Supplementary materials

Four-Component Relativistic Calculations of NMR Shielding Constants of the Transition Metal Complexes—Part 3: Fe, Co, Ni, Pd, and Pt Glycinates

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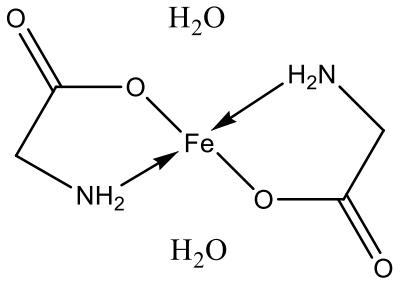
Cartesian coordinates (Angstroms) of chelate glycinates 1-6, optimized at the CCSD/TZP level.

Complex № 1:

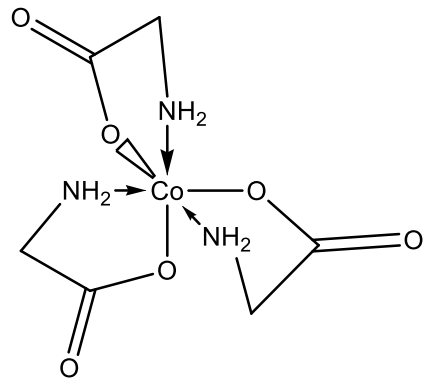
$[FeGly_2]\cdot 2H_2O$



Fe	2.135695000	6.565600000	4.329904000
N	0.131853000	6.843895000	4.358586000
N	4.139537000	6.287305000	4.301223000
O	2.149355000	8.124761000	5.502251000
O	2.365268000	7.506747000	2.506932000
O	0.862192000	9.824149000	6.254559000
O	2.122035000	5.006439000	3.157558000
O	1.906122000	5.624453000	6.152877000
O	3.409198000	3.307051000	2.405250000
C	1.048123000	8.808581000	5.597140000
C	− 0.125081000	8.253290000	4.744806000
C	3.223267000	4.322619000	3.062669000
C	4.396471000	4.877910000	3.915003000
H	1.901081000	8.310517000	2.227537000
H	2.090787000	6.767986000	1.926338000
H	− 0.369995000	6.582218000	3.507946000
H	− 0.218598000	6.208147000	5.079665000
H	− 1.074070000	8.384446000	5.293941000
H	− 0.201717000	8.870004000	3.830797000
H	2.370309000	4.820683000	6.432272000
H	2.180603000	6.363214000	6.733471000
H	4.641385000	6.548982000	5.151863000
H	4.489988000	6.923053000	3.580144000
H	5.345460000	4.746754000	3.365868000
H	4.473107000	4.261196000	4.829012000

Complex № 2:

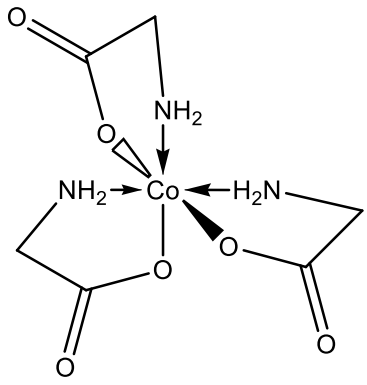
fac-[$CoGly_3$]



Co	5.325651000	9.330326000	7.733021000
O	4.097055000	12.978710000	7.137039000
O	5.010246000	11.129942000	8.039181000
O	2.093652000	7.173358000	8.010523000
O	3.526672000	8.888306000	7.743825000
O	6.891890000	9.326489000	11.299849000
O	5.557188000	8.940419000	9.529186000
N	4.978971000	9.771372000	5.832206000
N	5.623750000	7.384949000	7.499577000
N	7.228570000	9.881622000	7.786172000
C	4.044375000	10.939107000	5.871128000
C	4.389899000	11.798044000	7.098473000
C	4.449338000	6.732688000	8.158294000
C	3.219223000	7.633783000	7.962393000
C	7.461201000	10.330521000	9.194358000
C	6.594392000	9.470602000	10.128548000
H	5.802173000	10.008651000	5.272579000
H	4.520168000	8.994710000	5.350092000
H	4.091400000	11.537275000	4.946279000
H	3.019717000	10.553224000	6.004873000
H	5.700302000	7.058765000	6.532681000
H	6.479389000	7.082706000	7.971455000
H	4.262876000	5.720677000	7.762783000
H	4.654871000	6.669910000	9.240205000
H	7.909071000	9.158362000	7.539271000
H	7.404031000	10.666421000	7.154158000
H	8.524931000	10.269368000	9.477379000
H	7.119558000	11.375712000	9.281373000

