

**Table S1** Experimental Raman (top, bold, taken from Ref. 16) and calculated band frequencies (in units of  $\text{cm}^{-1}$ ) and corresponding assignments obtained by DFT calculations and subsequent normal mode analysis of  $[\text{Fe}(\text{btpa})]^{2+}$ .

Complex	<b>1333</b>	<b>1492</b>	<b>1575</b>	<b>1609</b>
LS Fe(II)(btpa) <sup>2+</sup>	1318 A	1490 B	1595 A	1631 B
	1323 B	1509 A	1600 B	1635 A
	Free py and bipy CH <sub>2</sub> rocking Bipy stretching N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending.	Bipyridine ring C-H in plane bending, Some N <sub>bipy</sub> -Fe-N <sub>sp3</sub> bending.	Bipyridine ring stretching, N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending.	Bipyridine ring stretching, Fe-N <sub>bipy</sub> stretching.
S-C <sub>1</sub> Fe(II)(btpa) <sup>2+</sup>	<b>1327</b>	<b>1484</b>	<b>1575</b>	<b>1597</b>
	1309	1487	1601	1629
	1315	Bipyridine ring stretching, C-H in plane bending, N <sub>bipy</sub> - Fe-N <sub>bipy</sub> bending.	1602	1632
HS-C <sub>2</sub> Fe(II)(btpa) <sup>2+</sup>	<b>1327</b>	<b>1484</b>	<b>1575</b>	<b>1597</b>
	1313 A	1494 B	1601 A	1629 A
	1315 B	1507 A	1605 B	1630 B
	Bipyridine Kekule stretching, N <sub>bipy</sub> - Fe-N <sub>bipy</sub> bending.	Bipyridine ring stretching, C-H in plane ending, N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending.	Bipyridine/axial pyridine ring stretching, N <sub>bipy</sub> -Fe-N <sub>sp3</sub> Bending.	Bipyridine ring stretching, Fe-N <sub>bipy</sub> stretching.

**Table S2** Calculated (DFT, B3LYP/CEP-31G) normal modes of  $M(\text{btpa})^{+2}$  cations.

Mode No	Ring mode	Zn(bpta) <sup>+2</sup>	Fe(btpa) <sup>+2</sup> Isomer HS-C <sub>2</sub>	Fe(bipa) <sup>+2</sup> Isomer HS-C <sub>1</sub>	Ru(bpta) <sup>+2</sup>	Fe(btpa) <sup>+2</sup> Isomer LS-C <sub>2</sub>	Fe(b(dpa)) <sup>+2</sup> Isomer LS	Fe(b(dpa)) <sup>+2</sup> Isomer HS
1		10 free and axial py libration	16 B free   and axial py libration	19 bipy, 7, free py libration	8 A free py libration	17 A free py libration	18 bz libration	11 bz libration
2		12 free and axial py libration	19 A free and axial py libration	26, All rings but Ax7 • py libration	21 A free py libration	18 B free py libration	20 bz libration	17 bz libration
3		16 Free py libration	20 B Free py libration	34 Ax7 py libration	23 Ay Axial and free py libration	35 A Axial py libration	35 Axial and bz libration	24 bz libration
4		20 Free py libration	29 A Bipy libration	36 Free py libration	35 B Axial and free py libration	37 B Axial py libration	36 Axial py libration	28 Axial py and bz libration
5		29 Bipy libration	37 A libration of free py and bipy	44 Bipy-half7, 7J and free libration	38 A Axial and free py libration	42 A Axial and free py libration	38 Axial and bz libration	35 Axial py and bz libration
6		36 libration of free py and bipy	38 A libration of free py and bipy	46 Bipy-half-Free and free py libration	42 B Axial and free py libration	48 B bipy and axial py libration	43 Axial and free py libration	40 Bz and bipy libration
7		40 libration of free and axial py	41 B libration of free py and bipy	52 libration of 7 and bipy	45 A Axial and free py libration	50 A bipy and axial py libration	49 bipy and axial py libration	43 all rings libration
8		48 libration of free py and bipy	47 A, libration of free and axial py	54 All rings libration	58 B, Axial and free py libration	54 B all ring libration	55 Axial and free py libration	56 all rings libration
9		52 libration of free and axial py	51, A, libration of free and	62 All rings libration	60 A All rings libration	60 By All rings	74 All rings	62 All rings

10	58	$N_{ax}$ -Zn- $N_{ax}$ bending Axial py libration	axial py	67	7 and free py libration	64, B All rings libration	59 B Axial and free py libration	75 All rings libration	64 Bz and axial libration
11	63	$N_{sp^3}$ -Zn- $N_{sp^3}$ bending Axial py libration	67 A Libration of axial py and $CH_2$	84	Ax7, 7, free py libration	76 A Axial py and bipy libration	84 A Libration of axial py and $CH_2$	79 Axial and free py libration	65 Bz and axial libration
12	81	Free and axial py libration	78 B libration of free and axial py	91	AxF, Ax7, 7 rings libration	81 B, bipy bowing Free and axial py libration	87 B, bipy bowing Free and axial py libration	81 All rings libration	74 Bz and axial libration
13	90	Axial and free libration	96 libration py and bipy	98	AxF, Free py libration	107 A Libration of all rings and bipy $CH_2$	108 A Libration of all rings and bipy $CH_2$	93 Axial and bz libration $N_{sp^3}$ -Fe- $N_{sp^3}$ bending	96 Bz and axial libration
14	99	Libration axial py + $N_{ax}$ -Zn- $N_{ax}$ bending	99, B Libration axial py + some $N_{ax}$ -Fe- $N_{ax}$ bending	105	AxF, Ax7 py libration Fe-N7 stretching $N_a$ -Fe- $N_{ax}$ bending	121B Libration axial py + some $N_{ax}$ -Ru- $N_{ax}$ bending	127 B Libration axial py + some $N_{ax}$ -Fe- $N_{ax}$ bending	117 Axial py libration	102 All rings libration
15	103	Libration axial py + $N_{ax}$ -Zn- $N_{ax}$ bending	110 A, Libration axial py + some $N_{ax}$ -Fe- $N_{ax}$ bending	110	Ax7, bipy-half7 libration $N_{ax}$ -Fe- $N_{ax}$ bending	124 B Libration axial py	135 B Axial and free py libration	127 Libration axial py + some $N_{ax}$ -Fe- $N_{ax}$ bending	104 All rings libration some $N_{ax}$ -Fe- $N_{ax}$ bending
16	114	Free and axial py. + some Zn- $N_{sp^3}$ and	120, B, Free and axial py. + some Fe- $N_{sp^3}$	121	Fe- $N_{ax}$ stretching (sym.)	132 A Axial and free py libration	136 A Axial and free py libration	130 Libration axial py	112 Axial py libration

17	Zn-N <sub>ax</sub> stretching	stretching	134	bipy bowing some Fe-N <sub>sp3</sub> and Fe-N7 stretching	145A bipy bowing	150 A Fe-Nax stretching Free and axial py libration	148 Fe-Nax stretching Free py libration	N <sub>ax</sub> -Fe-N <sub>ax</sub> bending
18	125 Fe-N <sub>sp3</sub> -stretching	123 A Fe-N <sub>sp3</sub> -stretching Fe-N <sub>ax</sub> stretching Bipy in-plane distortion	134 B, bipy bowing	138 AxF py libration Nsp3-Fe stretching bipy bowing	151 B Ru-N <sub>ax</sub> stretching Free and axial py libration	150 A, bipy bowing	151 bipy bowing	121 Axial py libration Fe-N <sub>ax</sub> stretching
19	130 bipy bowing	157 A Fe-N <sub>sp3</sub> stretching Libration free and axial py	158 Fe-N <sub>bipy</sub> stretching bipy in-plane distortion AxF libration N <sub>ax</sub> -Fe-N <sub>ax</sub> bending	181 N <sub>sp3</sub> - Ru-N <sub>sp3</sub> bending free and axial py libration	187 A free libration rocking bipy CH <sub>2</sub>	193 Fe-N <sub>sp3</sub> stretching bipy in-plane distortion Axial py libration	156 Axial py libration N <sub>sp3</sub> -Fe-N <sub>sp3</sub> N <sub>ax</sub> -Fe-N <sub>ax</sub> bending	
20	160 Zn-N <sub>sp3</sub> stretching	171 B Fe-N <sub>sp3</sub> stretching Libration free and axial py	169 Ax7 and 7 py libration	191 A free and axial py libration rocking axial py CH <sub>2</sub>	193A free and axial py libration rocking axial py CH <sub>2</sub>	201 Fe-N <sub>sp3</sub> stretching bipy in-plane distortion bz libration	168 Axial py libration Fe-N <sub>bipy</sub> stretching N <sub>ax</sub> -Fe-N <sub>ax</sub> bending	
21	1701 Zn - N <sub>sp3</sub> - stretching Axial py	188 A, Fe-N <sub>sp3</sub> stretching Libration free and	185 bipy torsion some Fe-N <sub>sp3</sub>	203 A bipy torsion	203 A, bipy torsion	210 bipy torsion	189 bipy torsion	

	libration	axial py	stretching	205 A	209 A	214	195
22	181 Bipy torsion	189, B bipy-libration Fe-N <sub>sp3</sub> - stretching	195 Ax F py libration N <sub>ax</sub> -Fe- N <sub>ax</sub> bending	205 A bipy torsion Axial py and free libration	209 A bipy torsion	214 All rings libration	195 Axial py libration Fe-N <sub>sp3</sub> stretching N <sub>ax</sub> -Fe-N <sub>ax</sub> bending
23	194 Axial and free py libration Zn-N <sub>ax</sub> stretching	1923 A Libration pyr Free/Ax Bipy torsion	202 Fe-N7, Fe-N <sub>sp3</sub> stretching Bipy torsion	215 B axial py libration rocking axial py CH <sub>2</sub> N <sub>ax</sub> -Ru-N <sub>ax</sub> bending rocking free py CH <sub>2</sub>	218 B axial py libration rocking axial py CH <sub>2</sub> N <sub>ax</sub> -Fe-N <sub>ax</sub> bending	221 Bz libration	203 Axial py libration Fe-N <sub>sp3</sub> stretching N <sub>ax</sub> -Fe-N <sub>ax</sub> bending and stretching
24	197. bipy libration Zn-N <sub>ax</sub> stretching	208.0, B, bipy libration + CH <sub>2</sub> <sub>bipy</sub> rocking	213 7, 7Ax and free py libration N <sub>ax</sub> -Fe- N <sub>ax</sub> bending	223 A axial py libration rocking axial py CH <sub>2</sub> N <sub>ax</sub> -Ru-N <sub>ax</sub> bending rocking free py	233 A axial py libration rocking axial py CH <sub>2</sub> N <sub>ax</sub> -Fe-N <sub>ax</sub> bending	222 All rings libration N <sub>ax</sub> -Fe-N <sub>sp3</sub> bending	210 Axial py libration Fe-N <sub>sp3</sub> stretching N <sub>ax</sub> -Fe-N <sub>ax</sub> bending and stretching
25	206 Libration free py Zn-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	219 A Libration axial py Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	219 bipy libration N <sub>ax</sub> -Fe- N <sub>bipy</sub> bending	235 B Ax py libration N <sub>ax</sub> -Ru-N <sub>ax</sub> bending	236 B axial and free py libration N <sub>ax</sub> -Fe-N <sub>ax</sub>	226 Ax py libration N <sub>ax</sub> -Fe-N <sub>sp3</sub> bending	214 bipy libration N <sub>ax</sub> -Fe-N <sub>ax</sub> bending and

26	214 Libration axial py Zn-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	225 B Libration axial py Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	228 Free, 7 py libration N <sub>ax</sub> -Fe- N <sub>bipy</sub> bending, Fe-N <sub>sp3</sub> stretching	246 B axial and free py libration N <sub>ax</sub> -Ru-N <sub>sp3</sub> bending	bending 251 B axial and free py libration N <sub>ax</sub> -Fe-N <sub>sp3</sub> bending	245 Ax py libration N <sub>ax</sub> -Fe-N <sub>sp3</sub> bending Fe-N <sub>ax</sub> stretching	stretching 232 Axial py and bz libration Fe-N <sub>bipy</sub> stretching N <sub>ax</sub> Fe-N <sub>ax</sub> bending
27	225 Zn-N <sub>ax</sub> stretching	234 A Libration axial py Fe-N <sub>bipy</sub> stretching	228 FeN <sub>bipy</sub> , Fe-N <sub>sp3</sub> stretching Ax F py libration.	247 A axial and bipy libration N <sub>ax</sub> -Ru-N <sub>bipy</sub> bending	255 A axial and bipy libration N <sub>ax</sub> -Fe-N <sub>bipy</sub> bending	259 Bipy libration N <sub>ax</sub> -Fe-N <sub>sp3</sub> bending	234 axial and bipy libration N <sub>ax</sub> -Fe-N <sub>bipy</sub> bending Fe-N <sub>bipy</sub> stretching
28	233 Zn-N <sub>bipy</sub> stretching Axial py libration	238 B Fe-N <sub>sp3</sub> stretching Fe-N <sub>ax</sub> bending	238 Fe-N <sub>sp3</sub> stretching	262 B axial libration and bipy py bowing N <sub>ax</sub> -Ru-N <sub>ax</sub> bending	271 B axial and bipy py libration	272 Fe-N <sub>ax</sub> stretching	241 Fe-N <sub>bipy</sub> stretching
29	246 bipy in-plane distortion Zn-N <sub>bipy</sub> stretching	253 B N <sub>ax</sub> -Fe stretching	247 Fe-N <sub>bipy</sub> stretching	272 A axial libration N <sub>ax</sub> -Ru-N <sub>ax</sub> bending	273 A bipy in-plane distortion Fe-N <sub>ax</sub> stretching	274 bipy in-plane distortion Fe-N <sub>bipy</sub>	247 N <sub>ax</sub> -Fe-N <sub>bipy</sub> bending Fe-N <sub>bipy</sub> stretching
30	248 Axial py libration Zn-N <sub>ax</sub> stretching	260 A Fe-N <sub>bipy</sub> and Fe-N <sub>sp3</sub> stretching	258 Fe-N <sub>bipy</sub> , Fe-N <sub>sp3</sub> stretching	294 A Ru-N <sub>sp3</sub> stretching N <sub>ax</sub> -Ru-N <sub>ax</sub> bending	296 A Fe-N <sub>sp3</sub> stretching N <sub>ax</sub> -Fe-N <sub>ax</sub>	308 Fe-N <sub>sp3</sub> Fe-N <sub>bipy</sub> stretching	256 All Fe-N stretching

