.091576000	1.106919000	-2.255337000
1	7.827792000	-1.061121000	1.304688000
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1	-14.104271000	-1.516421000	0.796983000
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1	9.953696000	-0.025826000	1.219681000
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1	11.672652000	-0.647258000	-1.251919000
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6	12.631946000	-0.912024000	0.683860000
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#### 4b

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1	1.283062000	-7.712091000	2.014723000
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6	0.243103000	-9.429707000	0.241691000
8	0.784988000	-10.088460000	1.154481000
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6	-0.595036000	10.116425000	0.550286000
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7	-0.129713000	9.173229000	-0.346500000
1	0.272884000	9.536595000	-1.204289000
8	-0.383147000	-10.055669000	-0.823392000
1	-0.330112000	-11.035340000	-0.743820000
6	-0.440516000	11.563465000	0.107885000
1	0.074169000	12.124960000	0.894903000
1	0.114805000	11.675945000	-0.828342000
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1	-11.649354000	-1.086921000	1.075704000
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6	10.137424000	-0.415023000	0.367619000
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1	-14.688572000	-1.502092000	-1.181528000
6	12.598477000	-0.732768000	0.937816000

1	12.431079000	-0.258027000	1.916661000
1	12.429451000	-1.811222000	1.078387000
6	14.057030000	-0.495253000	0.494769000
1	14.765722000	-0.895567000	1.231373000
1	14.259160000	-0.983230000	-0.468496000
1	14.261931000	0.577593000	0.377180000

**[4c]<sup>+</sup>**

7	1.207371000	1.520096000	-0.087437000
7	1.770840000	-1.327113000	0.013887000
7	-1.634337000	0.958432000	-0.063568000
7	-1.072466000	-1.889018000	0.006398000
6	0.729321000	2.835452000	-0.050981000
6	1.860635000	3.727600000	0.075266000
6	3.000729000	2.962557000	0.091233000
6	2.603432000	1.576461000	-0.017321000
1	1.787290000	4.800213000	0.159685000
1	4.019489000	3.303886000	0.188719000
6	3.494375000	0.491508000	-0.041023000
6	-0.611367000	3.252466000	-0.126714000
6	3.978271000	-1.983400000	-0.156559000
6	3.214576000	-3.123457000	-0.125230000
6	1.828453000	-2.724777000	-0.007641000
6	3.084286000	-0.849703000	-0.059886000
1	5.050605000	-1.913999000	-0.252457000
1	3.555679000	-4.144677000	-0.191873000
6	0.745797000	-3.615077000	0.070700000
6	-2.946246000	0.476351000	-0.125970000
6	-3.838525000	1.599874000	-0.306510000
6	-3.074936000	2.740553000	-0.337000000
6	-1.691375000	2.353055000	-0.171321000
1	-4.909113000	1.523483000	-0.414778000
1	-3.413560000	3.754903000	-0.476587000
6	-1.726528000	-4.088073000	0.265533000
6	-2.866652000	-3.324330000	0.236412000
6	-2.469683000	-1.943616000	0.063191000
6	-0.594768000	-3.199867000	0.110432000
1	-1.654272000	-5.156415000	0.396260000
1	-3.885993000	-3.662185000	0.340052000
6	-3.358646000	-0.862833000	-0.032952000
6	4.966874000	0.784275000	-0.046851000
6	5.568798000	1.392331000	-1.171495000
6	6.945365000	1.660964000	-1.186270000
6	7.730363000	1.327456000	-0.064988000
6	7.144907000	0.727211000	1.065212000
6	-0.904340000	4.720268000	-0.154702000
6	-1.656646000	5.327085000	0.875420000
6	-1.938294000	6.702205000	0.870268000
6	-1.473003000	7.508006000	-0.196194000
6	-0.721069000	6.908464000	-1.236270000
6	-0.437044000	5.537616000	-1.210574000
1	-2.013186000	4.723654000	1.706214000
1	-2.506314000	7.151624000	1.672940000
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6	-5.648712000	-0.737747000	1.033930000
6	-7.025923000	-1.006548000	1.029386000
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6	-6.795886000	-2.106145000	-1.142910000
6	-5.418197000	-1.841140000	-1.126147000
6	1.036235000	-5.086750000	0.114117000
6	1.704845000	-5.652206000	1.224708000
6	1.971465000	-7.027804000	1.268802000
6	1.581844000	-7.859453000	0.195919000
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6	0.644578000	-5.925951000	-0.954103000
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1	2.476771000	-7.464960000	2.124389000
1	0.624047000	-7.940242000	-1.743844000
1	0.140421000	-5.500608000	-1.817181000
6	5.768342000	0.451977000	1.067376000
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8	2.471264000	-9.871634000	1.226582000
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6	-2.422689000	9.721669000	0.577100000
8	-2.972807000	9.300750000	1.633451000
7	-1.717616000	8.902928000	-0.289280000