Complex № 3:

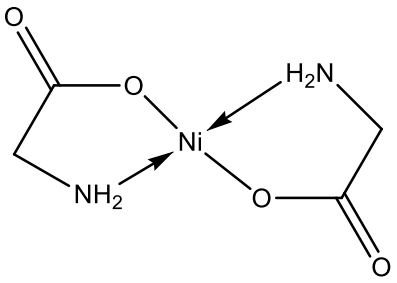
mer-[$CoGly_3$]



Co	−0.534710000	7.647190000	10.118207000
N	−1.709923000	7.448654000	11.646192000
N	0.602442000	8.240823000	8.655229000
N	0.097404000	5.786655000	10.087915000
O	0.829099000	8.049133000	11.326043000
O	1.188423000	8.506750000	13.504571000
O	−1.205167000	9.378677000	10.104043000
O	−0.672545000	11.487641000	9.512717000
O	−1.866066000	7.052106000	8.921366000
O	−2.496988000	5.290836000	7.652041000
C	0.445568000	8.266556000	12.572739000
C	−1.082887000	8.211695000	12.770880000
C	−0.452012000	10.292605000	9.526365000
C	0.805921000	9.709540000	8.859449000
C	−1.733813000	5.842827000	8.423367000
C	−0.438213000	5.120068000	8.865642000
H	−1.949772000	6.494699000	11.937273000
H	−2.585695000	7.890842000	11.339517000
H	0.082330000	8.082735000	7.782480000
H	1.512819000	7.774942000	8.566655000
H	−0.213046000	5.283093000	10.926426000
H	1.123155000	5.765706000	10.137354000
H	−1.462686000	9.247280000	12.740202000
H	−1.327330000	7.771368000	13.752209000
H	1.654061000	9.844573000	9.552337000
H	1.021362000	10.229786000	7.910797000
H	0.304691000	5.208738000	8.051352000
H	−0.629669000	4.044551000	9.022710000

Complex № 4:

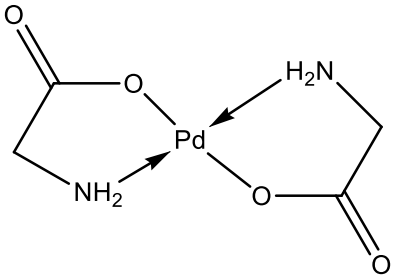
[$NiGly_2$]



Ni	1.843391000	1.309300000	4.127042000
N	0.329923000	2.468713000	4.177602000
N	3.356860000	0.149887000	4.076482000
O	−1.173150000	−0.225870000	6.000796000
O	0.881387000	0.138979000	5.138105000
O	4.859932000	2.844470000	2.253288000
O	2.805395000	2.479621000	3.115979000
C	−0.389577000	0.412704000	5.324809000
C	−0.858176000	1.654566000	4.536149000
C	4.076359000	2.205896000	2.929275000
C	4.544959000	0.964034000	3.717935000
H	0.497176000	3.185723000	4.881675000
H	0.216483000	2.968700000	3.298345000
H	−1.333579000	1.299584000	3.605669000
H	−1.603282000	2.225647000	5.112042000
H	3.189607000	−0.567123000	3.372409000
H	3.470300000	−0.350100000	4.955739000
H	5.020362000	1.319016000	4.648415000
H	5.290064000	0.392953000	3.142042000

Complex № 5:

