Electronic Supplementary Information for Dalton Transactions
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Supplementary Information - 1

Structural data of compounds [Ni(*S*-BBP-Gly)], [Ni(*S*-BBP-L-(and D-)-Ser)] and [Ni(*S*-BBP-L-(and D-)-aaIm)]

Table SI-1 Average deviations of coordinating atoms O(2), N(1), N(2), N(3) from the best least-squares plane defined by these atoms in complexes.

		Four donor atoms + Ni (X-ray)	Four donor atoms + Ni (MM)	Four donor atoms (X-ray)	Four donor atoms (MM)
[Ni(*S*-BBP-Gly]	Ni	0.049	0.0468	0.061	0.0585
	N(1)	-0.122	-0.1324	-0.109	-0.1204
	N(2)	0.092	0.1037	0.105	0.1160
	N(3)	-0.120	-0.1324	-0.108	-0.1211
	O(2)	0.100	0.1143	0.112	0.1255
	rms	0.100	0.1105	0.100	0.1208
[Ni(*S*-BBP-L-Ser]	Ni	0.021	0.0299	0.027	0.0374
	N(1)	0.010	-0.0897	0.005	-0.0822
	N(2)	-0.001	0.0715	-0.004	0.0791
	N(3)	0.010	-0.0864	0.005	-0.0789
	O(2)	-0.001	0.0747	-0.005	0.0820
	rms	0.010	0.0736	0.005	0.0806
[Ni(*S*-BBP-D-Ser]	Ni		0.0204		0.0255
	N(1)		-0.0315		-0.0262
	N(2)		0.0203		0.0256
	N(3)		-0.0317		-0.0268
	O(2)		0.0224		0.0274
	rms		0.0258		0.0265
[Ni(*S*-BBP-L-aaIm]	Ni	-0.015	0.0375	-0.018	0.0468
	N(1)	0.001	-0.0496	0.003	-0.0400
	N(2)	0.007	0.0293	-0.003	0.0390
	N(3)	0.001	-0.0492	0.003	-0.0400
	O(2)	0.007	0.0320	-0.003	0.0411
	rms	0.008	0.0404	0.003	0.0400
[Ni(*S*-BBP-D-aaIm]	Ni		0.0383		0.0479
	N(1)		-0.0456		-0.0356
	N(2)		0.0249		0.0349
	N(3)		-0.0465		-0.0374
	O(2)		0.0289		0.0381
	rms		0.0378		0.0365

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Conformations of the rings in complexes

