

Supporting Information

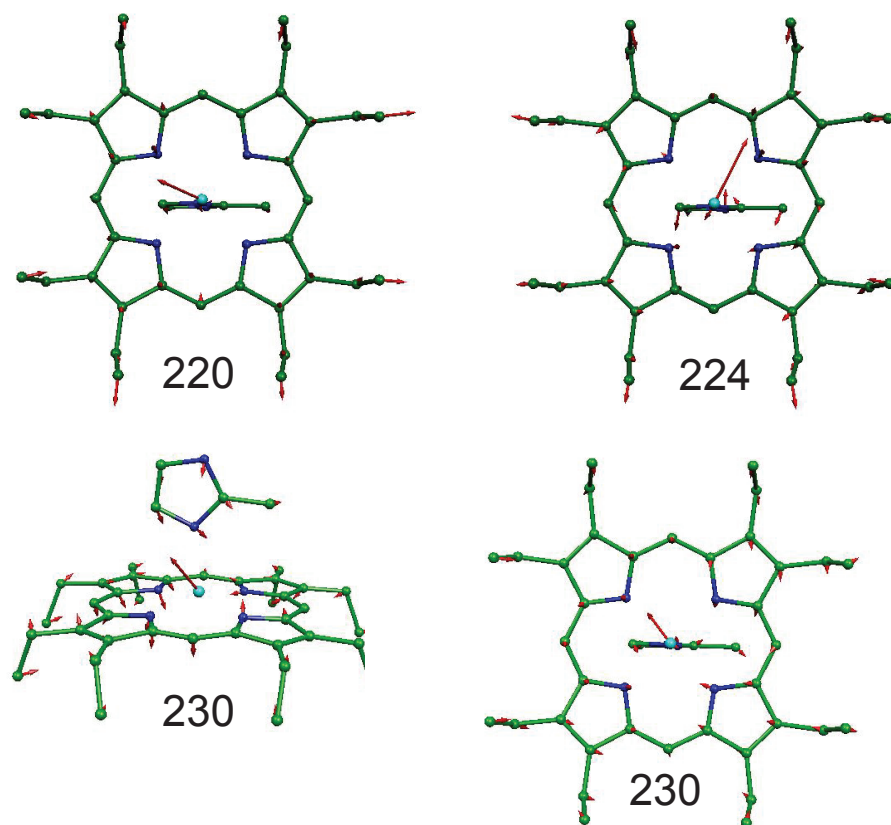


Figure S1. Three DFT-predicted in-plane Fe modes contributing to the experimental feature at 228 cm^{-1} in $[\text{Fe}(\text{OEP})(2\text{-MeHIm})]$. The 230 cm^{-1} mode has both in-plane and out-of-plane motion as shown in bottom pair of diagrams, which contributes to the experimental features at 231 cm^{-1} .