31	263 Zn-N <sub>bipy</sub> Bipy out-of-plane bending	269 A Fe-N <sub>bipy</sub> and Fe-N <sub>sp3</sub> stretching	265 Fe-N <sub>bipy</sub> , Fe-N <sub>sp3</sub> stretching	300 B Ru-N <sub>ax</sub> stretching bipy libration	bending 307 B Fe-N <sub>sp3</sub> stretching	319 Fe-N <sub>sp3</sub> Fe-N <sub>bipy</sub> stretching	268 Fe-N <sub>sp3</sub> Fe-N <sub>bipy</sub> stretching bipy out-of- plane bending
32	265 CH <sub>2</sub> -bipy rocking Bipy out-of-plane bending	273 A Fe-N <sub>sp3</sub> stretching	272 CH <sub>2</sub> -Ax -bipy Fe-N <sub>ax</sub> stretching (asymmetric) Fe-N <sub>bipy</sub> stretching	310 A Ru-N <sub>ax</sub> , Ru-N <sub>bipy</sub> stretching	324 A Bipy out-of- plane bending N <sub>bipy</sub> -Fe-N <sub>sp3</sub> bending	323 Bipy out-of- plane bending N <sub>bipy</sub> -Fe-N <sub>ax</sub>	269 All Fe-N stretching bipy out-of- plane bending
33	273 CH <sub>2</sub> -bipy rocking C1-C1' bend.	290 B CH <sub>2</sub> bipy rocking	277 Bipy out-of-plane bending CH <sub>2</sub> -bipy rocking Fe-N <sub>ax</sub> stretching	316 B Bipy out-of-plane bending N <sub>bipy</sub> -Ru-N <sub>sp3</sub> bending	330 B Bipy out-of- plane bending N <sub>bipy</sub> -Fe-N <sub>sp3</sub> bending	350 Fe-N <sub>ax</sub> Bipy out-of- plane bending	280 Bipy out-of- plane bending CH <sub>2</sub> -bipy rocking Fe-N <sub>ax</sub> stretching
34	324 Bipy in-plane distortion Some Zn-N <sub>sp3</sub> /N <sub>bipy</sub> stretching	319 A CH <sub>2</sub> -Free Bipy in-plane distortion Some Fe-N <sub>sp3</sub> stretching	317 CH <sub>2</sub> 7 rocking	331 A free CH <sub>2</sub> rocking Bipy in-plane distortion Ru-N <sub>sp3</sub> stretching , Ru-N <sub>ax</sub> stretching	337 A free py CH2 rocking some Fe-N <sub>sp3</sub> and Fe-N <sub>ax</sub> stretching	373 Bz CH <sub>2</sub> rocking	320 bipy in-plane distortion some Fe-N <sub>sp3</sub> and Fe-N <sub>bipy</sub> stretching
35	343 Axial py CH <sub>2</sub> rocking Some Zn-N <sub>sp3</sub> , Zn- N <sub>bipy</sub> stretching	332 B CH <sub>2</sub> -Free Bipy in-plane Some Fe-N <sub>sp3</sub> stretching	325 CH <sub>2</sub> 7, bipy 7- Fe-N <sub>sp3</sub> , Fe-N <sub>bipy</sub> stretching	361 A Ru-N <sub>sp3/bipy</sub> stretching Bipy in-plane distortion	359 B Fe-N <sub>ax</sub> stretching	376 Bz CH <sub>2</sub> rocking	345 Axial py CH <sub>2</sub> rocking Some Fe-N <sub>sp3</sub> and Fe-N <sub>bipy</sub> stretching

36	357 CH <sub>2</sub> Ax rocking Zn-N <sub>sp<sup>3</sup></sub> rocking	350 A Axial CH <sub>2</sub> rocking	344 Axiaily py, bipy CH <sub>2</sub> rocking Fe-N <sub>sp<sup>3</sup></sub> , Fe-N <sub>bipy</sub> stretching	378 A Ru-N <sub>sp<sup>3</sup>/bipy</sub> stretching Bipy libration	389 Fe-N <sub>sp<sup>3</sup>/bipy</sub> stretching Bipy libration	390 Fe-N <sub>sp<sup>3</sup>/bipy</sub> stretching Bipy in-plane distortion	352 Fe-N <sub>sp<sup>3</sup>/bipy</sub> stretching Bipy in-plane distortion
37	358 CH <sub>2</sub> Ax rocking Zn-N <sub>sp<sup>3</sup></sub> stretching	355 B CH <sub>2</sub> ax and free py rocking Fe-N <sub>bipy</sub> stretching	357 CH <sub>2</sub> AxF rocking Fe-N <sub>sp<sup>3</sup></sub> , Fe-N <sub>bipy</sub> stretching	380 B Ru-N <sub>sp<sup>3</sup>/bipy</sub> stretching Bipy libration	B 396 Fe-N <sub>sp<sup>3</sup>/bipy</sub> stretching	396 Fe-N <sub>sp<sup>3</sup>/bipy</sub> stretching	371 CH <sub>2</sub> axial py and bz rocking
38	A 362 CH <sub>2</sub> -Free rocking Zn-N <sub>ax</sub> stretching	360 A CH <sub>2</sub> ax and free py bowing, Fe-N <sub>bipy</sub> stretching	388 CH <sub>2</sub> Ax7 and 7 rocking Fe-N <sub>sp<sup>3</sup></sub> stretching	398 A CH <sub>2</sub> ax and free py, bowing Ru- N <sub>bipy</sub> stretching	406 A Fe-N <sub>sp<sup>3</sup>/bipy</sub> stretching	408 Fe-N <sub>sp<sup>3</sup>/bipy</sub> stretching	377 CH <sub>2</sub> bz rocking
39	16 365 CH <sub>2</sub> -free rocking Zn-N <sub>ax</sub> stretching	391 B CH <sub>2ax</sub> /bipy Fe-N <sub>sp<sup>3</sup>/bipy</sub> stretching	390 CH <sub>2</sub> free rocking	416 B Free py ring out-of-plane C-C- C bending	416 B Free py ring out-of-plane C- C-C bending	416 Bz out-of-plane C-C-C bending	396 All CH <sub>2</sub> rocking Fe-N <sub>sp<sup>3</sup>/N<sub>bipy</sub></sub> stretching Bipy in-plane distortion
40	16 414 CH <sub>2</sub> bipy rocking Zn-N <sub>sp<sup>3</sup>/N<sub>bipy</sub></sub> stretching Bipy in-plane distortion	A 417 Free ring out-of- plane C-C-C bending	417 CH <sub>2</sub> bipy and free rocking Free ring out-of- plane C-C-C bending Fe-N <sub>sp<sup>3</sup></sub> stretching	419 A Free py ring out-of-plane C-C- C bending	417 A Free py ring out-of-plane C- C-C bending	417 Bz out-of-plane C-C-C bending	413 Bz out-of- plane C-C-C bending
41	16 419 Free ring out-of- plane C-C-C	420 B Free ring out-of- plane C-C-C	420 Free py and 7 ring out-of-plane	438 B bipy in-plane distortion	437 B bipy in-plane distortion	427 bipy in-plane distortion	418 Bz out-of- plane C-C-C

42	16	419	Free ring out-of-plane C-C-C bending	432 A CH <sub>2</sub> -bipy rocking Axial py out-of-plane C-C-C bending Fe-N <sub>sp3</sub> stretching	C-C-C bending	Fe-N <sub>sp3</sub> stretching	Fe-N <sub>sp3</sub> stretching Bz out-of-plane C-C-C bending	bending
43	16	436	Axial py out-of-plane C-C-C bending	438 B Axial py out-of-plane C-C-C bending	424 7, free, Ax7 py ring out-of-plane C-C-C bending CH <sub>2</sub> -bipy and rocking	445 B Axial py ring out-of-plane C-C bending Fe-N <sub>sp3</sub> , Fe-N <sub>bipy</sub> stretching	440 Axial py ring out-of-plane C-C bending Fe-N <sub>sp3</sub> stretching	429 Bz and axial py out-of-plane C-C-C bending bipy CH <sub>2</sub> rocking
44	16	439	Axial py out-of-plane C-C-C bending	441 A CH <sub>2</sub> -bipy rocking Axial py out-of-plane C-C-C bending Fe-N <sub>sp3</sub> /N <sub>bipy</sub> stretching	435 Axial py rings out-of-plane C-C-C bending	465 B Axial py ring out-of-plane C-C bending Fe-N <sub>sp3</sub> , Fe-N <sub>bipy</sub> stretching	448 Axial py ring out-of-plane C-C bending Fe-N <sub>sp3</sub> stretching Axial CH <sub>2</sub> rocking	438 Axial py ring out-of-plane C-C bending Fe-N <sub>sp3</sub> stretching
45	16	440	Free and axial py out-of-plane C-C-C bending	443 B Axial py out-of-plane C-C-C bending	438 Ax7 py ring out-of-plane C-C-C bending	466 A Axial py out-of-plane C-C-C bending	454 Axial py out-of-plane C-C-C bending	439 Bz and axial py out-of-plane

46	16	445	Free and axial py out-of-plane C-C-C bending Zn-N <sub>sp3</sub> /N <sub>bipy</sub> .	bending CH <sub>2</sub> bipy rocking A 447 Axial/free py out-of-plane C-C-C bending Fe-N <sub>sp3</sub> bending	bending Fe-N <sub>sp3</sub> stretching Ax7 py ring out-of-plane C-C-C bending Fe-N <sub>sp3</sub> stretching	bending CH <sub>2</sub> bipy rocking 471 B Fe-N <sub>sp3</sub> stretching Axial/free py out-of-plane C-C-C bending	bending CH <sub>2</sub> bipy rocking 475 B Free py ring out-of-plane C-C-C bending	bending CH <sub>2</sub> bipy rocking 465 Axial py out-of-plane C-C-C bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	C-C-C bending 442 Axial py and bz ring out-of-plane C-C-C bending Fe-N <sub>sp3</sub> stretching
47	16	453	Bipy out-of-plane C-C-C bending	454 B Bipy out-of-plane C-C-C bending	455 Bipy ring out-of-plane C-C-C bending N <sub>bipy</sub> -Fe-N <sub>ax</sub> bending	475 A CH <sub>2</sub> free rocking Free py out-of-plane C-C-C bending	477 A Bipy and axial py ring out-of-plane C-C-C bending. N <sub>ax</sub> -Fe-N <sub>ax</sub> bending. Fe-N <sub>bipy</sub> bending and stretching	475 Axial py out-of-plane C-C-C bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	447 Axial py nad bipy out-of-plane C-C-C bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching Axial CH <sub>2</sub> rocking
48	16	457	Bipy out-of-plane C-C-C bending.	459. A Bipy out-of-plane C-C-C bending	459 AxF and 7 py ring out-of-plane C-C-C bending	484 A Ru-N <sub>sp3</sub> stretching bipy and axial out-of-plane C-C-C bending	483 Fe-N <sub>sp3</sub> stretching bipy and axial out-of-plane C-C-C bending	480 Axial py out-of-plane C-C-C bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	455 Bipy out-of-plane C-C-C bending N <sub>bipy</sub> -Fe-N <sub>ax</sub> bending
49	16	461	CH <sub>2</sub> Free rocking All rings out-of-plane C-C-C bending	466 B free/axial py out-of-plane C-C-C bending CH <sub>2</sub> free py rocking	461 AxF and bipy ring out-of-plane C-C-C bending Some Fe-N in-plane (bipy, sp3)	490 B bipy out-of-plane C-C-C bending	495 B Bipy ring out-of-plane C-C-C bending. N <sub>ax</sub> -Fe-N <sub>ax</sub> bending.	493 Bipy ring out-of-plane C-C-C bending.	461 Axial py ring out-of-plane C-C-C bending Some Fe-N in-plane (bipy,

