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SUPPORTING INFORMATION

Title: First-Row Transition Metal Bis(amidinate) Complexes; Planar Four-Coordination of Fe^{II} Enforced by Sterically Demanding Aryl Substituents

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IR data (nujol mull, KBr) for bis(amidinate) complexes 1–6

1: $\tilde{\nu} = 3060, 3043, 1580$ (m), 1438, 1416 (s), 1357, 1340, 1322, 1300, 1272, 1255, 1247, 1242 (m), 1225, 1189, 1180 (w), 1107 (m), 1095, 1060, 1030 (w), 963, 957, 952 (m), 932, 808, 803 (w), 788, 782 (m), 768, 697 (s), 671, 502, 435 (w) cm^{-1} .

2: $\tilde{\nu} = 3060$ (m), 1580 (w), 1360 (s), 1316 (s), 1269 (m), 1253 (m), 1239 (m), 1222 (w), 1181 (w), 1099 (w), 1055 (w), 1043 (w), 1027 (w), 955 (w), 933 (w), 802 (w), 784 (m), 765 (s), 697 (s), 423 (m) cm^{-1} .

3: $\tilde{\nu} = 3058$ (w), 1580 (w), 1461 (s), 1438 (s), 1413 (s), 1340 (m), 1321 (m), 1273 (m), 1256 (w), 1225 (w), 1106 (w), 963 (w), 804 (w), 782 (w), 766 (m), 696 (m) cm^{-1} .

4: $\tilde{\nu} = 3060$ (m), 1580 (w), 1360 (s), 1336 (w), 1318 (s), 1271 (m), 1253 (m), 1222 (w), 1181 (w), 1100(w), 1055 (w), 1043 (w), 1028 (w), 962 (w), 934 (w), 803 (w), 784 (m), 768 (s), 696 (s), 423 (m) cm^{-1} .

5: $\tilde{\nu} = 3073$ (m), 3055 (m), 3033 (m), 3025 (m), 2967 (s), 2902 (s), 1806 (w), 1580 (m), 1469 (s), 1436 (s), 1422 (s), 1380 (s), 1358 (s), 1341 (m), 1324 (s), 1300 (m), 1268 (s), 1251 (s), 1224 (m), 1190 (m), 1160 (m), 1107 (m), 1096 (m), 1061 (m), 1031 (w), 953 (m), 932 (m), 919 (w), 873 (w), 804 (m), 773 (s), 696 (s), 660 (m), 510 (w), 442 (w), 408 (w) cm^{-1} .

6: $\tilde{\nu} = 3068$ (m), 3040 (m), 3019 (m), 1618 (w), 1602 (w), 1580 (m), 1418 (s), 1361 (s), 1321 (s), 1275 (s), 1254 (m), 1231 (m), 1181 (w), 1159 (w), 1120 (w), 1097 (m), 1074 (w), 1054 (w), 1027 (m), 984 (w), 960 (m), 934 (w), 917 (w), 791 (m), 761 (s), 693 (s), 479 (w), 438 (w) cm^{-1} .

Table S.1 Total energies and S^2 values for bis(amidinate) complexes $[M\{HC(NH)_2\}_2]$

Complex ^[a]	Energy	E_{rel}	S	S^2_{ideal}	S^2_{act}
CrL ₂ perp	-383.53788	24.02	2	6.00	6.01
CrL ₂ plan	-383.57616	0.00	2	6.00	6.01
	-383.57616				
MnL ₂	-401.18484	0.00	2.5	8.75	8.76
MnL ₂ plan	-401.17444	6.53	2.5	8.75	8.75
	-401.18484				
FeL ₂ perp	-420.67651	0.00	2	6.00	6.01
FeL ₂ perp-is	-420.62254	33.87	1	2.00	2.01
FeL ₂ perp-ls	-420.57119	66.09	(restricted)		
FeL ₂ plan	-420.67267	2.41	2	6.00	6.01
FeL ₂ plan-is	-420.66538	6.99	1	2.00	2.01
FeL ₂ plan-ls	-420.61755	37.00	(restricted)		
	-420.67651				
CoL ₂	-442.30069	5.56	1.5	3.75	3.76
CoL ₂ perp	-442.30954	0.00	1.5	3.75	3.76
	-442.30954				
NiL ₂ perp	-466.49337	16.07	1	2.00	2.01
NiL ₂ plan	-466.51899	0.00	1	2.00	2.01
NiL ₂ plan_ls	-466.40334	72.57	(restricted)		
	-466.51899				

[a] perp = perpendicular; plan = planar