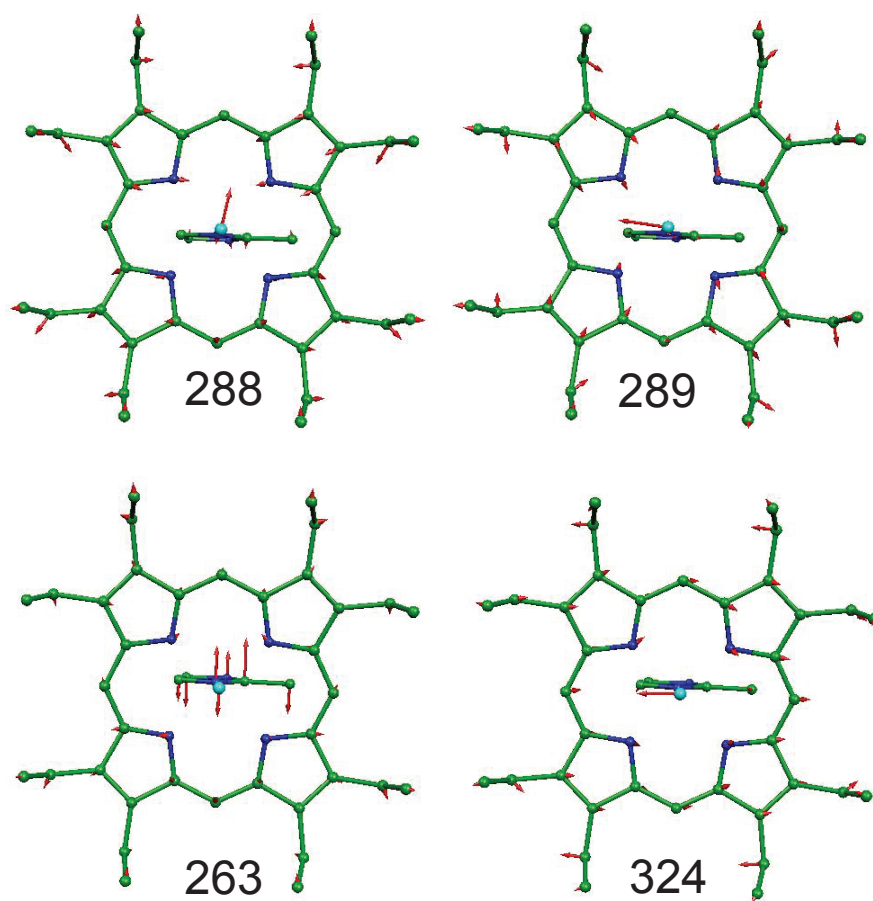


Figure S2. Other modes with significant in-plane Fe motion from the B3LYP calculations on Three DFT-predicted out-of-plane Fe modes contributing to the experimental feature at 220 cm^{-1} in $[\text{Fe}(\text{OEP})(2\text{-MeHIm})]$. .