50	16	A, 468. CH <sub>2</sub> Free rocking All rings out-of-plane C-C-C bending	469 A free/axial py out-of-plane C-C-C bending CH <sub>2</sub> free py rocking	468 7 and Ax7 py ring out-of-plane C-C-C bending	495 A bipy and axial out-of-plane C-C-C bending	497 A Bipy and axial py ring out-of-plane C-C-C bending. N <sub>ax</sub> -Fe-N <sub>ax</sub> bending. Fe-N <sub>bipy</sub> bending and stretching	498 Bipy ring out-of-plane C-C-C bending. N <sub>ax</sub> -Fe-N <sub>ax</sub> bending.	464 Axial py and bipy ring out-of-plane C-C-C bending	sp <sup>3</sup> ) stretching and bending
51	16	489 bipy in-plane zigzag N <sub>sp3</sub> -Zn-N <sub>bipy</sub> bending and stretching	491 B free py CH <sub>2</sub> rocking. Free py out-of-plane C-C-C bending bipy zigzag in-plane	490 bipy in-plane zigzag N <sub>sp3</sub> -Fe-N <sub>bipy</sub> bending and stretching	497 B free py CH <sub>2</sub> rocking. Free py out-of-plane C-C-C bending bipy zigzag in-plane	500 B axial py ring out-of-plane C-C-C bending. N <sub>ax</sub> -Fe-N <sub>ax</sub> bending. Fe-N <sub>isp3</sub> bending and stretching	504 All rings out-of-plane C-C-C bending.	491 bipy in-plane zigzag N <sub>sp3</sub> -Fe-N <sub>bipy</sub> bending and stretching Bz and axial py out-of-plane C-C-C bending	
52	16	512 CH <sub>2</sub> bipy rocking bipy and free py out-of-plane C-C-C bending Zn-N <sub>sp3</sub> stretching	503 B CH <sub>2</sub> bipy rocking Axial py out-of-plane C-C-C bending	499 Ax7 and 7 py out-of-plane C-C-C bending	505 B Bipy and axial py ring out-of-plane C-C-C bending. N <sub>ax</sub> -Ru-N <sub>ax</sub> bending. Ru-N <sub>bipy</sub> bending and stretching	506 Bipy and axial py ring out-of-plane C-C-C bending. N <sub>ax</sub> -Fe-N <sub>ax</sub> bending. Fe-N <sub>bipy</sub> bending and stretching	507 Bipy and axial py ring out-of-plane C-C-C bending. N <sub>bip</sub> -Fe-N <sub>ax</sub> bending.	499 Bz CCC in-phase bending Fe-N <sub>sp3</sub> stretching	
53	16,6	512 Axial py out-of-plane C-C-C bending + free py	508 A Axial py out-of-plane C-C-C bending + free py	510 Ax7 py out-of-plane C-C-C bending	516 A Axial and free py ring out-of-plane C-C-C bending.	509 axial py ring out-of-plane C-C-C bending.	512 Axial py and bz C-C-C bending.	507 axial py ring out-of-plane C-C-C bending.	

		CCC in-phase bending Zn-N <sub>sp3</sub> bending +stretching	CCC in-phase bending Fe-N <sub>sp3</sub> bending +stretching	Fe-N <sub>bipy</sub> stretching N <sub>sp3</sub> -Fe-N <sub>bipy</sub> bending	All CH <sub>2</sub> rocking	Nax-Fe-Nax bending. Fe-N <sub>sp3</sub> bending and stretching		All CH <sub>2</sub> rocking
54	16,6	B, 513.3 Axial py "out-of-plane C-C-C bending + free py CCC in-phase bending Zn-N <sub>sp3</sub> bending+stretching	509 B Axial py "out-of-plane C-C-C bending + free py CCC in-phase bending Fe-N <sub>sp3</sub> bending+stretching	519 CH <sub>2</sub> bipy rocking Fe-N <sub>sp3</sub> stretching Free py out-of-plane C-C-C bending	520.8 B Axial py ring out-of-plane C-C-C bending. Bipy in-plane zig-zagging Fe-N <sub>sp3</sub> bending+stretching	523 B Axial py ring out-of-plane C-C-C bending. Bipy in-plane zig-zagging Fe-N <sub>sp3</sub> bending+stretching	508 Bz CCC in-phase bending	
55	16,6	521 Free py out-of-plane C-C-C bending + axial py CCC in-phase bending N <sub>bipy</sub> -Zn-N <sub>sp3</sub> bending	518 B Free py out-of-plane C-C-C bending + axial py CCC in-phase bending Fe-N <sub>sp3</sub> stretching	520 7 py out-of-plane C-C-C bending CH <sub>2all</sub> rocking	527 axial py ring out-of-plane C-C-C bending. N <sub>sp3</sub> -Ru-N <sub>sp3</sub> bending and stretching	523 axial py ring out-of-plane C-C-C bending. N <sub>sp3</sub> -Fe-N <sub>sp3</sub> bending and stretching	512 axial py ring out-of-plane C-C-C bending. N <sub>sp3</sub> -Fe-N <sub>sp3</sub> bending and stretching	
56	16,6	528 All CH <sub>2</sub> rocking Bipy "out-of-plane C-C-C bending	536.3 A All CH <sub>2</sub> rocking Bipy out-of-plane C-C-C bending	533 Bipy and free py out-of-plane C-C-C bending	533 B Bipy and free py out-of-plane C-C-C bending Ru-N <sub>sp3</sub> stretching	534 B Fe-N <sub>sp3</sub> bipy in-plane bending	536 N <sub>sp3</sub> -Fe-N <sub>sp3</sub> bending bipy in-plane bending	
57	6	607 py free, axial and bipy CCC in-phase bending	607 A py free, axial and bipy CCC in-phase bending	606 Bipy, AxF and free py phase bending	607 A Bipy and free py CCC in-phase bending	609 A Bipy and free py CCC in-phase bending	596 Bz CCC in-phase bending Fe-N <sub>sp3</sub>	



64	6	650 N <sub>ax</sub> -Zn stretching Axial py CCC in-phase bending	648 B N <sub>ax</sub> -Fe stretching Axial py CCC in-phase bending	651 Bipy, 7, AxF py CCC in-phase bending Fe-N <sub>bipy</sub> , Fe-N <sub>Ax</sub> Free, Fe-N7 stretching	654 B Axial CCC in-phase bending Ru-N <sub>axial</sub> stretching	655 B Axial CCC in-phase bending Fe-N <sub>axial</sub> stretching	653 Axial CCC in-phase bending Fe-N <sub>axial</sub> stretching	647 N <sub>ax</sub> -Fe stretching Axial py CCC in-phase bending
65	6	651 N <sub>ax</sub> -Zn stretching Axial py CCC in-phase bending	653 B Bipy in-phase bending Fe-N <sub>bipy</sub> stretching	653 Axial py and bipy in-phase bending Fe-N <sub>bipy</sub> and Fe-N <sub>Ax</sub> stretching	658 A Axial CCC in-phase bending Ru-N <sub>axial</sub> stretching	656 Axial CCC in-phase bending Fe-N <sub>axial</sub> stretching	655 Axial CCC in-phase bending Fe-N <sub>axial</sub> stretching	653 Bipy in-phase bending Fe-N <sub>bipy</sub> stretching
66	6	655 Bipy in-phase bending Zn-N <sub>bipy</sub> stretching	658 B Bipy and axial py in-phase bending Fe-N <sub>bipy</sub> stretching	657 Bipy and 7 py in-phase bending Fe-N <sub>bipy</sub> stretching	667 B bipy CCC in-phase bending Ru-N <sub>bipy</sub> stretching	665 B bipy CCC in-phase bending Fe-N <sub>bipy</sub> stretching	666 bipy CCC in-phase bending Fe-N <sub>bipy</sub> stretching	656 Bipy and axial py in-phase bending Fe-N <sub>bipy</sub> stretching
67	6,4	679 Zn-N <sub>bipy</sub> Free py puckering Axial py/bipy – CCC in-phase bending	679 A Fe-N <sub>bipy</sub> Free py puckering Axial py/bipy – CCC in-phase bending	672 All rings CCC in phase bending and ring puckering	685 B Ru-N <sub>bipy</sub> /N <sub>sp3</sub> Free py puckering Axial py/bipy – CCC in-phase bending	698 A All rings CCC in phase bending. Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	680 Bz puckering bipy CCC in-phase bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	670 Bz puckering bipy CCC in-phase bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching

68	6	679 B All rings CCC in-phase bending Zn-N <sub>sp3</sub> stretching	693 A Bipy/free py CCC in-phase bending N <sub>sp3</sub> -Fe stretching CH <sub>2</sub> Free rocking	678 All rings CCC in-phase bending, puckering of Free py	701 A All rings CCC in phase bending. Ru-N <sub>sp3</sub> /N <sub>bipy</sub> stretching	703 B All rings CCC in phase bending. Fe-N <sub>sp3</sub> stretching	680 Bz puckering bipy CCC in-phase bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	678 Bz puckering bipy and axial py CCC in-phase bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching
69	6	724 N <sub>bipy</sub> /N <sub>sp3</sub> -Zn stretching Bipy CCC in-phase bending	727 A N <sub>bipy</sub> /N <sub>sp3</sub> -Fe stretching Bipy CCC in-phase bending	722 bipy symmetric CCC in-phase bending Fe-N <sub>bipy</sub> /N <sub>sp3</sub> stretching	736 A Bipy CCC in-phase bending Ru-N <sub>bipy</sub> stretching	735 A Bipy CCC in-phase bending Fe-N <sub>bipy</sub> stretching	720 Bz puckering bipy CCC in-phase bending Fe-N <sub>bipy</sub> stretching	716 Bz puckering bipy CCC in-phase bending Fe-N <sub>bipy</sub> stretching
70	4	754 Axial py, bipy puckering	754 A Axial py puckering	751 Ax7 py puckering	750 B Axial and free py puckering	752 B Axial and free py puckering	724 Bz puckering	722 Bz puckering
71	4	758 Axial py puckering	756 B Axial py puckering	754 AxF py puckering	753 A Axial and free py puckering	753 A Axial and free py puckering	735 Bz C-H out of plane in phase bipy CCC in-phase bending Fe-N <sub>bipy</sub> stretching	729 Bz puckering bipy CCC in-phase bending Fe-N <sub>bipy</sub> stretching
72	4	761 Axial py, bipy puckering	760 A bipy puckering	762 bipy puckering CH <sub>2</sub> bipy rocking	754 B Axial and free py puckering	755 B Axial and free py puckering	755 Axial puckering	754 Ax py and bipy puckering
73	4	770 Free py puckering	762 B free puckering	763 7 py puckering	756 B Axial py and bipy	756 A Axial and free	755 Axial	757 Axial

74	4	770.	Free py puckering	770 A	Free py puckering	771 A	Free py puckering	762 B	bipy puckering	763	bipy puckering	761	Axial py and bipy puckering
75	11	786	bipy C-H out of plane in phase	786 A	bipy C-H out of plane in phase	787 A	bipy C-H out of plane in phase	793 A	bipy C-H out of plane in phase	786	Bz C-H out of plane in phase	783	Bz C-H out of plane in phase
76	11	799	Free py C-H out of plane in phase	799 B	Free and axial py C-H out-of-plane in phase	802 A	Free and axial py C-H out-of-plane in phase	802 A	Free py C-H out-of-plane in phase	786	Bz C-H out of plane in phase	784	Bz C-H out of plane in phase
77	11	801	Free py C-H out of plane in phase	801 A	Free and axial py C-H out-of-plane in phase	803 B	Free and axial py C-H out-of-plane in phase	803 A	Free py C-H out-of-plane in phase	794	bipy C-H out of plane in phase	786	bipy C-H out of plane in phase
78	11	815	Axial py C-H out of plane in phase	812 B	Free and axial py C-H out-of-plane in phase	811 A	Free and axial py C-H out-of-plane in phase	810	Free and axial py C-H out-of-plane in phase	814	Axial py C-H out-of-plane in phase	811	Axial py C-H out-of-plane in phase
79	11	815	Axial py C-H out of plane in phase	814 A	Free and axial py C-H out-of-plane in phase	813 B	Axial py C-H out-of-plane in phase	813 A	Axial py C-H out-of-plane in phase	814	Axial py C-H out-of-plane in phase	812	Axial py C-H out-of-plane in phase
80	11	834		830 B	837	817	823 B	827	829				

81	11	840	Axial py breathing Bipy C-H out-of-plane in phase Zn-N <sub>ax</sub> stretching	838 A All rings C-H out-of-plane in phase	834 B All rings C-H out-of-plane in phase	Free and axial py C-H out-of-plane in phase	830 Bz and axial py C-H out-of-plane in phase	All rings C-H out-of-plane in phase
82	11	84X	Axial py breathing Bipy C-H out-of-plane in phase Zn-N <sub>ax</sub> stretching	839 bipy, 7, Ax py C-H out-of-plane in phase	837 B Free and axial py C-H out-of-plane in phase	Free and axial py C-H out-of-plane in phase	841 Axial py breathing Bipy C-H out-of-plane in phase	835 All rings C-H out-of-plane in phase
83	11, 1	851	Bipy C-H out-of-plane in phase	842 Ax7, 7 py C-H out-of-plane in phase Fe-Nax7	843 A bipy and axial py C-H out-of-plane in phase bipy and axial CH <sub>2</sub> -C stretching	bipy C-H out-of-plane in phase	845 Axial py breathing Fe-N <sub>sp3</sub> stretching	844 bipy C-H out-of-plane in phase + axial py breathing
84	11,1	854	N <sub>sp3</sub> -CH <sub>2</sub> bipy stretching, bipy in-plane stretching Zn-N <sub>sp3</sub> stretching	860 Bipy and free py C-H out-of-plane in phase	846 B Bipy C-H out-of-plane in phase Axial py breathing	Bipy C-H out-of-plane in phase Axial py breathing	850 bipy C-H out-of-plane in phase	851 Bipy C-H out-of-plane in phase Axial py breathing
85	11	863	N <sub>sp3</sub> -CH <sub>2</sub> bipy stretching, bipy in-plane stretching	871 N-CH <sub>2</sub> stretching, All rings C-H out-of-plane in phase	859 B N <sub>sp3</sub> -CH <sub>2</sub> bipy stretching, bipy in-plane	N <sub>sp3</sub> -CH <sub>2</sub> bipy stretching, bipy in-plane	857 N <sub>sp3</sub> -CH <sub>2</sub> bipy stretching, bipy in-plane	857 All N-CH <sub>2</sub> stretching bipy in-plane