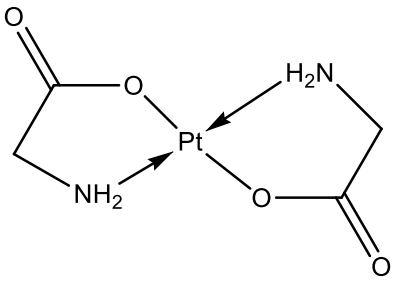
[$PdGly_2$]



Pd	−1.968411000	4.523000000	3.364486000
N	−1.128694000	5.709758000	1.966875000
N	−2.808128000	3.336242000	4.762097000
O	−3.483935000	4.450814000	2.124764000
O	−4.262955000	5.374274000	0.224980000
O	−0.452887000	4.595186000	4.604207000
O	0.326133000	3.671726000	6.503992000
C	−2.238772000	6.266983000	1.146857000
C	−3.438088000	5.291293000	1.114166000
C	−0.498734000	3.754707000	5.614806000
C	−1.698050000	2.779017000	5.582115000
H	−0.550450000	6.437905000	2.380964000
H	−0.509848000	5.138217000	1.394302000
H	−2.586322000	7.193770000	1.634224000
H	−1.914508000	6.506844000	0.121981000
H	−3.386372000	2.608095000	4.348008000
H	−3.426974000	3.907783000	5.334670000
H	−1.350500000	1.852230000	5.094748000
H	−2.022314000	2.539156000	6.606991000

Complex № 6:

[$PtGly_2$]



Pt	0.062782000	0.034358000	0.026475000
N	−1.335952000	0.534297000	−1.361883000
N	1.461516000	−0.465581000	1.414833000
O	1.136124000	1.439974000	−0.896616000
O	1.169813000	2.755613000	−2.723215000
O	−1.010560000	−1.371258000	0.949566000
O	−1.044249000	−2.686897000	2.776165000
C	−0.647943000	1.213961000	−2.502809000
C	0.656730000	1.897942000	−2.030491000
C	0.773507000	−1.145245000	2.555759000
C	−0.531166000	−1.829226000	2.083441000
H	−0.371354000	0.446959000	−3.247993000
H	−1.305907000	1.949342000	−2.995471000
H	−1.876533000	−0.277190000	−1.676699000
H	−2.018044000	1.167254000	−0.930479000
H	2.002097000	0.345906000	1.729649000
H	2.143608000	−1.098538000	0.983429000
H	1.431471000	−1.880626000	3.048421000
H	0.496918000	−0.378243000	3.300943000