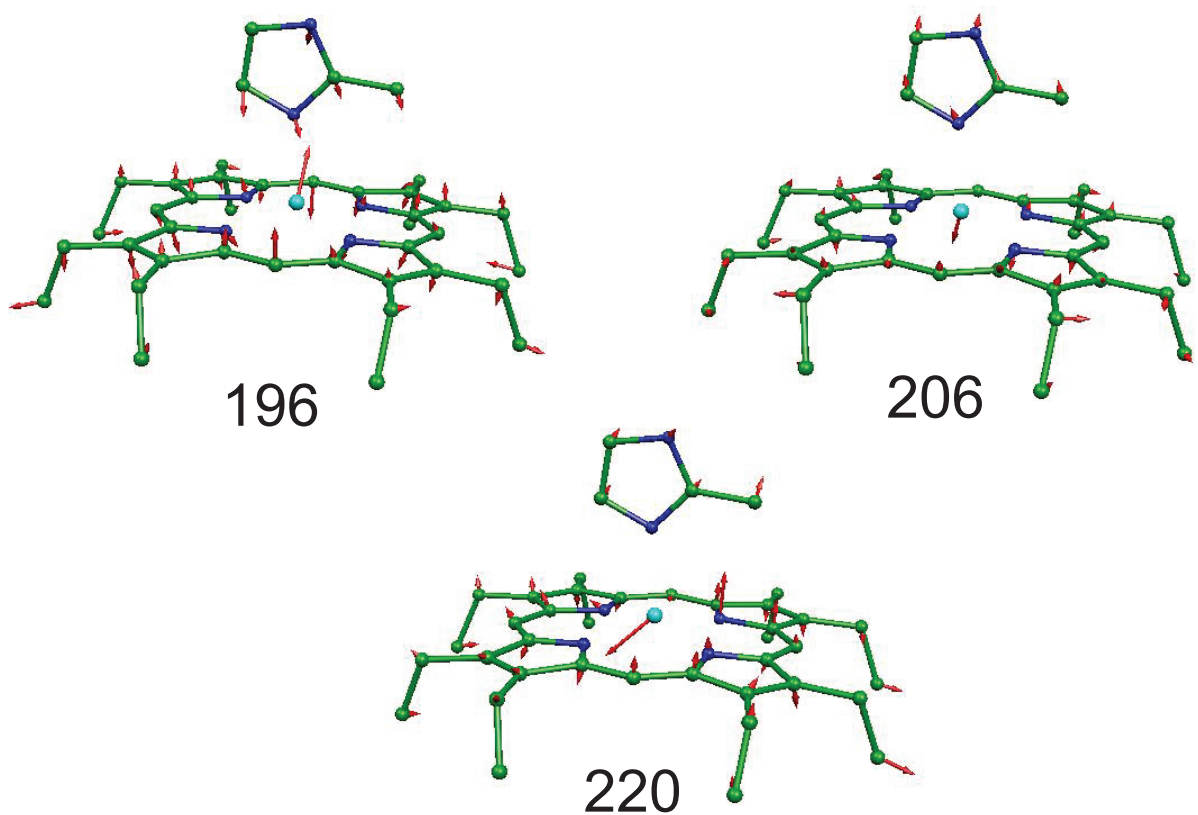


Figure S3. Three DFT-predicted out-of-plane Fe modes contributing to the experimental feature at 220 cm⁻¹ in [Fe(OEP)(2-MeHIm)].

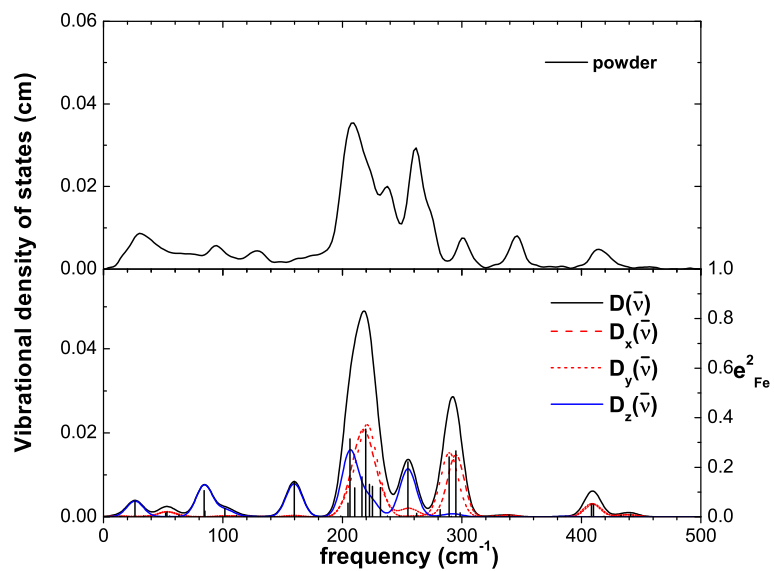
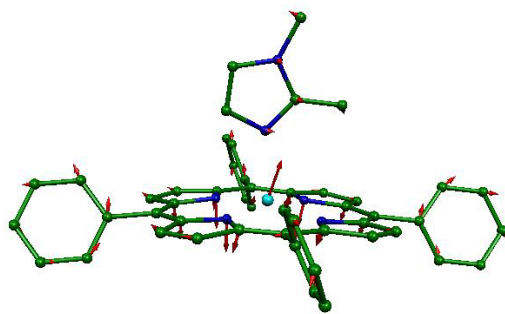


Figure S4. Comparison of the experimental VDOS determined from NRVS measurements on [Fe(TPP)(1,2-Me₂Im)] (upper panel) with the VDOS predicted on the basis of DFT calculations (lower panel). The spectra in the top panel have been normalized so that the following relationship is followed: $D(\bar{\nu}) = D_{\text{ip}}(\bar{\nu}) + D_{\text{oop}}(\bar{\nu})$.



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Figure S5. The out-of-plane Fe mode, predicted at 254 cm^{-1} , contributing to the experimental feature at 238 cm^{-1} in $[\text{Fe}(\text{TPP})(1,2\text{-Me}_2\text{Im})]$.