		Zn-N <sub>sp3</sub> stretching	CH <sub>2</sub> -C py stretching	stretching Ru-N <sub>sp3</sub> stretching	stretching Fe-N <sub>sp3</sub> stretching	stretching Fe-N <sub>sp3</sub> stretching	stretching Fe-N <sub>sp3</sub> stretching
86	11,1,1 0	868 All rings C-H out-of-plane in phase	876 Bipy, 7, free py combination of ring breathing and C <sub>6</sub> libration Fe-N <sub>sp3</sub> stretching	866 A N <sub>sp3</sub> -CH <sub>2</sub> bipy stretching, bipy in-plane stretching Ru-N <sub>sp3</sub> stretching	871 A N <sub>sp3</sub> -CH <sub>2</sub> bipy stretching, Fe-N <sub>sp3</sub> stretching	880 Bz C-H out-of-plane in phase CH <sub>2</sub> -C Bz stretching Fe-N <sub>sp3</sub> stretching	864 All rings C-H out-of-plane in phase Fe-N <sub>sp3</sub> stretching
87	11,10	872 All rings C-H out-of-plane in phase.	879 Bipy, free, 7 py C-H out-of-plane in phase	882 B Bipy C-H out-of-plane in phase	887 B bipy C <sub>6</sub> libration	887 All rings C-H out-of-plane in phase Fe-N <sub>sp3</sub> stretching.	881 All rings C-H out-of-plane in phase Fe-N <sub>sp3</sub> stretching.
88	11,10	900 bipy C <sub>6</sub> libration	905 bipy C <sub>6</sub> libration	885 B Free C <sub>6</sub> libration Ru-N <sub>sp3</sub> stretching	891 A bipy C-H out of plane in-phase	887 bipy C-H out of plane in-phase	900 Bz and bipy C-H out of plane in-phase
89	10	946 Free C <sub>6</sub> libr. CH <sub>2</sub> free py rocking	946 Ax7 C <sub>6</sub> libration CH <sub>2</sub> free rocking	937 A Free py C <sub>6</sub> libration Free CH <sub>2</sub> wagging	946 A Free py C <sub>6</sub> libration	902 Bz C <sub>6</sub> libration	903 Bz and bipy C-H out of plane in-phase
90	10	949 Free C <sub>6</sub> libr. CH <sub>2</sub> free py rocking	948 Ax7 C <sub>6</sub> libration CH <sub>2</sub> free rocking	942 B Axial C <sub>6</sub> libration Axial CH <sub>2</sub> -Nsp3 stretching Bipy CH <sub>2</sub> wagging	946 B Ax and free py C <sub>6</sub> libration	902 Bz C <sub>6</sub> libration	905 Bz C <sub>6</sub> libration
91	10	954	949	944 A	949 A	929	938

		Axial and free py C <sub>6</sub> libration	Axial py and Free py C <sub>6</sub> libration	Ax C <sub>6</sub> libration	Ax and free py C <sub>6</sub> libration	Ax py C <sub>6</sub> libration	N <sub>sp<sup>3</sup></sub> -Bz CH <sub>2</sub> stretching	N <sub>sp<sup>3</sup></sub> -Bz CH <sub>2</sub> stretching
92	10	957 Axial py C <sub>6</sub> libration	954 B Axial py Free py C <sub>6</sub> libration	955 Bipy, Ax7 py C <sub>6</sub> - libration	948 B Axial py C <sub>6</sub> libration.	949.0 B Axial and free py C <sub>6</sub> -libr.	937 N <sub>sp<sup>3</sup></sub> -Bz CH <sub>2</sub> stretching	946 N <sub>sp<sup>3</sup></sub> -bipy CH <sub>2</sub> stretching
93	10	957 Axial and free py C <sub>6</sub> libration	956.0 □ A All rings C <sub>6</sub> libration	958 Free, AxF py C <sub>6</sub> - libration	948 B Ax py C <sub>6</sub> -libr.	954 A Axialpy C <sub>6</sub> -libr.	950 Axial py C <sub>6</sub> -lib	949 Axial py C <sub>6</sub> -lib + N <sub>sp<sup>3</sup></sub> -axial CH <sub>2</sub> stretching
94	10	964 bipy C <sub>6</sub> libration	957 B All rings C <sub>6</sub> libration	963.7 7 py C <sub>6</sub> -libration	951 B Free by and bipy C <sub>6</sub> libration	958 B CH <sub>2</sub> bipy wagging	950 Axial py- C <sub>6</sub> - libration	954 Axial py- C <sub>6</sub> - libration
95	10	965 bipy1 and free py C <sub>6</sub> libration	960 All rings C <sub>6</sub> libration	969 All rings C <sub>6</sub> libration	957 A free py C <sub>6</sub> -lib	961 A bipy and free py C <sub>6</sub> libration. CH <sub>2</sub> bipy wagging	952 Axial py- C <sub>6</sub> - libration All CH <sub>2</sub> wagging	959 Axial py- C <sub>6</sub> - libration
96	10	968 All rings C <sub>6</sub> libration	974.0 B All rings C <sub>6</sub> libration	970 Ax7, bipy C <sub>6</sub> - libration CH <sub>2</sub> Ax7 - rocking	961 B free py C <sub>6</sub> -libr.	964 Free py C <sub>6</sub> -libr.	955 N <sub>sp<sup>3</sup></sub> -CH <sub>2</sub> Ax stretching Bz CH <sub>2</sub> rocking	963 Ax C <sub>6</sub> - libration All CH <sub>2</sub> rocking
97	10, 17	969 bipy and axial py C-H out-of-plane + CH <sub>2</sub> rocking	976 A Free and axial py C-H out-of-plane + CH <sub>2</sub> rocking	980 AxF, bipy, 7 py C <sub>6</sub> -libration CH <sub>2</sub> AxF - rocking	972 A Ax and free py C <sub>6</sub> libr. Bipy C-H out of plane	983 A Axial and free py CH <sub>2</sub> wagging all rings C <sub>6</sub> libration	967 All rings C <sub>6</sub> libration	972 Ax C <sub>6</sub> - libration All CH <sub>2</sub> rocking
98	17,10	990	984 B	988	981 B	985 B	970	973

99	17,12	bipy and axial py C-H out-of-plane + CH <sub>2</sub> rocking	axial py C-H out-of-plane + CH <sub>2</sub> wagging	Fe-N7 stretching 7 CCC trigonal bending bipy C-H out-of-plane	Ax and free py C6 libr. Bipy C-H out of plane "17"	axial py C-H out-of-plane + CH <sub>2</sub> wagging	All rings C6 libration	bipy and axial py C-H out-of-plane + axial CH <sub>2</sub> wagging
100	12,17,10	Free py CCC trigonal bending + Bipy C-H out of plane	990 A Bipy C-H out-of-plane + CH <sub>2</sub>	988 Bipy C-H out of plane free CCC trigonal bending bipy C-H out-of-plane	988 B Bipy C-H out of plane free CCC trigonal bending	988.1 A bipy Oop 17 free c3t	985 Bz C6 libration	981 Bz C6 libration
101	12,17,10	Free py CCC trigonal bending + Bipy C-H out of plane	993 B free py CCC trigonal bending	992 Free py CCC trigonal bending	990 A Bipy C-H out of plane free CCC trigonal bending	992 B bipy C-H out-of-plane	985 Bz C6 libration	986 Bz and bipy C6 libration
102	12, 17	Free py CCC trigonal bending + Bipy C-H out of plane	994 B Bipy C-H out-of-plane + CH <sub>2</sub> rocking	999 Bipy C-H out-of-plane + CH <sub>2</sub> rocking	992 B bipy C-H out of plane free CCC trigonal bending	995 B free py CCC trigonal bending	989 Bipy in-plane stretching N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending	988 Bz and bipy C6 libration
103	12,5	Free py CCC trigonal bending + Bipy C-H out of plane Axial py CH <sub>2</sub> rocking	996 A Bipy C-H out-of-plane + CH <sub>2</sub> rocking	1004 bipy trigonal C-H out-of-plane	996 A Bipy and axial py C-H out of plane free CCC trigonal bending	998 A bipy C-H out of plane free CCC trigonal bending	990 Bipy C-H out-of-plane + CH <sub>2</sub> rocking	997 Bipy C-H out-of-plane + CH <sub>2</sub> rocking
		1006 Bipy C-H out of plane	1001 A bipy trigonal C-H out-of-plane	1008 trig. bending. 7	1001 A Bipy C-H out-of-plane + CH <sub>2</sub>	1004 A bipy trigonal bending	1001 bipy trigonal C-H out-of-plane	1003 bipy trigonal C-H out-of-plane +

		Axial py CH <sub>2</sub> rocking			rocking	trigonal C-H out-of-plane		trigonal C-H out-of-plane	1005	bz trig. bending
104	12,5,1	1015 bipy CCC trigonal bending (asym) Zn-N <sub>bipy</sub> stretching	1015 B bipy trigonal bending Fe-N <sub>bipy</sub> stretching.	1012 bipy trig. bending (asym) Fe-N <sub>bipy</sub>	1017 A Free and axial C-H out-of-plane	1017 B free py trigonal bending trigonal C-H out-of-plane	1005 Bz trig. bending	1005 Bz trig. bending	1005 Bz trig. bending	1005 Bz trig. bending
105	12, 5	1017 Free py C-H out-of-plane	1016 A Axial py trig. bending Fe-N <sub>axial</sub> stretching.	1014 trig. bending bipy/axial py Fe-N <sub>bipy</sub> /N <sub>ax</sub> stretching	1018 B Free py C-H out-of-plane	1017 A free py trigonal bending trigonal C-H out-of-plane	1005 Bz trig. bending	1006 bipy trigonal C-H out-of-plane +bz trig. bending	1006 bipy trigonal C-H out-of-plane +bz trig. bending	1006 bipy trigonal C-H out-of-plane +bz trig. bending
106	12, 5	1018 Free py C-H out-of-plane	1017 B Axial py trig. bending Fe-N <sub>axial</sub> stretching.	1017 Trig. bending axial py Fe-N <sub>bipy</sub> /N <sub>ax</sub> stretching	1019 A Axial py C-H out-of-plane	1023 B Axial py trigonal bending and trigonal C-H out-of-plane bending Fe-N <sub>ax</sub> stretching	1023 Axial py trig. stretching + out-of-plane C-H stretch Fe-N <sub>ax</sub> stretching	1013 Axial py trig. bending Fe-N <sub>axial</sub> stretching.	1013 Axial py trig. bending Fe-N <sub>axial</sub> stretching.	1013 Axial py trig. bending Fe-N <sub>axial</sub> stretching.
107	12,5	1021 Axial py CCC trigonal bending Zn-N <sub>ax</sub> stretching (sym)	1018 A Free py trigonal C-H out-of-plane	1019 Free py trigonal C-H out-of-plane	1022 B Free and axial C-H out-of-plane	1024 A Axial py trigonal bending trigonal out-of-plane C-H	1023 Axial py trigonal out-of-plane C-H	1015 Asym. Bipy and axial trigonal bending Fe-N <sub>ax</sub> /N <sub>bipy</sub> stretching	1015 Asym. Bipy and axial trigonal bending Fe-N <sub>ax</sub> /N <sub>bipy</sub> stretching	1015 Asym. Bipy and axial trigonal bending Fe-N <sub>ax</sub> /N <sub>bipy</sub> stretching
108	12,5	1023 Axial py CCC trigonal bending Zn-N <sub>ax</sub> stretching (asym)	1019 B Free py trigonal C-H out-of-plane	1021 Sym bipy trig. bending + axial py trig. C-H out-of-plane Fe-N <sub>bipy</sub> /N <sub>ax</sub> stretching	1024 B Axial py CCC trigonal bending Ru-N <sub>ax</sub> stretching	1024 B Axial py trigonal bending Trigonal out-of-plane C-H	1024 Axial py trig. bending Fe-N <sub>ax</sub> stretching (asym)	1017 Axial py trig. bending Fe-N <sub>axial</sub> stretching.	1017 Axial py trig. bending Fe-N <sub>axial</sub> stretching.	1017 Axial py trig. bending Fe-N <sub>axial</sub> stretching.
109	12	1024 bipy CCC trigonal bending (sym)	1024 A bipy trigonal bending+ axial py	1022 Sym bipy trig. bending + axial py	1028 A Axial py CCC trigonal bending	1025 A Axial py trigonal bending	1024 Axial py trig. bending	1023 Axial py trigonal out-of-plane C-	1023 Axial py trigonal out-of-plane C-	1023 Axial py trigonal out-of-plane C-