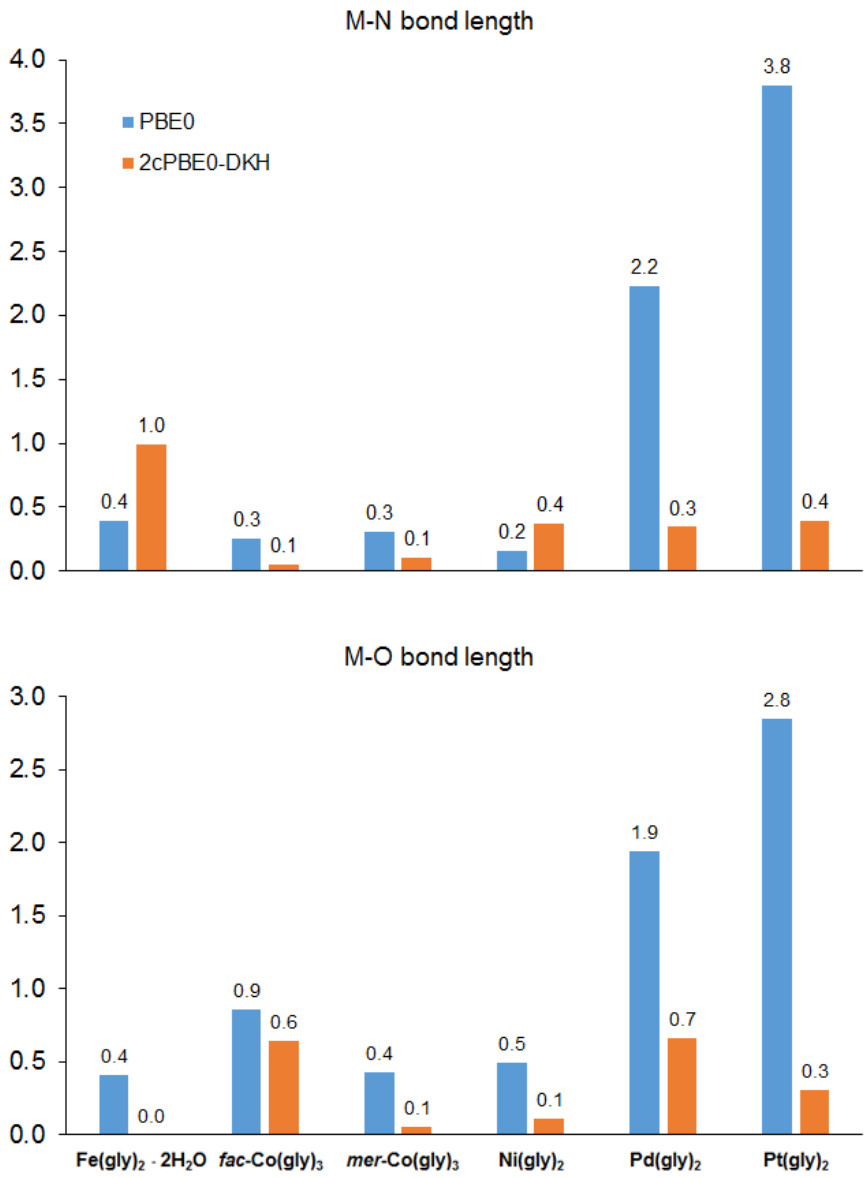


Figure S1. Normalized Absolute Deviation (%) of M-N and M-O bond lengths of glycinates **1-6**, evaluated at non-relativistic (PBE0/ATZP) and relativistic (2cPBE0-DKH/ATZP) levels as compared to CCSD geometry.

Table S1. Relativistic corrections (ppm) to the ^{1}H, ^{13}C, ^{15}N ^{57}Fe, ^{59}Co, ^{61}Ni, ^{105}Pd and ^{195}Pt anisotropy tensors of **1–6**, evaluated at the (4c)PBE0/pc-1//aug-pcS-2//dyall.ae3z level.

	Fe(gly)$_2$ · 2H$_2$O			***fac*-Co(gly)$_3$**			***mer*-Co(gly)$_3$**			**Ni(gly)$_2$**			**Pd(gly)$_2$**			**Pt(gly)$_2$**		
	non-rel	rel	Δrel	non-rel	rel	Δrel	non-rel	rel	Δrel	non-rel	rel	Δrel	non-rel	rel	Δrel	non-rel	rel	Δrel
σM	13758.9	14405.4	646.5	917.2	881.6	−35.6	2012.5	2139.3	126.8	8478.3	8893.7	415.4	4121.9	4141.0	19.1	4796.0	5331.6	535.6
σ^{15}N *trans* to NH$_2$	139.7	164.5	24.8	63.6	85.4	21.8	73.5	86.0	12.5	54.5	77.1	22.6	40.2	57.8	17.6	30.4	64.4	34.0
σ^{15}N *trans* to O							82.8	93.0	10.2									
σ^{13}C C=O	80.9	77.2	−3.7	68.9	66.7	−2.2	64.5	62.1	−2.4	64.2	74.1	9.9	65.2	66.8	1.6	68.8	75.3	6.5
σ^{13}C CH$_2$	69.3	64.8	−4.5	48.3	48.2	−0.1	50.8	50.6	−0.2	38.4	33.7	−4.7	41.7	40.9	−0.8	40.0	38.0	−2.0
σ^{1}H NH$_2$	46.11	46.02	−0.09	21.50	22.66	1.16	23.35	24.35	1.00	17.33	17.56	0.23	15.39	15.35	−0.04	16.86	15.81	−1.05
σ^{1}H CH$_2$	14.30	13.59	−0.71	5.03	5.33	0.30	4.41	4.67	0.26	5.40	5.90	0.50	8.14	8.03	−0.11	9.31	9.04	−0.27