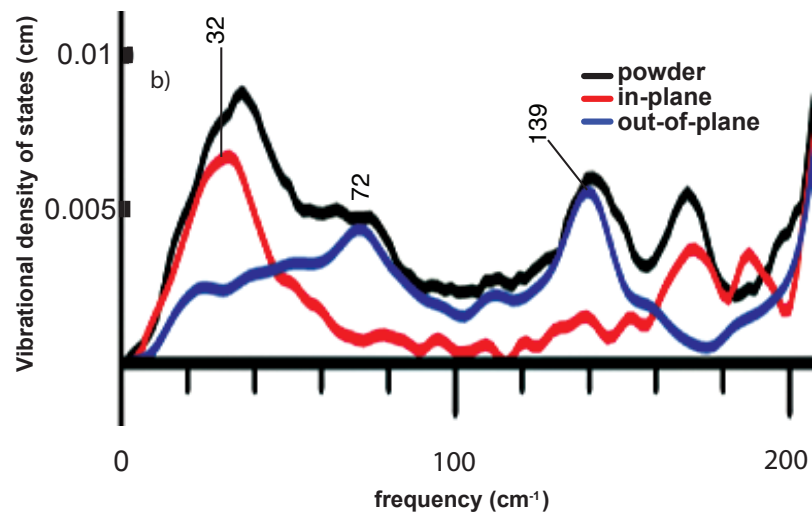
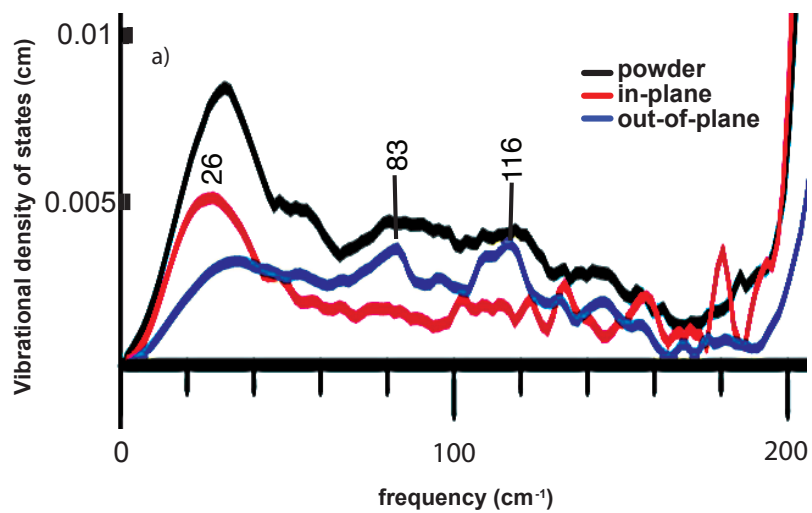


Figure S6. Expanded view of the 0 – 200 cm⁻¹ region for (top) [Fe(TPP)(2-MeHIm)] and (bottom) that for [Fe(OEP)(2-MeHIm)].

Captions for Supporting Information Figures and Tables

Figure S1. Three DFT-predicted in-plane Fe modes contributing to the experimental feature at 228 cm^{-1} in $[\text{Fe}(\text{OEP})(2\text{-MeHIm})]$. The 230 cm^{-1} mode has both in-plane and out-of-plane motion as shown in bottom pair of diagrams, which contributes to the experimental features at 231 cm^{-1} .

Figure S2. Other modes with significant in-plane Fe motion from the B3LYP calculations on $[\text{Fe}(\text{OEP})(2\text{-MeHIm})]$.

Figure S3. Three DFT-predicted out-of-plane Fe modes contributing to the experimental feature at 220 cm^{-1} in $[\text{Fe}(\text{OEP})(2\text{-MeHIm})]$.

Figure S4. Comparison of the experimental VDOS determined from NRVS measurements on $[\text{Fe}(\text{TPP})(1,2\text{-Me}_2\text{Im})]$ (upper panel) with the VDOS predicted on the basis of DFT calculations (lower panel). The spectra in the top panel have been normalized so that the following relationship is followed: $D(\bar{\nu}) = D_{\text{ip}}(\bar{\nu}) + D_{\text{oop}}(\bar{\nu})$.

Figure S5. The out-of-plane Fe mode, predicted at 254 cm^{-1} , contributing to the experimental feature at 238 cm^{-1} in $[\text{Fe}(\text{TPP})(1,2\text{-Me}_2\text{Im})]$.

Figure S6. expanded scale

Table S1. Predicted e_{Fe}^2 values for four calculated compounds.