		Zn-N <sub>bipy</sub> stretching	trigonal C-H out-of-plane Fe-N <sub>bipy</sub> stretching	trig. C-H out-of-plane Fe-N <sub>bipy</sub> stretching	Ru-N <sub>ax</sub> stretching Some bipy CCC trigonal bending and Fe-N <sub>bipy</sub> stretching	Fe-N <sub>ax</sub> stretching	Fe-N <sub>ax</sub> stretching (sym)	H
110	12	1027 Axial py C-H out-of-plane	1025 B Axial py trigonal out-of-plane C-H	1023 Sym bipy trig. bending + axial py trig. C-H out-of-plane Fe-N <sub>bipy</sub> stretching	1032 B Bipy CCC trigonal bending and Fe-N <sub>bipy</sub> stretching	1033 B Bipy trigonal bending Fe-N <sub>bipy</sub> stretching	1033 Asym bipy trig. bending Fe-N <sub>bipy</sub> stretching	1025 Axial py trigonal out-of-plane C-H + sym bipy trig. bending Fe-N <sub>bipy</sub> stretching
111	12	1027 Axial py C-H out-of-plane	1026 A bipy trig. bending + axial py trig. C-H out-of-plane Fe-N <sub>bipy</sub> stretching	1044 free py trigonal C-H out-of-plane	1047 A Bipy CCC trigonal bending and Fe-N <sub>bipy</sub> stretching	1041 A Bipy trigonal bending Fe-N <sub>bipy</sub> stretching	1033 Bz trigonal out-of-plane C-H	1026 Axial py trigonal out-of-plane C-H + sym bipy trig. bending Fe-N <sub>bipy</sub> stretching
112	12	1058 free py C-H in plane bending	1058 B free py bending	1059 free py trigonal bending	1055 B Free py C-H in plane bending bipy C-H out-of-plane	1059 B free py trigonal bending	1033 Bz trigonal out-of-plane C-H	1032 Bz trigonal out-of-plane C-H
113	12	1058 free py C-H in plane bending	1058 A free py bending	1063 free py trigonal C-H out-of-plane	1055.7 A bipy C-H Oop	1059 A free py trigonal bending	1040 Sym bipy trig. bending Fe-N <sub>bipy</sub> stretching	1034 <b>0.2</b> Bz trigonal out-of-plane C-H
114	5	1061 Free py C-H out-of-	1063 B free py trigonal C-H	1065 Bipy C-H trig out-	1057 A bipy C-H out-of-	1060 A Bipy trigonal C-	1042 Bz C-H in	1042 Bz C-H in

	plane	out-of-plane	of-plane	plane	H out-of-plane	plane bending	plane bending
115	17	1061 Free py C-H out-of-plane	1063 A free py trigonal C-H out-of-plane	1065 7 py C-H trig out-of-plane	1058 A Free py C-H in-plane	1042 phenyl stretching	1042 Bz C-H in-plane bending
116	5	1067 bipy C-H out-of-plane	1064 A Bipy C-H trigonal out-of-plane	1066 Axial C-H in-plane trigonal bending	1059 A Free py C-H in-plane Axial py C-H out-of-plane	1057 Bz trig. C-H out-of-plane	1056 Bz trig. C-H out-of-plane
117	5	1068 bipy C-H out-of-plane	1066B Bipy C-H trigonal out-of-plane	1066 Bipy C-H trig out-of-plane	1062 A Free C-H out-of-plane	1057 Bz trig. C-H out-of-plane	1057 phenyl trig. C-H out-of-plane
118	5	1069 Axial C-H in-plane Bipy C-H out-of-plane	1066 A Axial trigonal C-H out-of-plane	1067 Axial pyridine C-H trig out-of-plane	1062 B Free C-H out-of-plane	1057 Axial and bipy C-H out-of-plane Bz C-H in-plane	1064 Axial py C-H in-plane bending
119	5	1068.6 A Axial C-H in-plane	1067 B Axial pyridine C-H trigonal out-of-plane	1067 Axial pyridine C-H trig out-of-plane	1064 A Axial py C-H out-of-plane	1059 Bipy C-H out-of-plane, Bz C-H in-plane bending	1065 Bipy C-H trig out-of-plane
120	15	1070 Axial C-H out-in-plane	1068 B Axial pyridine C-H trigonal out-of-plane	1069 Axial C-H in-plane trigonal bending	1064 B Axial py C-H out-of-plane	1061 Bipy trigonal C-H out-of-plane	1066 Bipy C-H trig out-of-plane
121	15	1070 Axial C-H out-of-plane	1067 A Axial pyridine C-H trigonal out-of-plane	1070 7 py trigonal out-of-plane C-H	1069 A Axial py C-H out-of-plane Some Fe-N <sub>ax</sub> stretching	1061 Bipy trigonal out-of-plane stretching	1067 Bipy+axial C-H out-of-plane
122	18	1089 Free py and bipy C-	1093 B Free py and bipy C-	1077 N <sub>sp3</sub> -	1071 B Axial py C-H	1066 Axial trigonal	1067 axial C-H out-

		H in-plane bending Free and axial-CH <sub>2</sub> rocking N <sub>sp<sup>3</sup></sub> -Zn- N <sub>sp<sup>3</sup></sub> Bending	H in-plane bending Axial CH <sub>2</sub> rocking N <sub>bipy</sub> -Fe- N <sub>sp<sup>3</sup></sub> Bending	bipy_half_free CH <sub>2</sub> stretching Free CH <sub>2</sub> rocking	out-of-plane Some Ru-N <sub>ax</sub> stretching	stretching Free CH <sub>2</sub> rocking	C-H out-of-plane	of-plane
123	18	1090 Free py and bipy C- H in-plane bending Free and axial-CH <sub>2</sub> rocking N <sub>sp<sup>3</sup></sub> -Zn- N <sub>sp<sup>3</sup></sub> bending	1093.6 A N <sub>sp<sup>3</sup></sub> - bipy CH <sub>2</sub> CH <sub>2</sub> Ax/Free py rocking N <sub>sp<sup>3</sup></sub> -Fe- N <sub>sp<sup>3</sup></sub> bending	1084 N <sub>sp<sup>3</sup></sub> - bipy CH <sub>2</sub> stretching CH <sub>2</sub> Ax/Free rocking N <sub>sp<sup>3</sup></sub> -Fe- N <sub>sp<sup>3</sup></sub> bending	1082 A N <sub>sp<sup>3</sup></sub> - bipy CH <sub>2</sub> stretching v CH <sub>2</sub> Ax/Free rocking N <sub>sp<sup>3</sup></sub> -Ru- N <sub>sp<sup>3</sup></sub> bending	1088 B N <sub>sp<sup>3</sup></sub> - bipy CH <sub>2</sub> stretching CH <sub>2</sub> Ax/Free rocking N <sub>sp<sup>3</sup></sub> -Fe- N <sub>sp<sup>3</sup></sub> bending	1067 Axial trigonal C- H out-of-plane	1068 axial C-H out- of-plane stretching and C-H trig out-of- plane
124	18	1108 N <sub>sp<sup>3</sup></sub> - free- CH <sub>2</sub> stretching N <sub>sp<sup>3</sup></sub> -Fe- N <sub>ax</sub> bending Axial py C-H in- plane bending	1105 B bipy/axial py C-H in-plane bending CH <sub>2</sub> rocking	1100 CH <sub>2</sub> 7-N <sub>sp<sup>3</sup></sub> Stretching CH <sub>2</sub> AxF rocking Ax7 C-H in-plane bending N <sub>sp<sup>3</sup></sub> -Fe- N <sub>ax</sub> bending	1088 B N <sub>sp<sup>3</sup></sub> - bipy CH <sub>2</sub> stretching v CH <sub>2</sub> Ax/Free rocking N <sub>sp<sup>3</sup></sub> -Ru- N <sub>sp<sup>3</sup></sub> bending	1099 B bipy/axial py C- H in-plane bending CH <sub>2</sub> rocking, N <sub>sp<sup>3</sup></sub> -CH <sub>2</sub> free py rocking	1074 Axial py C-H in-plane bending Some Fe-N <sub>ax</sub> stretching	1073 bipy/axial py C-H in-plane bending CH <sub>2</sub> rocking
125	18	1108 N <sub>sp<sup>3</sup></sub> - free- CH <sub>2</sub> stretching N <sub>sp<sup>3</sup></sub> -Fe- N <sub>ax</sub> bending Axial py C-H in- plane bending	1105 A bipy/axial py C-H in-plane bending CH <sub>2</sub> rocking	1109 CH <sub>2</sub> free-N <sub>sp<sup>3</sup></sub> Stretching CH <sub>2</sub> AxF rocking AxF C-H in-plane bending N <sub>sp<sup>3</sup></sub> -Fe- N <sub>ax</sub> bending	1100 B Bipy and free py C-H in-plane bending Ru <sub>bipy</sub> stretching	1100 A bipy/axial py C- H in-plane bending CH <sub>2</sub> rocking, free py CH <sub>2</sub> rocking v	1075 Axial py C-H in-plane bending Some Fe-N <sub>ax</sub> stretching	1074 bipy/axial py C-H in-plane bending CH <sub>2</sub> rocking
126	18	1108 bipy C-H in-plane bending Zn-N <sub>bipy</sub> stretching	1109 B bipy/axial py C-H in-plane bending CH <sub>2</sub> rocking	1110 bipy C-H in-plane bending (asymmetric)	1104 B bipy C-H in-plane bending Ru-N <sub>bipy</sub> stretching	1105 B bipy C-H in- plane bending plane Fe-N <sub>bipy</sub>	1085 N <sub>sp<sup>3</sup></sub> - Bz CH <sub>2</sub> stretching CH <sub>2</sub> Ax/bipy rocking	1090 N <sub>sp<sup>3</sup></sub> - Bz CH <sub>2</sub> stretching CH <sub>2</sub> Ax/bipy rocking



134	15	free py C-H in-plane bending	free py C-H in-plane bending	free py C-H in-plane bending	free py C-H in-plane bending	free py Axial and free py C-H in plane	Axial py C-H in plane "18"	Axial py C-H in plane
135	15,9	119 free py C-H in-plane bending	1191 B free py C-H in-plane bending	1195 7 py C-H in-plane bending	1192 B free py C-H in-plane bending	1192 B free py Axial and free py C-H in plane	1157 bipy C-H in plane N <sub>bipy</sub> -Fe-N <sub>sp3</sub> bending	1156 bipy C-H in plane N <sub>bipy</sub> -Fe-N <sub>sp3</sub> bending
136	15,9	1198 axial py C-H in-plane bending	1197 A axial py C-H in-plane bending	1196 Ax F py C-H in-plane bending	1196 A axial py C-H in-plane bending 15	1197 B axial py C-H in-plane bending 1	1198 axial py C-H in-plane bending	1197 axial py C-H in-plane bending 15
137	15,9	1211 bipy py C-H in-plane bending	1197 B axial py C-H in-plane bending	1197 Ax7 py C-H in-plane bending	1197 B Axial py C-H in-plane bending	1197 A Axial py C-H in-plane bending	1198 axial py C-H in-plane bending	1198 axial py C-H in-plane bending
138	15,9	1215 bipy py C-H in-plane bending	1211 B bipy C-H in-plane bending	1211 bipy C-H in-plane bending (asymmetric)	1209 B bipy C-H in-plane bending	1209 A bipy py C-H in-plane bending	1199 Bz C-H in-plane bending	1198 Bz C-H in-plane bending
139	15	1240 Free py C-CH2 stretching and all CH2 rocking	1212 A bipy C-H in-plane bending	1215 bipy C-H in-plane bending (symmetric)	1210 A bipy C-H in-plane bending	1211 B bipy C-H in-plane bending	1199 Bz C-H in-plane bending	1198 Bz C-H in-plane bending
140	15,	1241	1231 A All CH2 rocking	1238 Bipy C-CH2 stretching and CH2 rocking	1225 A All CH2 rocking	1222 A All CH2 rocking	1209 bipy C-H in-plane bending	1212 bipy C-H in-plane bending
			1240 B	1244	1235 B	1223	1212	1212

141	Free py C-CH2 stretching and all CH <sub>2</sub> rocking	free py ring stretching	Bipy and free py C-CH2 stretching and CH <sub>2</sub> rocking	All CH <sub>2</sub> rocking	All CH <sub>2</sub> rocking	bipy C-H in plane bending	bipy + Bz C-H in-plane bending
142	15, 9, 14?	1247 A Axial py/bipy ring stretching CH <sub>2</sub> free/bipy rocking	1250 Bipy and free py C-CH2 stretching and CH <sub>2</sub> rocking	1232 B Free py ring stretching + CH <sub>2</sub> - C stretching	1243 A Free py ring stretching + CH <sub>2</sub> - C stretching	1215 Bz C-H in plane bending	1213 bipy + Bz C-H in-plane bending
143	15, 14?	1252 A Axial py/bipy ring stretching rocking	1254 Ax F py ring stretching + CH <sub>2</sub> - C stretching	1249 A Free py ring stretching + CH <sub>2</sub> - C stretching	1243 B Free py ring stretching + CH <sub>2</sub> - C stretching	1215 Bz C-H in plane bending	1213 Bz C-H in-plane bending
144	15, 14?	1253 Free py and bipy C-CH2 and ring stretching and CH <sub>2</sub> rocking	1256 7 py ring stretching + CH <sub>2</sub> - C stretching	1259 A Bipy and axial py C-H in-plane bending	1261A bipy CH <sub>2</sub> - C stretching + C-H in-plane bending	1224 Bz CH <sub>2</sub> - C stretching + C-H in-plane bending	1223 Bz CH <sub>2</sub> - C stretching + C-H in-plane bending
145	15, 14	1260 B Axial py/bipy ring stretching	1260 Ax7 and 7 ring stretching + CH <sub>2</sub> - C stretching	1263 B Axial py C-H in-plane bending Axial py and bipy CH <sub>2</sub> -C stretching	1266 B Axial py C-H in-plane bending Axial py and bipy CH <sub>2</sub> -C stretching	1225 Bz CH <sub>2</sub> - C stretching + C-H in-plane bending	1226 Bz CH <sub>2</sub> - C stretching + C-H in-plane bending
145	15, 14	1262 Axial py C-CH2 and ring stretching and CH <sub>2</sub> rocking	1265 Ax F py ring stretching + CH <sub>2</sub> - C stretching	1265 B All rings C-H in-plane bending Axial py and bipy CH <sub>2</sub> -C stretching	1267 A Axial py ring stretching + CH <sub>2</sub> - C stretching	1230 bipy C-CH2 stretching and CH <sub>2</sub> rocking	1234 bipy C-CH2 stretching and CH <sub>2</sub> rocking