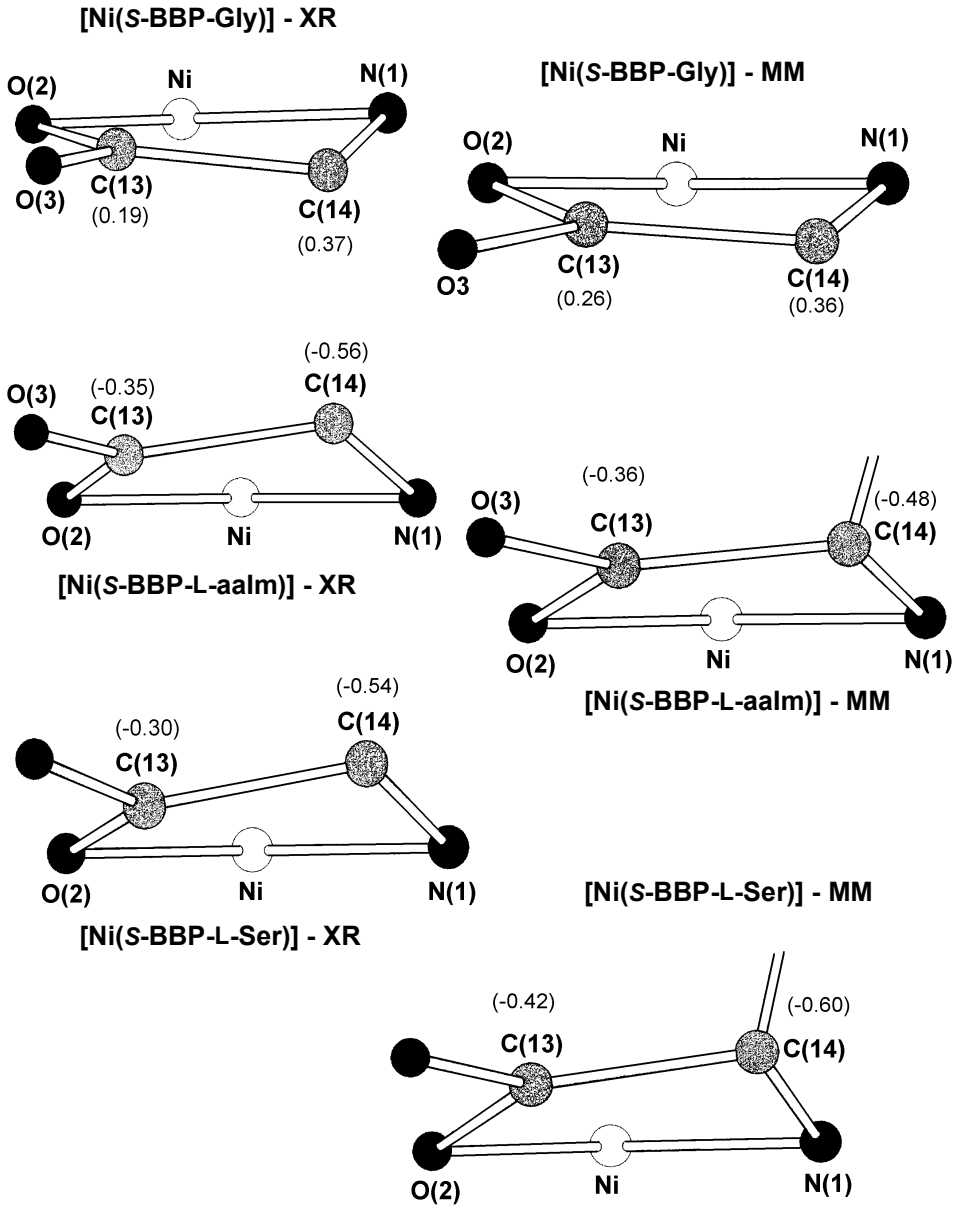

Figure SI-1a Relative positions of atoms of Ring A [Ni-N(1)-C(14)-C(12)-O(2)], to the plane defined by O(2)-Ni-N(1). The distances of atoms C(13) and C(14) to this plane are included between () in Å, and considered with a positive sign when the atom is on the same side of the coordination plane as the benzyl group. XR: X-ray structure; MM: structure calculated by Molecular Mechanics.

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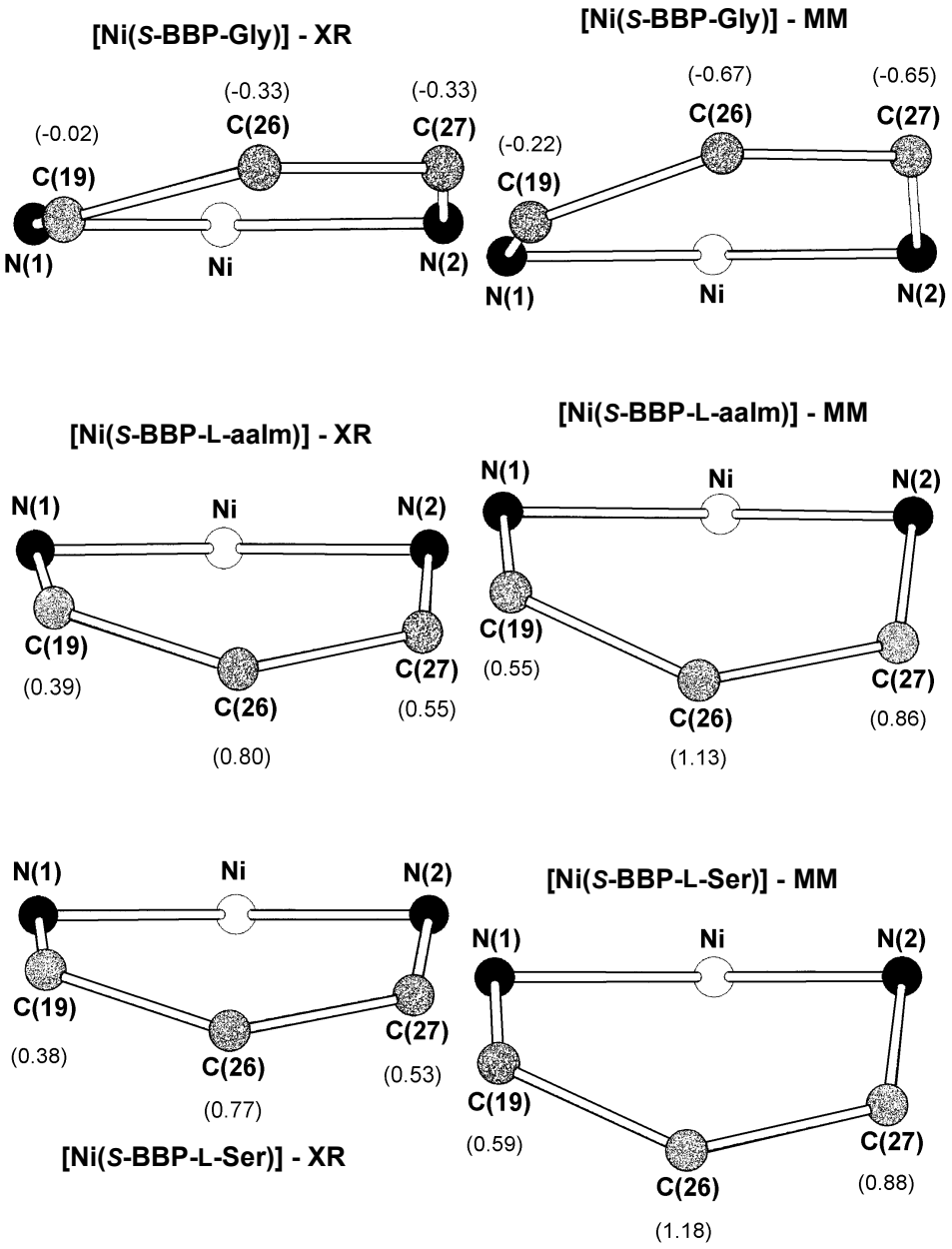