Table S2. Optimized Cartesian Coordinate (pdb format) for $[\text{Fe}(\text{OEP})(2\text{-MeHIm})]$

Table S3. Optimized Cartesian Coordinate (pdb format) for [Fe(OEP)(1,2-Me₂Im)]

Table S4. Optimized Cartesian Coordinate (pdb format) for [Fe(TPP)(2-MeHIm)]

Table S5. Optimized Cartesian Coordinate (pdb format) for [Fe(TPP)(1,2-Me₂Im)]

Table S1. Predicted frequencies and e_{Fe}^2 values for four calculated compounds

[Fe(TPP)(2-MeHIm)]		[Fe(TPP)(1,2-Me ₂ Im)]		[Fe(OEP)(2-MeHIm)]		[Fe(OEP)(1,2-Me ₂ Im)]	
frequency	e_{Fe}^2	frequency	e_{Fe}^2	frequency	e_{Fe}^2	frequency	e_{Fe}^2
27	0.03	26	0.06	36	0.08	31	0.03
28	0.03	52	0.02	39	0.03	33	0.06
52	0.02	53	0.02	116	0.06	37	0.03
53	0.02	84	0.11	128	0.02	115	0.06
83	0.08	85	0.02	160	0.02	157	0.03
87	0.07	102	0.03	160	0.02	158	0.03
125	0.02	160	0.14	160	0.04	173	0.30
163	0.06	205	0.05	180	0.06	175	0.02
197	0.07	206	0.31	196	0.15	204	0.02
201	0.14	210	0.12	206	0.05	211	0.02
203	0.09	216	0.16	220	0.21	214	0.10
212	0.17	220	0.35	224	0.36	219	0.06
215	0.02	223	0.13	230	0.40	221	0.29
220	0.28	225	0.12	243	0.02	224	0.05
222	0.36	232	0.12	249	0.02	233	0.43
223	0.06	255	0.22	252	0.02	238	0.02
228	0.21	282	0.03	263	0.06	240	0.04
242	0.02	289	0.24	280	0.05	247	0.04
247	0.02	295	0.27	288	0.18	254	0.16
262	0.04	299	0.02	289	0.27	276	0.48
266	0.21	408	0.05	320	0.02	280	0.03
292	0.27	410	0.05	321	0.03	281	0.18
295	0.25			324	0.21	337	0.02
298	0.02			341	0.02	340	0.04
408	0.06					352	0.03
411	0.05						