146	15, 14	1262	Axial py C-CH2 and ring stretching and CH <sub>2</sub> rocking	1271 B	Ax py ring stretching	1277	Bipy and 7 py CH <sub>2</sub> - C stretching + C-H in-plane	1270 A	All rings C-H in-plane Axial py and bipy CH <sub>2</sub> -C stretching	1270 B	bipy CH <sub>2</sub> - C stretching + C-H in-plane	1230	bipy C-CH2 stretching and CH <sub>2</sub> rocking	1241	bipy C-CH2 stretching and CH <sub>2</sub> rocking
147	15,14	1285	Axial py ring stretching and CH <sub>2</sub> rocking	1294 B	Ax/free py stretching	1288	Ax7 Kekule stretching + CH <sub>2</sub> -C stretching	1286 A	Axial Kekule stretching + axial py CH <sub>2</sub> -C stretching	1291 B	Axial Kekule stretching + axial py CH <sub>2</sub> -C stretching	1261	bipy CH <sub>2</sub> - C stretching + C-H in-plane	1247	bipy + axial CH <sub>2</sub> - C stretching + C-H in-plane
148	14,15	1286	Axial py ring stretching and CH <sub>2</sub> rocking	1295 A	Free /axial py stretching	1289	AxF py Kekule stretching + CH <sub>2</sub> rocking	1291 B	Axial Kekule stretching + axial py CH <sub>2</sub> -C stretching	1292 A	Axial py ring stretching + CH <sub>2</sub> - C stretching	1263	Axial Kekule stretching + axial py CH <sub>2</sub> -C stretching	1259	bipy + axial CH <sub>2</sub> - C stretching + C-H in-plane
149	14, 15	130	Free and axial Kekule stretching	1297 A	free/axial py Kekule stretching	1296	Ax7 + 7 py Kekule stretching	1297 A	Axial Kekule stretching	1296 A	Free py Kekule stretching 14	1265	Axial Kekule stretching + axial py CH <sub>2</sub> -C stretching	1262	bipy + axial CH <sub>2</sub> - C stretching + C-H in-plane
150	14, 15	1302	Free Kekule stretching	1299 A	Axial py Kekule stretching	1299	Kekule AxF py Kekule stretching	1297 B	Axial Kekule stretching	1297 B	Free py Kekule 14	1265	bipy CH <sub>2</sub> - C stretching + C-H in-plane	1268	axial CH <sub>2</sub> - C stretching + C-H in-plane
151	14, 15	1302	Axial py Kekule stretching N <sub>ax</sub> -Zn-N <sub>ax</sub> bending	1301 B	free/axial py Kekule stretching	1300	Free, Ax7 py Kekule stretching	1298 B	Free and axial py Kekule stretching	1299 B	Axial py Kekule stretching	1290	Axial py Kekule stretching + C-H in-plane	1281	bipy + axial CH <sub>2</sub> - C stretching + C-H in-plane

152	14,15	130? Axial and free py Kekule stretching N <sub>ax</sub> -Zn-N <sub>ax</sub> bending	1303 B free/axial py Kekule stretching	1301 Axial and free Kekule stretching	1300 A Bipy and free py Kekule stretching	1300 A Axial py Kekule stretching + C- H in-plane	1295 axial CH <sub>2</sub> - C stretching + C- H in-plane
153	14	1313 bipy Kekule stretching N <sub>bipy</sub> -Zn-N <sub>bipy</sub> bending	1309A bipy free/axial py Kekule stretching	1309 bipy Kekule stretching N <sub>sp3</sub> -Fe- N <sub>bipy</sub> bending	1303 B Bipy and free py Kekule stretching	1298 Axial py Kekule stretching N <sub>ax</sub> -Fe- N <sub>bipy</sub> bending	1300 Axial py Kekule stretching N <sub>ax</sub> -Fe- N <sub>bipy</sub> bending
154	14	1320 bipy Kekule stretching N <sub>sp3</sub> -Zn- N <sub>bipy</sub> bending	1313 A Free py/bipy Kekule stretching N <sub>bipy</sub> -Fe- N <sub>bipy</sub> bending	1315 bipy Kekule stretching N <sub>bipy</sub> -Fe- N <sub>bipy</sub> bending	1305 A Free py and bipy Kekule stretching N <sub>bipy</sub> -Ru- N <sub>bipy</sub> bending	1299 Axial py Kekule stretching N <sub>ax</sub> -Fe- N <sub>bipy</sub> bending	1302 Axial py Kekule stretching N <sub>ax</sub> -Fe- N <sub>bipy</sub> bending
155	14,	1327 free py C-H in plane CH <sub>2</sub> bipy_free rocking	1315 B Free py/bipy Kekule stretching N <sub>bipy</sub> -Ru- N <sub>sp3</sub> bending	1319 free py C-H in plane CH <sub>2</sub> bipy_free rocking	1313 B Free py and bipy Kekule stretching N <sub>bipy</sub> -Ru- N <sub>sp3</sub> bending	1309 Bipy Kekule stretching N <sub>bipy</sub> -Fe- N <sub>bipy</sub> bending	1310 Bipy Kekule stretching N <sub>bipy</sub> -Fe- N <sub>bipy</sub> bending
156	14	1328 free py C-H in plane CH <sub>2</sub> bipy_free rocking	1325 B Free/axial py Kekule stretching CH <sub>2</sub> rocking	1320.3 7 py Kekule + in- plane C-H CH <sub>2</sub> bipy 7 rocking Ax7 Kekule + in-	1319 A bipy Kekule stretching Free py C-H in- plane bending	1314 Bipy Kekule stretching Bipy CH <sub>2</sub> rocking	1311 Bipy Kekule stretching Bipy CH <sub>2</sub> rocking N <sub>bipy</sub> -Fe- N <sub>sp3</sub>

157	14	1339	Axial py Kekule stretching Axial py CH <sub>2</sub> rocking	1331 A	Axial py Kekule stretching Axial py CH <sub>2</sub> rocking	plane C-H	1339	Ax and free py Kekule stretching + C-H in-plane bending	1323 B	bipy Kekule stretching Free py C-H in-plane bending	1318 A	Free py and bipy CH <sub>2</sub> rocking Bipy stretching N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending	1318	Bipy Kekule stretching N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending	1322	Bipy Kekule stretching Bipy CH <sub>2</sub> rocking	bending
158	14	1340	Axial py Kekule stretching Axial py CH <sub>2</sub> rocking	1333 B	Free py CH <sub>2</sub> rocking	1344	Ax7 py Kekule stretching + C-H in-plane CH <sub>2</sub> Ax7 rocking	1332.4 A	Axial py C-H in-plane Axial py CH <sub>2</sub> rocking	1323 B	Free py and bipy CH <sub>2</sub> rocking Bipy stretching N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending	1322	Bipy Kekule stretching N <sub>bipy</sub> -Fe-N <sub>sp3</sub> bending	1325	Bipy Kekule stretching Bipy CH <sub>2</sub> rocking		
159	14	1353	Free and bipy C-H in-plane CH <sub>2</sub> free/bipy rocking	1352 B	Axial py Kekule stretching Axial py CH <sub>2</sub> rocking	1348	Bipy and 7 py Kekule stretching + C-H in-plane	1335 B	Axial py C-H in-plane bending Axial py CH <sub>2</sub> rocking	1332 B	Axial py C-H in-plane bending Axial py CH <sub>2</sub> rocking	1323	Axial py C-H in-plane bending Axial py CH <sub>2</sub> rocking	1334	Axial py C-H in-plane bending Axial py CH <sub>2</sub> rocking		
160	14	1354	Free and bipy C-H in-plane CH <sub>2</sub> free/bipy rocking.	1352 B	free py C-H in-plane free py rocking C-H/CH <sub>2</sub>	1361	bipy Kekule stretching + C-H in-plane	1347 A	Free py C-H in-plane Free py CH <sub>2</sub> rocking	1334 A	Axial py C-H in-plane free py rocking C-H/CH <sub>2</sub> "9"γ	1333	Axial py C-H in-plane Axial py CH <sub>2</sub> rocking	1342	Axial py C-H in-plane Axial py CH <sub>2</sub> rocking		
161	14	1356	bipy C-H in-plane bending N <sub>bipy</sub> -Zn-N <sub>bipy</sub>	1359.0 A	bipy C-H in-plane bending N <sub>bipy</sub> -Fe-N <sub>bipy</sub>	1362	free Kekule stretching + C-H in-plane	1354.4 A	bipy C-H in-plane + Kekule stretching bending N <sub>bipy</sub> -Ru-N <sub>bipy</sub>	1362 A	bipy C-H in-plane bending Fe-N <sub>bipy</sub>	1358	Bz C-H in-plane Bz CH <sub>2</sub> rocking	1359	bipy C-H in-plane bending Fe-N <sub>bipy</sub>		
162	14	1380		1387 A		1382		1370 A		1376 A		1359		1364			

163	14	Free CH <sub>2</sub> rocking	Free py Kekule stretching Free py CH <sub>2</sub> rocking	Free CH <sub>2</sub> rocking	bipy C-H in-plane + CH <sub>2</sub> rocking	bipy C-H in-plane + CH <sub>2</sub> rocking	Bz C-H in-plane Bz CH <sub>2</sub> rocking
164	14	1380 Free CH <sub>2</sub> rocking	1388 B bipy CH <sub>2</sub> rocking	1393 CH <sub>2</sub> bipy and 7 py rocking	1382 B Free py C-H in-plane + CH <sub>2</sub> rocking	1383 B bipy C-H in-plane + CH <sub>2</sub> rocking	1364 Bz C-H in-plane Bipy Kekule stretching N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending
164	14	1390 Bipy Kekule stretching + bipy CH <sub>2</sub> rocking	1394 A free py C-H in-plane free py rocking C-H/CH <sub>2</sub>	1395 bipy and AxF CH <sub>2</sub> rocking	1384 A bipy C-H in-plane + CH <sub>2</sub> rocking	1392 A Free py C-H in-plane + CH <sub>2</sub> rocking	1369 Bz C-H in-plane Bz CH <sub>2</sub> rocking
165	14	1398 Bipy Kekule stretching + bipy CH <sub>2</sub> rocking	1397 B free py C-H in-plane free py rocking CH <sub>2</sub>	1412 Bipy and 7 py CH <sub>2</sub> rocking	1388 B bipy C-H in-plane + Kekule stretching, CH <sub>2</sub> rocking	1393 B bipy C-H in-plane + Kekule stretching, CH <sub>2</sub> rocking	1374 Bz CH <sub>2</sub> rocking
166	14, 19	1411 Axial py C-H in-plane Axial py CH <sub>2</sub> rocking	1410 A Axial py C-H in-plane Axial py CH <sub>2</sub> rocking	1417 AxF CH <sub>2</sub> rocking AxF py C-H in-plane	1403 A Axial py C-H in-plane + CH <sub>2</sub> rocking	1401 A Axial py C-H in-plane + CH <sub>2</sub> rocking	1383 Bz CH <sub>2</sub> rocking + Bz stretching
167	14, 19	1415	1414 B	1433	1409 B	1407 B	1383 Bipy CH <sub>2</sub> rockin