Figure SI-1b Relative positions of atoms of Ring B [Ni-N(1)-C(19)-C(26)-C(27)-N(2)], to the plane defined by N(1)-Ni-N(2). The distances of atoms C(19), C(26) and C(27) to this plane are included between () in Å, and are considered with a positive sign when the atom is on the same side of the coordinating plane as the benzyl group. XR: X-ray structure; MM: structure calculated by Molecular Mechanics.

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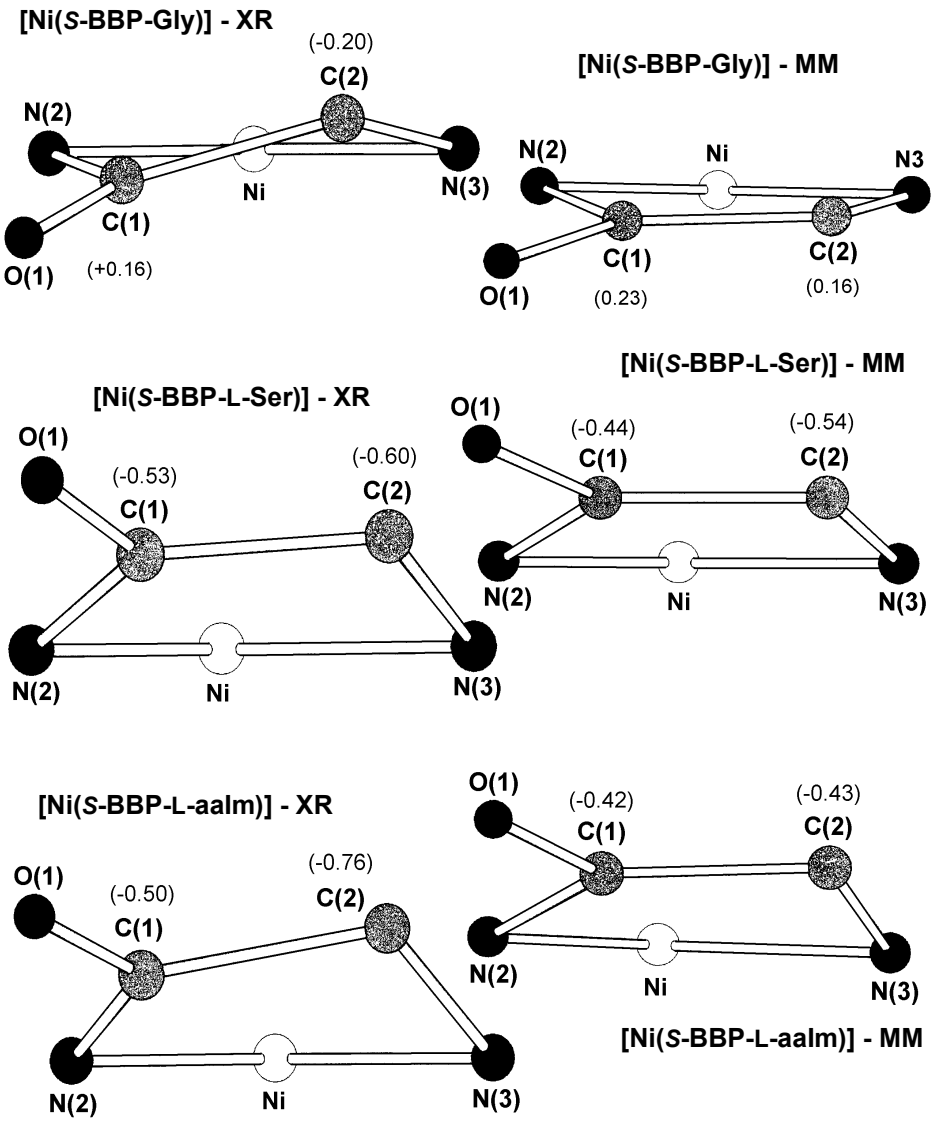
Figure SI-1c Relative positions of atoms of Ring C [Ni-N(3)-C(2)-C(1)-N(2)], to the plane