1	-1.322062000	9.357721000	-1.105559000
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1	1.666931000	-10.976635000	-0.752988000
6	-2.499111000	11.183653000	0.168306000
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1	-1.934677000	11.412273000	-0.740750000
1	-3.548645000	11.456775000	0.009477000
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1	-7.235430000	-2.633519000	-1.983565000
1	-4.802628000	-2.157930000	-1.962637000
1	5.317186000	-0.009327000	1.940694000
1	4.966154000	1.641584000	-2.039609000
1	7.749593000	0.470012000	1.928712000
1	7.398101000	2.114762000	-2.062415000
79	0.067907000	-0.184482000	-0.032520000
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9	-9.421819000	-3.102382000	-0.798285000
9	-9.642221000	-2.059286000	1.182872000
6	9.190643000	1.656585000	-0.069281000
9	9.457007000	3.006810000	0.271910000
9	9.936051000	0.890087000	0.838967000
9	9.791670000	1.474594000	-1.328540000

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7	1.307364000	1.524662000	-0.108605000
7	1.766081000	-1.443590000	0.019268000
7	-1.659033000	1.068881000	-0.035021000
7	-1.200997000	-1.902239000	-0.015977000
6	0.867897000	2.842461000	-0.084614000
6	2.045877000	3.700354000	0.014189000
6	3.156542000	2.886837000	0.036323000
6	2.694132000	1.503496000	-0.047431000
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1	4.186932000	3.198108000	0.123967000
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6	1.744873000	-2.831691000	0.005817000
6	3.082758000	-1.005004000	-0.034581000
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6	0.589046000	-3.658270000	0.047856000
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6	-3.051440000	-3.258496000	0.167613000
6	-2.588825000	-1.878731000	0.032161000
6	-0.762296000	-3.217154000	0.061805000
1	-1.925399000	-5.146468000	0.291565000
1	-4.082393000	-3.566726000	0.259004000
6	-3.413933000	-0.723452000	-0.019986000
6	5.006198000	0.577009000	-0.037806000
6	5.641437000	1.191764000	-1.141257000
6	7.028331000	1.404510000	-1.147069000
6	7.797298000	1.004080000	-0.037167000
6	7.182017000	0.394862000	1.074160000
6	-0.711116000	4.770103000	-0.168619000
6	-1.387923000	5.435494000	0.877562000
6	-1.602259000	6.824059000	0.856496000
6	-1.142134000	7.585553000	-0.243200000
6	-0.468296000	6.929679000	-1.301476000
6	-0.252408000	5.546077000	-1.258953000
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6	1.248913000	-7.943703000	0.148918000
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9	-9.578747000	-2.714339000	-0.743732000
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6	9.268049000	1.269037000	-0.015324000
9	9.606058000	2.508626000	0.589636000
9	9.996156000	0.304897000	0.705409000
9	9.843651000	1.320425000	-1.296527000