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SCALE2 0.000000 1.000000 -0.000000 0.000000										
SCALE3 0.000000 0.000000 1.000000 0.000000										
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HETATM	3	N3	UNK	0	1	1.469	1.474	-0.052	1.00	0.00
HETATM	4	N4	UNK	0	1	1.486	-1.445	-0.073	1.00	0.00
HETATM	5	N5	UNK	0	1	-1.435	-1.464	-0.061	1.00	0.00
HETATM	6	C6	UNK	0	1	-2.812	1.240	-0.138	1.00	0.00
HETATM	7	C7	UNK	0	1	-1.265	2.803	-0.095	1.00	0.00
HETATM	8	C8	UNK	0	1	1.252	2.824	-0.095	1.00	0.00
HETATM	9	C9	UNK	0	1	2.821	1.284	-0.124	1.00	0.00
HETATM	10	C10	UNK	0	1	2.837	-1.232	-0.130	1.00	0.00
HETATM	11	C11	UNK	0	1	1.294	-2.798	-0.118	1.00	0.00
HETATM	12	C12	UNK	0	1	-1.220	-2.815	-0.114	1.00	0.00
HETATM	13	C13	UNK	0	1	-2.789	-1.274	-0.144	1.00	0.00
HETATM	14	C14	UNK	0	1	-3.513	2.516	-0.230	1.00	0.00
HETATM	15	C15	UNK	0	1	-2.545	3.493	-0.203	1.00	0.00
HETATM	16	C16	UNK	0	1	2.524	3.533	-0.180	1.00	0.00
HETATM	17	C17	UNK	0	1	3.506	2.570	-0.201	1.00	0.00
HETATM	18	C18	UNK	0	1	3.543	-2.507	-0.201	1.00	0.00
HETATM	19	C19	UNK	0	1	2.578	-3.486	-0.199	1.00	0.00
HETATM	20	C20	UNK	0	1	-2.491	-3.523	-0.209	1.00	0.00
HETATM	21	C21	UNK	0	1	-3.472	-2.559	-0.232	1.00	0.00
HETATM	22	C22	UNK	0	1	-0.011	3.429	-0.086	1.00	0.00
HETATM	23	H23	UNK	0	1	-0.020	4.514	-0.117	1.00	0.00
HETATM	24	C24	UNK	0	1	3.448	0.030	-0.133	1.00	0.00
HETATM	25	H25	UNK	0	1	4.533	0.037	-0.177	1.00	0.00
HETATM	26	C26	UNK	0	1	0.042	-3.424	-0.111	1.00	0.00
HETATM	27	H27	UNK	0	1	0.049	-4.510	-0.142	1.00	0.00
HETATM	28	C28	UNK	0	1	-3.420	-0.023	-0.160	1.00	0.00
HETATM	29	H29	UNK	0	1	-4.504	-0.033	-0.225	1.00	0.00
HETATM	30	C30	UNK	0	1	-5.000	2.685	-0.374	1.00	0.00
HETATM	31	H31	UNK	0	1	-5.290	3.686	-0.031	1.00	0.00
HETATM	32	H32	UNK	0	1	-5.521	1.979	0.288	1.00	0.00
HETATM	33	C33	UNK	0	1	-5.510	2.484	-1.815	1.00	0.00
HETATM	34	H34	UNK	0	1	-6.598	2.612	-1.868	1.00	0.00
HETATM	35	H35	UNK	0	1	-5.265	1.482	-2.184	1.00	0.00
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HETATM	37	C37	UNK	0	1	-2.729	4.982	-0.312	1.00	0.00
HETATM	38	H38	UNK	0	1	-2.023	5.494	0.356	1.00	0.00
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HETATM	44	C44	UNK	0	1	2.687	5.025	-0.274	1.00	0.00
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HETATM	53	H53	UNK	0	1	5.265	3.760	0.040	1.00	0.00
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HETATM	56	H56	UNK	0	1	5.054	3.325	-2.436	1.00	0.00
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HETATM	58	C58	UNK	0	1	5.034	-2.673	-0.303	1.00	0.00
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HETATM	65	C65	UNK	0	1	2.768	-4.974	-0.299	1.00	0.00
HETATM	66	H66	UNK	0	1	2.066	-5.486	0.374	1.00	0.00
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HETATM	68	C68	UNK	0	1	2.583	-5.527	-1.727	1.00	0.00
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HETATM	87	C87	UNK	0	1	-0.739	-0.026	3.460	1.00	0.00