168	14, 19	1450	Axial py C-H in-plane Axial py CH <sub>2</sub> rocking	Axial py C-H in-plane Axial py rocking CH <sub>2</sub>	bipy and 7 py C-H in-plane 7 py CH <sub>2</sub> rocking	Axial py C-H in-plane + CH <sub>2</sub> rocking	Axial py C-H in-plane rocking	Bz ring stretching	Bz CH <sub>2</sub> rocking + Bz ring stretching
169	19	1452	bipy C-H in-plane bipy CH <sub>2</sub> rocking	1445A bipy C-H in-plane bipy CH <sub>2</sub> rocking	1444 bipy C-H in-plane CH <sub>2</sub> bipy rocking	1431 A bipy C-H in-plane bipy rocking CH <sub>2</sub>	1433 A bipy C-H in-plane bipy rocking CH <sub>2</sub>	1386 Bz ring stretching	1391 bipy rocking CH <sub>2</sub>
170	19, 3	1456	Bipy and free Kekule stretching + C-H in-plane	1450 B bipy C-H in-plane bipy CH <sub>2</sub> rocking	1452 bipy C-H in-plane bipy CH <sub>2</sub> rocking	1445 B bipy C-H in-plane bipy rocking CH <sub>2</sub>	1446 B bipy C-H in-plane + CH <sub>2</sub> rocking	1393 Bipy Kekule stretching bending Bipy CH <sub>2</sub> rocking	1396 Bipy Kekule stretching bending Bipy CH <sub>2</sub> rocking
171	19, 3	1456	All rings Kekule stretching + C-H in-plane	1456 B Free py C-H in-plane	1454 Free py C-H in-plane + CH <sub>2</sub> rocking	1451 A Free py C-H in-plane + Kekule stretching, CH <sub>2</sub> rocking	1452 A Free py C-H in-plane + CH <sub>2</sub> rocking	1406 Axial py C-H in-plane Axial py CH <sub>2</sub> rocking	1405 Axial py C-H in-plane Axial py CH <sub>2</sub> rocking
172	19, 3	1466	Axial py C-H in-	1464 B Axial py C-H in-	1463 Ax F C-H in-plane	1464 B C-H in-plane +	1465 B Axial py C-H	1438 bipy C-H in-	1444 bipy C-H in-

	plane	plane	+ CH <sub>2</sub> rocking	Kekule stretching, CH <sub>2</sub> rocking	in-plane + CH <sub>2</sub> rocking	plane Axial py and bipy CH <sub>2</sub> rocking	plane bipy CH <sub>2</sub> rocking
173	19, 3	1466 Axial py C-H in- plane	1468 Ax7 and 7 C-H in-plane + CH <sub>2</sub> rocking	1465.0 A Axial py C-H in- plane + Kekule stretching, CH <sub>2</sub> rocking	1465 A Axial py C-H in-plane + CH <sub>2</sub> rocking	1450 bipy C-H in- plane + ring stretching bipy CH <sub>2</sub> rocking	1451 bipy C-H in- plane + ring stretching bipy CH <sub>2</sub> rocking
174	19, 3	1483 Free py C-H in- plane free CH <sub>2</sub> rocking	1484 AxF and free CH <sub>2</sub> δ	1483 A Free py C-H in- plane + Kekule stretching	1488 B Free py C-H in- plane + CH <sub>2</sub> rocking	1467 Axial py C-H in-plane + ring stretching Axial CH <sub>2</sub> rocking	1464 Axial py C-H in-plane + ring stretching Axial CH <sub>2</sub> rocking
175	19, 3	1483 Free py C-H in- plane free CH <sub>2</sub> rocking	1484 Free py C-H in- plane all CH <sub>2</sub> δ	1485 B bipy CH <sub>2</sub> δ bipy C-H in-plane	1489 A Free py C-H in- plane + CH <sub>2</sub> rocking	1468 Axial py C-H in-plane + ring stretching Axial CH <sub>2</sub> rocking	1464 Axial py C-H in-plane + ring stretching Axial CH <sub>2</sub> rocking
176	19, 3	1485 bipy C-H in-plane bending CH <sub>2</sub> rocking	1487 Bipy and free py C-H in-plane bending All CH <sub>2</sub> δ Some N <sub>bipy</sub> -Fe- N <sub>sp3</sub> bending	1489 B Free py C-H in- plane Free/bipy CH <sub>2</sub> δ	1490 B bipy C-H in- plane + CH <sub>2</sub> rocking	1477 Bz C-H in- plane + ring stretching Bz CH <sub>2</sub> rocking	1477 Bz C-H in- plane + ring stretching Bz CH <sub>2</sub> rocking

177	19, 3	1491 All CH <sub>2</sub> δ.	1492 A Free CH <sub>2</sub> δ	1490 All CH <sub>2</sub> δ	1489 A Free py C-H in-plane bending Free/bipy CH <sub>2</sub> δ	1490 B Free py C-H in-plane Free/bipy CH <sub>2</sub> δ	1477 Bz C-H in-plane + ring stretching Bz CH <sub>2</sub> rocking	1478 Bz C-H in-plane + ring stretching Bz CH <sub>2</sub> rocking
178	19, 3	1492 free CH <sub>2</sub> δ	1494 B bipy C-H in-plane All CH <sub>2</sub> δ Some N <sub>bipy</sub> -Fe-N <sub>sp3</sub> bending	1497 All CH <sub>2</sub> δ	1497 B Free py CH <sub>2</sub> δ	1502 B Axial py C-H in-plane "14" + CH <sub>2</sub> rocking	1487 bipy C-H in-plane "14" + CH <sub>2</sub> δ	1486 bipy C-H in-plane "14" + CH <sub>2</sub> δ
179	19, 3	1500 bipy C-H in-plane "14" + CH <sub>2</sub> rocking	1497 A Axial py C-H in-plane 14 Ax CH <sub>2</sub> δ	1501 Ax7 py C-H in-plane Bipy and 7 CH <sub>2</sub> δ	1498.3 B Axial py C-H in-plane Ax py CH <sub>2</sub> δ	1503 A Axial py C-H in-plane "14" + CH <sub>2</sub> rocking	1489 bipy C-H in-plane "14" + CH <sub>2</sub> δ	1494 bipy C-H in-plane "14" + all CH <sub>2</sub> δ
180	19, 3	1500 Axial py C-H in-plane 14 Ax CH <sub>2</sub> δ	1499 B Axial py C-H in-plane 14 Ax CH <sub>2</sub> δ	1502 Ax F py C-H in-plane Ax F and free CH <sub>2</sub> δ	150. A Axial py, bipy C-H in-plane Ax/bipy CH <sub>2</sub> δ	1503 B Axial py, bipy C-H in-plane Ax/bipy CH <sub>2</sub> δ	1497 Axial py, bipy C-H in-plane Ax/bipy CH <sub>2</sub> δ	1496 all CH <sub>2</sub> δ
181	19, 3	1501 Axial py C-H in-plane 14 Ax CH <sub>2</sub> δ	1504.0 A Free py CH <sub>2</sub> δ bipy py C-H in-plane	1505 7 and Ax7 py C-H in-plane 7 and Ax7 CH <sub>2</sub> δ	1502 B Axial py, bipy C-H in-plane All CH <sub>2</sub> δ	1508 B Ax and free py CH <sub>2</sub> δ	1500 bipy C-H in-plane "14" + CH <sub>2</sub> δ	1497 Axial py C-H in-plane All CH <sub>2</sub> δ
182	19	1514 Ax CH <sub>2</sub> δ Axial py C-H in-plane	1507 All CH <sub>2</sub> δ Bipy C-H in-plane Some N <sub>bipy</sub> -Fe-N <sub>bipy</sub> bending	1509 Bipy and free CH <sub>2</sub> δ	1505 A All CH <sub>2</sub> δ Bipy C-H in-plane	1506.0 B All CH <sub>2</sub> δ Bipy C-H in-plane	1501 Axial py C-H in-plane Ax/bipy CH <sub>2</sub> δ	1499 Axial py C-H in-plane bending All CH <sub>2</sub> δ
183	19	1516 Ax CH <sub>2</sub> δ Axial py C-H in-plane	1516 B All CH <sub>2</sub> δ	1512 Bipy, Ax7 and free CH <sub>2</sub> δ	1509 A All CH <sub>2</sub> δ Bipy C-H in-plane	1514 A All CH <sub>2</sub> δ Bipy C-H in-plane	1505 Axial py C-H in-plane	1505 Axial py C-H in-plane

		plane			plane 19/14	plane 19/14	bipy CH <sub>2</sub> δ	All CH <sub>2</sub> δ
184	19	1524 bipy CH <sub>2</sub> δ	1520 A All CH <sub>2</sub> δ	1514 Bipy, Ax7 and free CH <sub>2</sub> δ bipy C-H in-plane in-phase	1519 A All CH <sub>2</sub> δ	1527 A All CH <sub>2</sub> δ	1508 Bz and Ax CH <sub>2</sub> δ	1506 Bipy and axial py ring stretching All CH <sub>2</sub> δ
185	19	1525 bipy CH <sub>2</sub> δ	1524 A bipy CH <sub>2</sub> δ	1516 7 py nad bipy CH <sub>2</sub> δ	1526.2 B All CH <sub>2</sub> δ	1531 All CH <sub>2</sub> δ	1509 Bipy ring stretching Ax CH <sub>2</sub> δ	1510 Bipy ring stretching and CH <sub>2</sub> δ
186	8	1600 Axial py and bipy ring stretching N <sub>bipy</sub> -Zn- N <sub>bipy</sub> bending N <sub>ax</sub> -Zn- N <sub>ax</sub> bending	1598 A Ax py ring stretching	1597. Ax F ring stretching N <sub>ax</sub> .Fe- N <sub>ax</sub> bending	1587 A bipy ring stretching N <sub>bipy</sub> -Ru- N <sub>bipy</sub> bending	1596 A bipy ring stretching N <sub>bipy</sub> .Fe- N <sub>bipy</sub> bending	1517 Axial py C-H in-plane bipy CH <sub>2</sub> δ	1515 Axial py CH <sub>2</sub> δ
187		1602 Axial and free ring stretching	1600 B Ax py ring stretching	1600 Ax7 and bipy (A) ring stretching N <sub>bipy</sub> .Fe- N <sub>bipy</sub> bending	1593 B bipy ring stretching N <sub>sp3</sub> -Ru- N <sub>bipy</sub> bending	1598 B Axial py and bipy ring stretching	1519 Bz ring stretching + C- H in-plane + CH <sub>2</sub> δ	1517 Bz ring stretching + C- H in-plane + bz and axial CH <sub>2</sub> δ
188	8	1601 Free ring stretching	1601 A Bipy free py ring stretching N <sub>bipy</sub> .Fe- N <sub>bipy</sub> bending	1601 Free py ring stretching	1595 A Axial ring stretching	1599 A Axial py and bipy ring stretching	1520 Bz ring stretching + C- H in-plane + CH <sub>2</sub> δ	1519 Bz ring stretching + C- H in-plane + CH <sub>2</sub> δ
189	8	1602	1602 B	1602	1596 B	1600 B	1522	1520

190	8	Axial and free py ring stretching	Bipy free py ring stretching	All rings ring stretching $N_{\text{bipy}}\text{-Fe-}N_{\text{sp}^3}$ bending	Axial ring stretching	bipy ring stretching $N_{\text{bipy}}\text{-Fe-}N_{\text{bipy}}$ bending	Bz ring stretching + C-H in-plane + Bz and axial py $\text{CH}_2 \delta$	Bz ring stretching + C-H in-plane + all $\text{CH}_2 \delta$
191	8	1602 Axial and free ring stretching	1602 A Bipy free py ring stretching $N_{\text{sp}^3}\text{-Fe-}N_{\text{sp}^3}$ bending	1602 7, bipy, free py – ring stretching	1601 A Free py ring stretching	1602 A Free py ring stretching	1595 bipy ring stretching bending $N_{\text{sp}^3}\text{-Fe-}N_{\text{bipy}}$	1598 Axial py ring stretching $N_{\text{sp}^3}\text{-Fe-}N_{\text{sp}^3}$ bending
192	8	1608 bipy ring stretching bending $N_{\text{sp}^3}\text{-Zn-}N_{\text{bipy}}$	1605 B bipy ring stretching $N_{\text{bipy}}\text{-Fe-}N_{\text{sp}^3}$ bending	1606 Bipy ring stretching	1602 Free py ring stretching	1602 B Free py ring stretching	1598 Bipy and axial py ring stretching bending $N_{\text{sp}^3}\text{-Fe-}N_{\text{bipy}}/N_{\text{ax}}$	1599 Bipy and axial py ring stretching bending $N_{\text{sp}^3}\text{-Fe-}N_{\text{bipy}}/N_{\text{ax}}$
193	8	1616 Free ring ring stretching	1616 B Free ring stretching	1615.3 Free ring stretching	1615 B Free py ring stretching	1616 B Free py ring stretching	1599 Axial py ring stretching	1601 Bipy py ring stretching bending $N_{\text{bipy}}\text{-Fe-}N_{\text{bipy}}$
194	8	1627 Free ring ring stretching $\text{Zn-}N_{\text{bipy}}$	1629 A bipy ring stretching $\text{Fe-}N_{\text{bipy}}$	1629 Bipy ring stretching Some $\text{Fe-}N_{\text{bipy}}$	1617 A Free py ring stretching	1616 A Free py ring stretching	1600 Bipy py ring stretching bending $N_{\text{sp}^3}\text{-Fe-}N_{\text{bipy}}$	1604 Bipy py ring stretching bending $N_{\text{bipy}}\text{-Fe-}N_{\text{sp}^3}$
					1626 B bipy ring stretching $\text{Ru-}N_{\text{bipy}}$	1631 B bipy ring stretching Fe-	1625 Bz ring stretching	1625 Bz ring stretching

