

Electronic supplementary materials *Mendeleev Commun.*, 2020, **30**, 476–478

**Four-component relativistic computational NMR study of ferrous,
cobalt and nickel bisglycinates**

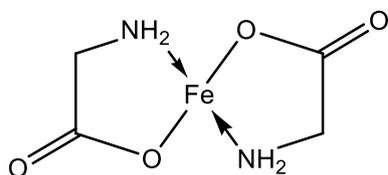
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TABLE OF CONTENTS

Cartesian coordinates (Angstroms) of 1-3 optimized at the M062X/ aug-cc-pVTZ level.....	2
Solvent corrections to ¹ H, ¹³ C and ¹⁵ N NMR chemical shifts of ferrous, cobalt, and nickel bisglycinates, calculated at the PBE0/ATZP level within the Integral Equation Formalism Polarizable Continuum Model, ppm.....	5

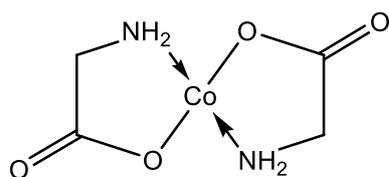
**Cartesian coordinates (Angstroms) of 1-3 optimized at the M062X/
aug-cc-pVTZ level.**

Compound: 1



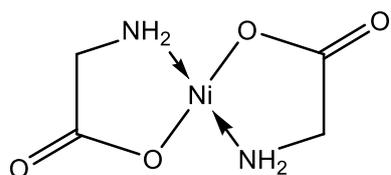
Fe	0.000000	0.000000	0.000000
O	0.059308	1.591124	0.966632
O	-1.189135	3.219288	1.860350
O	-0.059308	-1.591124	-0.966632
O	1.189135	-3.219288	-1.860350
N	-2.025994	0.275892	-0.014935
N	2.025994	-0.275892	0.014935
C	-1.063175	2.233050	1.183147
C	-2.280146	1.659121	0.444076
C	1.063175	-2.233050	-1.183147
C	2.280146	-1.659121	-0.444076
H	-2.430847	0.093810	-0.925910
H	-2.447785	-0.396876	0.615928
H	-3.155252	1.734470	1.084818
H	-2.447634	2.297953	-0.422289
H	2.430847	-0.093810	0.925910
H	2.447785	0.396876	-0.615928
H	3.155252	-1.734470	-1.084818
H	2.447634	-2.297953	0.422289

Compound: **2**



Co	0.000000	0.000000	0.000000
O	0.087802	1.571026	0.883670
O	-1.064679	3.320842	1.663373
O	-0.087802	-1.571026	-0.883670
O	1.064679	-3.320842	-1.663373
N	-1.931581	0.314672	-0.107472
N	1.931581	-0.314672	0.107472
C	-1.024907	2.286079	1.088455
C	-2.277245	1.637445	0.486414
C	1.024907	-2.286079	-1.088455
C	2.277245	-1.637445	-0.486414
H	-2.226377	0.241847	-1.080310
H	-2.412594	-0.448309	0.366953
H	-3.027186	1.527446	1.265071
H	-2.675065	2.301162	-0.277395
H	2.226377	-0.241847	1.080310
H	2.412594	0.448309	-0.366953
H	3.027186	-1.527446	-1.265071
H	2.675065	-2.301162	0.277395

Compound: **3**



Ni	-0.043465	-0.104997	0.055855
O	-0.160726	-0.027855	-1.794054
O	-1.591324	-0.180401	-3.507912
O	0.072770	-0.169969	1.906296
O	1.521229	-0.229331	3.610889
N	-2.005427	-0.248128	0.059711
N	1.914755	0.082526	0.053940
C	-1.330111	-0.212668	-2.331186
C	-2.445730	-0.538703	-1.325061
C	1.260488	-0.202677	2.433917
C	2.407517	-0.249315	1.411497
H	-2.658191	-1.602512	-1.416247
H	-3.346780	0.006314	-1.594204
H	-2.314010	-0.945810	0.727319
H	-2.377886	0.636547	0.388072
H	2.795370	-1.266524	1.411693
H	3.206796	0.413165	1.733437
H	2.330671	-0.493279	-0.669350
H	2.131780	1.042071	-0.193784

Solvent corrections to ^1H , ^{13}C and ^{15}N NMR chemical shifts of ferrous, cobalt, and nickel bisglycinates, calculated at the PBE0/ATZP level within the Integral Equation Formalism Polarizable Continuum Model, ppm.

Solvent		Carbon-tetra-chloride	Chloroform	Pyridine	Ethanol	Aceto-nitrile	DMSO	Formic Acid	Water	Form-amide	n-Methyl-Formamide
ϵ		2.23	4.71	12.98	24.85	35.69	46.83	51.10	78.36	108.94	181.56
Ferrous bisglycinate	^1H (CH_2)	-0.09	-0.14	-0.17	-0.18	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19
	^1H (NH_2)	0.03	0.09	0.13	0.15	0.15	0.16	0.16	0.16	0.16	0.17
	^{13}C (CH_2)	0.5	0.8	1.0	1.1	1.1	1.2	1.2	1.2	1.2	1.2
	^{13}C ($\text{C}=\text{O}$)	2.7	4.3	5.5	5.8	5.9	6.0	6.0	6.1	6.1	6.2
	^{15}N	-2.3	-3.6	-4.4	-4.6	-4.7	-4.8	-4.8	-4.8	-4.8	-4.8
Cobalt bisglycinate	^1H (CH_2)	0.24	0.41	0.54	0.58	0.60	0.61	0.61	0.62	0.62	0.63
	^1H (NH_2)	1.74	3.04	4.08	4.41	4.52	4.58	4.60	4.67	4.70	4.74
	^{13}C (CH_2)	1.2	2.1	2.7	2.9	2.9	3.0	3.0	3.0	3.1	3.1
	^{13}C ($\text{C}=\text{O}$)	3.6	6.0	7.9	8.5	8.7	8.8	8.8	8.9	9.0	9.1
	^{15}N	4.4	7.9	11.0	12.0	12.3	12.5	12.6	12.8	12.9	13.0
Nickel bisglycinate	^1H (CH_2)	0.07	0.11	0.14	0.15	0.15	0.15	0.15	0.16	0.16	0.16
	^1H (NH_2)	0.09	0.14	0.16	0.16	0.17	0.17	0.17	0.17	0.17	0.17
	^{13}C (CH_2)	0.7	1.1	1.4	1.5	1.5	1.5	1.5	1.5	1.5	1.5
	^{13}C ($\text{C}=\text{O}$)	2.9	4.7	5.9	6.3	6.4	6.5	6.5	6.6	6.6	6.7
	^{15}N	-1.5	-2.3	-2.8	-2.9	-3.0	-3.0	-3.0	-3.1	-3.1	-3.1