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HETATM	89	H89	UNK	0	1	-0.605	-0.048	5.566	1.00	0.00
HETATM	90	C90	UNK	0	1	1.242	-0.007	4.484	1.00	0.00
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HEADER										
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SCALE3	0.000000	0.000000	1.000000			0.000000				
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HETATM	3	N3	UNK	0	1	-0.097	-0.004	2.059	1.00	0.00
HETATM	4	N4	UNK	0	1	-0.710	-0.011	4.185	1.00	0.00
HETATM	5	C5	UNK	0	1	0.675	-0.010	4.167	1.00	0.00
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HETATM	7	C7	UNK	0	1	1.034	-0.008	2.850	1.00	0.00
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HETATM	9	C9	UNK	0	1	-2.578	0.002	2.505	1.00	0.00
HETATM	10	H10	UNK	0	1	-3.100	-0.886	2.884	1.00	0.00
HETATM	11	H11	UNK	0	1	-2.660	0.010	1.420	1.00	0.00
HETATM	12	H12	UNK	0	1	-3.096	0.886	2.898	1.00	0.00
HETATM	13	C13	UNK	0	1	-1.555	0.010	5.368	1.00	0.00
HETATM	14	H14	UNK	0	1	-2.293	-0.796	5.328	1.00	0.00
HETATM	15	H15	UNK	0	1	-2.081	0.967	5.461	1.00	0.00
HETATM	16	H16	UNK	0	1	-0.929	-0.133	6.251	1.00	0.00
HETATM	17	N17	UNK	0	1	1.548	1.477	-0.201	1.00	0.00
HETATM	18	N18	UNK	0	1	-1.332	1.459	-0.674	1.00	0.00
HETATM	19	N19	UNK	0	1	-1.310	-1.478	-0.677	1.00	0.00
HETATM	20	N20	UNK	0	1	1.568	-1.460	-0.197	1.00	0.00
HETATM	21	C21	UNK	0	1	2.895	1.277	-0.056	1.00	0.00
HETATM	22	C22	UNK	0	1	1.345	2.828	-0.261	1.00	0.00
HETATM	23	C23	UNK	0	1	-1.134	2.813	-0.679	1.00	0.00
HETATM	24	C24	UNK	0	1	-2.636	1.241	-1.034	1.00	0.00
HETATM	25	C25	UNK	0	1	-2.619	-1.278	-1.032	1.00	0.00
HETATM	26	C26	UNK	0	1	-1.095	-2.830	-0.677	1.00	0.00
HETATM	27	C27	UNK	0	1	1.385	-2.813	-0.261	1.00	0.00
HETATM	28	C28	UNK	0	1	2.913	-1.242	-0.057	1.00	0.00
HETATM	29	C29	UNK	0	1	3.586	2.561	-0.006	1.00	0.00
HETATM	30	C30	UNK	0	1	2.618	3.528	-0.132	1.00	0.00
HETATM	31	C31	UNK	0	1	-2.376	3.496	-1.022	1.00	0.00
HETATM	32	C32	UNK	0	1	-3.312	2.515	-1.248	1.00	0.00
HETATM	33	C33	UNK	0	1	-3.279	-2.561	-1.239	1.00	0.00
HETATM	34	C34	UNK	0	1	-2.329	-3.529	-1.013	1.00	0.00
HETATM	35	C35	UNK	0	1	2.668	-3.497	-0.139	1.00	0.00
HETATM	36	C36	UNK	0	1	3.622	-2.516	-0.014	1.00	0.00
HETATM	37	C37	UNK	0	1	0.099	3.438	-0.454	1.00	0.00
HETATM	38	H38	UNK	0	1	0.098	4.523	-0.484	1.00	0.00
HETATM	39	C39	UNK	0	1	-3.222	-0.022	-1.190	1.00	0.00
HETATM	40	H40	UNK	0	1	-4.265	-0.030	-1.490	1.00	0.00
HETATM	41	C41	UNK	0	1	0.146	-3.439	-0.453	1.00	0.00
HETATM	42	H42	UNK	0	1	0.159	-4.524	-0.483	1.00	0.00
HETATM	43	C43	UNK	0	1	3.513	0.022	0.026	1.00	0.00
HETATM	44	H44	UNK	0	1	4.592	0.030	0.147	1.00	0.00
HETATM	45	C45	UNK	0	1	5.073	2.745	0.117	1.00	0.00
HETATM	46	H46	UNK	0	1	5.480	2.021	0.836	1.00	0.00
HETATM	47	H47	UNK	0	1	5.285	3.736	0.539	1.00	0.00
HETATM	48	C48	UNK	0	1	5.829	2.603	-1.219	1.00	0.00
HETATM	49	H49	UNK	0	1	5.662	1.615	-1.663	1.00	0.00
HETATM	50	H50	UNK	0	1	6.909	2.734	-1.074	1.00	0.00
HETATM	51	H51	UNK	0	1	5.489	3.351	-1.943	1.00	0.00
HETATM	52	C52	UNK	0	1	2.796	5.021	-0.173	1.00	0.00

