

The calculated vibrations of high-spin and low-spin isomer of [Mn(III)(pyrrol)3tren]

	low-sj	high-ε	
1	45	37	
2	49	41	
3	56	50	
4	86	77	
5	93	80	
6	101	90	pyrrole libration (flipping and around Mn_N bond, twist of N(CH2)3 "cap" around pseudo C3 axis
7	120	114	
8	129	121	
9	130	128	
10	166	142	
11	189	150	
12	196	157	pyrrole libration with some Mn-Npyrr stretching, and N-Mn-N bending, N(CH2)3 "cap" twist, CH2 rocking
13	200	168	
14	215	178	
15	218	203	
16	237	215	
17	247	218	
18	258	234	
19	287	263	
20	307	274	
21	312	288	
22	357	305	Mn-N stretching and bending, combined with CH2 rocking out-of-plane C-H imine vibrations,
23	362	340	
24	372	348	
25	377	360	
26	400	378	
27	402	394	
28	426	405	
29	432	408	
30	436	418	
31	441	431	
32	463	439	
33	469	448	pronounced Mn-N stretching combined with CH2 rocking and C-H methine out-of-plane
34	490	463	
35	496	478	
36	499	490	
37	564	554	imine C-H out-of-plane, NCH2 rocking, some N-Mn-N bending
38	571	559	
39	572	570	
40	611	609	
41	612	612	pyrrole puckering
42	615	615	
43	696	691	
44	698	692	
45	700	696	
46	715	715	Namine-C stretching
47	777	786	
48	791	789	
49	799	798	pyrrole C-H out-of-plane
50	800	802	
51	802	804	
52	803	807	
53	870	865	
54	873	874	pyrrole C-H out-of-plane with some CH2 rocking

55	875	875	
56	875	876	
57	880	883	
58	885	887	
59	898	897	pyrrole stretching, C-H out-of-plane
60	901	898	
61	901	899	
62	911	912	ethyl C-C stretching
63	912	916	
64	932	934	
65	936	936	C-H pyrrole out-of-plane, pyrrole ring deformation,
66	937	940	Some Mn-N stretching
67	976	973	
68	984	984	
69	988	991	
70	995	994	C-H pyrrole in-plane
71	996	997	
72	1001	999	
73	1010	1012	
74	1056	1061	
75	1065	1062	C-H pyrrole in-plane and CH2 wagging,
76	1067	1065	some Mn-N stretching
77	1068	1067	
78	1072	1068	
79	1072	1069	
80	1095	1086	
81	1096	1094	pyrrole ring breathing, C-H in-plane, CH2 wagging,
82	1098	1096	Mn-N stretching
83	1099	1099	
84	1101	1106	
85	1106	1113	
86	1187	1189	CH2 wagging
87	1191	1192	
88	1213	1210	
89	1214	1214	
90	1222	1218	CH2 twist, C-H methine in-plane, in-plane in-phase
91	1240	1239	
92	1260	1261	
93	1261	1263	
94	1280	1281	
95	1284	1286	
96	1302	1296	
97	1305	1298	
98	1322	1330	
99	1327	1335	
100	1334	1338	pyrrole stretching, CH2 - twisting and wagging
101	1347	1345	
102	1348	1350	
103	1359	1359	
104	1362	1361	
105	1365	1363	
106	1365	1369	
107	1382	1383	
108	1384	1383	CH2 wagging
109	1408	1407	

110	1409	1409	
111	1410	1410	<hr/>
112	1413	1416	CH2 wagging + ring stretching
113	1416	1420	* Mn-Nypr (some)
114	1421	1423	
115	1453	1450	
116	1458	1454	
117	1460	1457	<hr/>
118	1493	1494	
119	1494	1495	CH2 scissoring
120	1498	1496	
121	1500	1500	
122	1502	1503	
123	1506	1508	<hr/>
124	1516	1511	
125	1520	1521	ring stretching, C-Nmethine stretching,
126	1525	1537	CH2
127	1596	1615	pyrrole ring stretching
128	1618	1621	
129	1623	1629	<hr/>
130	2964	2945	C-H stretching
131	2964	2962	
132	2970	2965	
133	3009	2984	
134	3011	3009	
135	3013	3013	
136	3067	3058	
137	3070	3067	
138	3072	3076	
139	3104	3081	
140	3107	3084	
141	3109	3109	
142	3133	3111	
143	3133	3126	
144	3138	3134	
145	3229	3222	
146	3229	3228	
147	3229	3232	
148	3249	3236	
149	3250	3248	
150	3250	3253	
151	3270	3259	
152	3271	3271	
153	3271	3275	

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