defined by N(2)-Ni-N(3). The distances of atoms C(1) and C(2) to this plane are included between () in Å, and are considered with a positive sign when the atom is on the same side of the coordinating plane as the benzyl group. XR: X-ray structure; MM: structure calculated by Molecular Mechanics.

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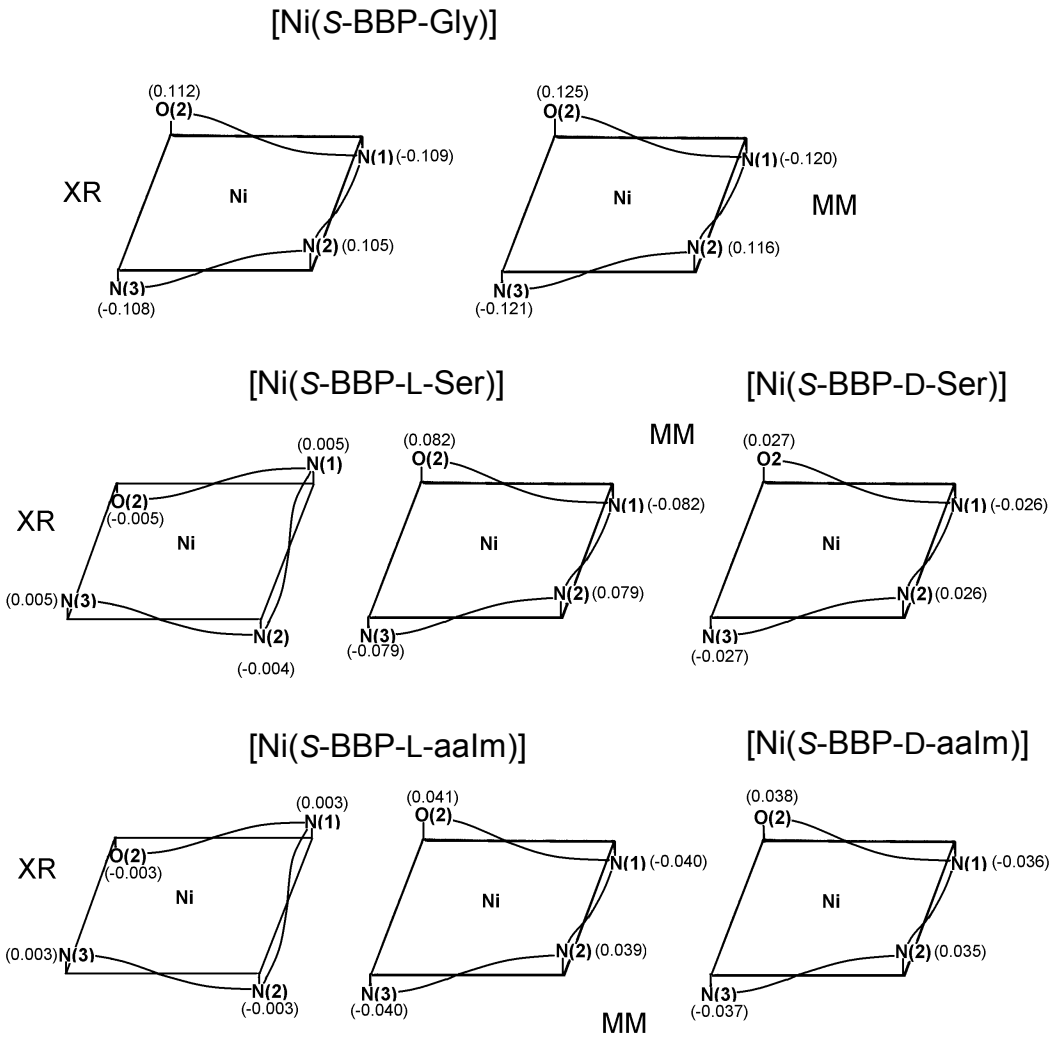

Figure SI-2 Relative positions of atoms in the coordination plane. The deviations included are those of the 5th column in Table SI-1.