195	8	1630	Free ring ring stretching stretching Zn-N <sub>bipy</sub>	1630 B bipy ring stretching stretching Fe-N <sub>bipy</sub>	stretching 1629 A bipy ring stretching Ru-N <sub>bipy</sub> stretching	N <sub>bipy</sub> 1635 A bipy ring stretching stretching Fe-N <sub>bipy</sub>	1625 Bz ring stretching	1625 Bz ring stretching
196	8	1636	Axial py ring stretching stretching Zn-N <sub>Ax</sub>	1633 A Axial py ring stretching stretching Fe-N <sub>Ax</sub>	1636 B Ax py ring stretching Ru-N <sub>ax</sub> stretching	1638 B Axial py ring stretching	1628 Bipy py ring stretching Fe-N <sub>bipy</sub> stretching	1631 Bipy py ring stretching Fe-N <sub>bipy</sub> stretching
197	8	1636	Axial py ring stretching stretching Zn-N <sub>Ax</sub>	1634 B Axial py ring stretching stretching Fe-N <sub>Ax</sub>	1636 A Ax py ring stretching Ru-N <sub>ax</sub> stretching	1638 A Axial py ring stretching	1629 Bipy py ring stretching Fe-N <sub>bipy</sub> stretching	1635 Bipy py ring stretching Fe-N <sub>bipy</sub> stretching
198		3032	CH <sub>2</sub> Ax C-H v <sub>s</sub>	3037 B CH <sub>2</sub> Ax py C-H stretching v <sub>s</sub>	3028 CH <sub>2</sub> 7, bipy-half7 C-H v <sub>s</sub>	3051 A CH <sub>2</sub> Free/Ax C-H v <sub>s</sub>	1633 Axial py ring stretching Fe-N <sub>ax</sub> stretching	1638 Axial py ring stretching Fe-N <sub>ax</sub> stretching
199		3033	CH <sub>2</sub> Ax C-H v <sub>s</sub>	3043 A CH <sub>2</sub> Ax py C-H stretching	3035 CH <sub>2</sub> 7, bipy-half7 and Ax7 py C-H v <sub>s</sub>	3052 B CH <sub>2</sub> Free py C- H stretching	1634 Axial py ring stretching Fe-N <sub>ax</sub> stretching	1638 Axial py ring stretching Fe-N <sub>ax</sub> stretching
200		3041	CH <sub>2</sub> bipy	3045 A CH <sub>2</sub> Free	3038 CH <sub>2</sub> 7, bipy-half7	3060 B CH <sub>2</sub> axial py C-	1641 Bz ring	1641 Bz ring

	C-H $\nu_s$	C-H stretching $\nu_s$	and Ax7 py C-H $\nu_s$	C-H $\nu_s$	H stretching	stretching	stretching
201	3041 CH <sub>2</sub> bipy C-H $\nu_s$	3056 B CH <sub>2</sub> Free C-H stretching	3053 CH <sub>2</sub> bipy – half_rec C-H $\nu_s$	3061 bipy CH <sub>2</sub> C-H $\nu_s$	3064 A CH <sub>2</sub> bipy C-H $\nu_s$	1641 Bz ring stretching	1642 Bz ring stretching
202	3077 CH <sub>2</sub> Free C-H $\nu_s$	3071 B bipy CH <sub>2</sub> C-H stretching $\nu_s$	3075 CH <sub>2</sub> AxF C-H $\nu_s$	3078 bipy CH <sub>2</sub> C-H $\nu_s$	3066 B bipy CH <sub>2</sub> C-H stretching	3057 CH <sub>2</sub> free/Ax C-H $\nu_s$	3044 CH <sub>2</sub> free/Ax C-H $\nu_s$
203	3077 CH <sub>2</sub> Free C-H $\nu_s$	3078 A CH <sub>2</sub> bipy C-H stretching	3091 CH <sub>2</sub> bipy 7 C-H $\nu_{as}$	3087 CH <sub>2</sub> free/Ax C-H $\nu_s$	3067 A All CH <sub>2</sub> C-H stretching	3058 CH <sub>2</sub> free/Ax C-H $\nu_s$	3047 CH <sub>2</sub> free/Ax C-H $\nu_s$
204	3085 Ax C-H $\nu_{as}$	3091 B CH <sub>2</sub> Ax/Free C-H stretching $\nu$	3093 CH <sub>2</sub> Free py C-H $\nu_s$	3103 CH <sub>2</sub> Ax/Free C-H $\nu_{as}$	3131 B CH <sub>2</sub> Ax C-H $\nu_{as}$	3068 bipy CH <sub>2</sub> C-H $\nu_s$	3050 bipy CH <sub>2</sub> C-H $\nu_s$
205	3085 Ax C-H $\nu_{as}$	3104 A CH <sub>2</sub> Ax/Free C-H stretching $\nu$	3101 CH <sub>2</sub> 7 C-H $\nu_a$	3113 CH <sub>2</sub> Free C-H $\nu_{as}$	3131 A All CH <sub>2</sub> C-H stretching	3068 bipy CH <sub>2</sub> C-H $\nu_s$	3055 bipy CH <sub>2</sub> C-H $\nu_s$
206	3099 bipy CH <sub>2</sub> C-H $\nu_{as}$	3106 B CH <sub>2</sub> Ax/Free C-H stretching $\nu$	3106. CH <sub>2</sub> bipy- half_free C-H $\nu_{as}$	3114 CH <sub>2</sub> bipy C-H $\nu_{as}$	3134 B All CH <sub>2</sub> C-H stretching	3072 Bz CH <sub>2</sub> C-H $\nu_s$	3064 Bz CH <sub>2</sub> C-H $\nu_s$
207	3099 Bipy CH <sub>2</sub> C-H $\nu_{as}$	3116 A CH <sub>2</sub> Ax/Free C-H stretching $\nu$	3123 CH <sub>2</sub> Ax7 C-H $\nu_{as}$	3128 CH <sub>2</sub> Ax C-H $\nu_{as}$	3135 A lAxial py CH <sub>2</sub> C-H stretching	3074 Bz CH <sub>2</sub> C-H $\nu_s$	3071 Bz CH <sub>2</sub> C-H $\nu_s$
208	3145	3128 A	3164	3148	3138 B	3114	3100

	free CH <sub>2</sub> C-H v <sub>as</sub>	bipy CH <sub>2</sub> C-H stretching	Free and Ax F CH <sub>2</sub> C-H v <sub>as</sub>	Bipy CH <sub>2</sub> C-H v <sub>as</sub>	Axial py CH <sub>2</sub> C-H stretching	Ax C-H v <sub>as</sub>	CH <sub>2</sub> free/Ax C-H v
209	3145 free CH <sub>2</sub> C-H v <sub>as</sub>	3146 B free py C-H stretchin	3169 Free and Ax F CH <sub>2</sub> C-H v <sub>as</sub>	3161 A Free CH <sub>2</sub> C-H v <sub>as</sub>	3138 A Axial py CH <sub>2</sub> C-H stretching	3114 Ax C-H v <sub>as</sub>	3102 CH <sub>2</sub> free/Ax C-H
210	3186 Free C-H stretching	3186 B Free py C-H stretching	3177 7 C-H stretching	3184. B Free C-H stretching	3187 A Free C-H	3124 CH <sub>2</sub> bipy C-H v <sub>as</sub>	3106 CH <sub>2</sub> bipy C-H v <sub>as</sub>
211	3186 Free C-H stretching	3187 A Free py C-H stretching	3182 C-H free stretching	3185A Free C-H stretching	3187 B Free py C-H stretching	3125 CH <sub>2</sub> bipy C-H v <sub>as</sub>	3111 CH <sub>2</sub> bipy C-H v <sub>as</sub>
212	3202 Free C-H stretching	3202 B Free py C-H stretching	3197 7 C-H stretching	3203 Free C-H stretching	3203 B Free py C-H stretching	3147 CH <sub>2</sub> Bz C-H v <sub>as</sub>	3144 CH <sub>2</sub> Bz C-H v <sub>as</sub>
213	3202 Free C-H stretching	3203 A Free py C-H stretching	3200 Free C-H stretching	3203.0 Free C-H stretching	3203 Ax – CH stretching	3148 CH <sub>2</sub> Bz C-H v <sub>as</sub>	3144 CH <sub>2</sub> Bz C-H v <sub>as</sub>
214	3208 Ax C-H stretching	3205A Ax py C-H stretching	3203 Ax7 C-H stretching	3207 A Ax-CH stretching	3207 B Axial py C-H stretching	3157 Bz C-H stretching	3155 Bz C-H stretching
215	3208 Ax-C-H stretching	3206 B Ax py C-H stretching	3204 Ax F C-H stretching	3208 B Ax C-H stretching	3207 A Axial py C-H stretching	3157 Bz C-H stretching	3158 Bz C-H stretching
216	3208	3209 B	3207	3209 B	3209.1 B	3168	3162

	bipy C-H stretching	bipy C-H stretching	bipy C-H stretching	Bipy C-H stretching	bipy C-H stretching	bipy C-H stretching	Bz C-H stretching
217	3209 bipy C-H stretching	3210 A bipy C-H stretching	3209 bipy C-H stretching	3210 A Bipy C-H stretching	3210 B bipy C-H stretching	3168 Bz C-H stretching	3164 Bz C-H stretching
218	3213 Free py C-H stretching	3213 B Free py C-H stretching	3212 Free py C-H stretching	3214 B Free C-H stretching	3214 A Free py C-H stretching	3193 Bz C-H stretching	3192 Bz C-H stretching
219	3213 Free py C-H stretching	3213 A Free py C-H stretching	3214 7 py – C-H stretching	3214 A Free C-H stretching	3214 Free C-H stretching	3193 Bz C-H stretching	3192 Bz C-H stretching
220	3219 Axial py C-H stretching	3215 B Axial py C-H stretching	3215.4 Ax 7 C-H stretching	3220 Bipy + Ax C-H stretching	3220 B Axial py C-H stretching	3207 Axial py C-H stretching	3205 Axial py C-H stretching
221	3219 Axial py C-H stretching	3218 B Axial py C-H stretching	3215.4 Ax 7 C-H stretching	3220 Bipy + Ax C-H stretching	3220 A Axial py C-H stretching	3207 Axial py C-H stretching	3206 Axial py C-H stretching
222	3223 bipy C-H stretching	3223 B bipy C-H stretching	3221 bipy C-H stretching	3221 Ax C-H stretching	3221 B Ax C-H stretching	3208 Axial py C-H stretching	3206 Axial py C-H stretching
223	3227 bipy C-H stretching	3225 A Axial py C-H stretching	3224 Ax F C-H stretching	3223 A bipy C-H stretching	3234 A bipy C-H stretching	3208 Bz C-H stretching	3206 Bz C-H stretching
224	3228 Axial py C-H stretching	3226 A bipy C-H stretching	3225 bipy C-H stretching	3234 A Ax C-H stretching	3235 B Axial py C-H stretching	3210 bipy C-H stretching	3209 bipy C-H stretching
225	3228 Axial py C-H stretching	3228 B Axial py C-H stretching	3227 Ax 7 C-H stretching	3235 A Ax C-H stretching	3235 A bipy iph + Ax iph	3211 bipy C-H stretching	3210 bipy C-H stretching

226	3235 Free C-H in-phase stretching	3235 B bipy C-H stretching in-phase	3234 7 C-H in-phase stretching	3235 B Free C-H in-phase	3236 B bipy C-H stretching	3220 Axial py C-H stretching	3214 Axial py C-H stretching
227	3235 Free C-H in-phase stretching	3236 B bipy C-H stretching in-phase	3235 Free C-H in-phase stretching	3236 B Bipy B C-H in-phase	3237 B Free py C-H stretching	3220 Axial py C-H stretching	3217 Axial py C-H stretching
228	3237 bipy C-H stretching in-phase	3236 A bipy C-H stretching in-phase	3236 C-H in-phase stretching	3236 A Free C-H in-phase	3237 A Free C-H in-phase	3221 bipy C-H stretching	3222 bipy C-H stretching
229	3243 bipy C-H stretching in-phase	3236 A bipy C-H stretching in-phase	3241 Ax F C-H in-phase stretching	3237 A Bipy C-H in-phase	3237 A bipy C-H stretching	3224 bipy C-H stretching	3225 Axial py C-H stretching
230	3245 Axial py C-H stretching in-phase	3242 A Axial py C-H stretching in-phase	3241 bipy C-H in-phase stretching	3251 B Ax C-H in-phase	3262 B Axial py C-H stretching	3227 Bz C-H stretching	3225 bipy C-H stretching
231	3245 Axial py C-H stretching in-phase	3244 B Axial py C-H stretching in-phase	3243 Ax 7 py C-H in-phase stretching	3253 A Ax C-H in-phase	3262 A C-H in-phase	3227 Bz C-H stretching	3226 Bz C-H stretching
232						3226 Bz C-H stretching	3226 Bz C-H stretching
233						3236	3228

234						Axial C-H stretching	Axial C-H stretching
235						3236 bipy C-H stretching	3236 bipy C-H stretching
236						3237 bipy C-H stretching	3240 bipy C-H stretching
237						3259 Axial C-H stretching	3242 Axial C-H stretching
						3259 Axial C-H stretching	3243 Axial C-H stretching

- As in corresponding modes of benzene ring

|| Tentative assignment of symmetry modes

#### Abbreviations

| bz - phenyl ring of benzyl moiety in b(dpa) ligand

| free and axial py – axially co-ordinated and non-coordinated pyridines

• Ax7 – axially co-ordinated pyridine ring of picoline bound to N<sub>sp3</sub> to which the additional, seventh weakly co-ordinated pyridine is bound in HS C<sub>1</sub> isomer of Fe(btpa)<sup>+2</sup>, the corresponding pyridine bound to N<sub>sp3</sub> linked to non-co-ordinating pyridine is denoted as AxF  
 | 7 – seventh, weakly co-ordinated pyridineHS C<sub>1</sub> isomer of Fe(btpa)<sup>+2</sup>. Bipy-half-free and bipy-half7 denote the respective rings of bipyridine.