HETATM	53	H53	UNK	0	1	3.724	5.293	0.345	1.00	0.00
HETATM	54	H54	UNK	0	1	1.986	5.507	0.389	1.00	0.00
HETATM	55	C55	UNK	0	1	2.833	5.604	-1.600	1.00	0.00
HETATM	56	H56	UNK	0	1	3.666	5.181	-2.173	1.00	0.00
HETATM	57	H57	UNK	0	1	2.956	6.694	-1.574	1.00	0.00
HETATM	58	H58	UNK	0	1	1.910	5.377	-2.144	1.00	0.00
HETATM	59	C59	UNK	0	1	-2.556	4.987	-1.092	1.00	0.00
HETATM	60	H60	UNK	0	1	-3.411	5.225	-1.737	1.00	0.00
HETATM	61	H61	UNK	0	1	-1.681	5.445	-1.572	1.00	0.00
HETATM	62	C62	UNK	0	1	-2.772	5.647	0.285	1.00	0.00
HETATM	63	H63	UNK	0	1	-3.676	5.257	0.768	1.00	0.00
HETATM	64	H64	UNK	0	1	-2.881	6.734	0.186	1.00	0.00
HETATM	65	H65	UNK	0	1	-1.928	5.447	0.954	1.00	0.00
HETATM	66	C66	UNK	0	1	-4.758	2.680	-1.628	1.00	0.00
HETATM	67	H67	UNK	0	1	-5.031	1.931	-2.384	1.00	0.00
HETATM	68	H68	UNK	0	1	-4.902	3.655	-2.109	1.00	0.00
HETATM	69	C69	UNK	0	1	-5.729	2.564	-0.436	1.00	0.00
HETATM	70	H70	UNK	0	1	-5.635	1.589	0.055	1.00	0.00
HETATM	71	H71	UNK	0	1	-6.769	2.682	-0.764	1.00	0.00
HETATM	72	H72	UNK	0	1	-5.519	3.335	0.315	1.00	0.00
HETATM	73	C73	UNK	0	1	-4.724	-2.745	-1.612	1.00	0.00
HETATM	74	H74	UNK	0	1	-4.858	-3.724	-2.089	1.00	0.00
HETATM	75	H75	UNK	0	1	-5.011	-2.002	-2.368	1.00	0.00
HETATM	76	C76	UNK	0	1	-5.691	-2.639	-0.415	1.00	0.00
HETATM	77	H77	UNK	0	1	-5.467	-3.404	0.336	1.00	0.00
HETATM	78	H78	UNK	0	1	-6.731	-2.771	-0.738	1.00	0.00
HETATM	79	H79	UNK	0	1	-5.607	-1.662	0.073	1.00	0.00
HETATM	80	C80	UNK	0	1	-2.491	-5.023	-1.076	1.00	0.00
HETATM	81	H81	UNK	0	1	-1.613	-5.471	-1.560	1.00	0.00
HETATM	82	H82	UNK	0	1	-3.346	-5.273	-1.717	1.00	0.00
HETATM	83	C83	UNK	0	1	-2.692	-5.680	0.304	1.00	0.00
HETATM	84	H84	UNK	0	1	-1.847	-5.468	0.967	1.00	0.00
HETATM	85	H85	UNK	0	1	-2.789	-6.768	0.209	1.00	0.00
HETATM	86	H86	UNK	0	1	-3.598	-5.299	0.790	1.00	0.00
HETATM	87	C87	UNK	0	1	2.866	-4.987	-0.186	1.00	0.00
HETATM	88	H88	UNK	0	1	2.067	-5.485	0.380	1.00	0.00
HETATM	89	H89	UNK	0	1	3.801	-5.247	0.325	1.00	0.00
HETATM	90	C90	UNK	0	1	2.902	-5.565	-1.614	1.00	0.00
HETATM	91	H91	UNK	0	1	1.972	-5.349	-2.151	1.00	0.00
HETATM	92	H92	UNK	0	1	3.039	-6.653	-1.592	1.00	0.00
HETATM	93	H93	UNK	0	1	3.725	-5.130	-2.192	1.00	0.00
HETATM	94	C94	UNK	0	1	5.113	-2.679	0.102	1.00	0.00
HETATM	95	H95	UNK	0	1	5.342	-3.670	0.514	1.00	0.00
HETATM	96	H96	UNK	0	1	5.512	-1.955	0.825	1.00	0.00
HETATM	97	C97	UNK	0	1	5.861	-2.512	-1.236	1.00	0.00
HETATM	98	H98	UNK	0	1	5.529	-3.259	-1.966	1.00	0.00
HETATM	99	H99	UNK	0	1	6.942	-2.628	-1.098	1.00	0.00
HETATM	100	H100	UNK	0	1	5.676	-1.524	-1.671	1.00	0.00
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CONNECT	33	34	73	
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CONNECT	35	36	87	
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CONNECT	62	63	64	65
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CONNECT	64			
CONNECT	65			
CONNECT	66	67	68	69

HEADER	CSD ENTRY [Fe(TPP)(2-MeHIm)] Table S4									
CRYST1	1.0000	1.0000	1.0000	90.00	90.00	90.00	Unknown			
SCALE1	1.000000	-0.000000	-0.000000			0.000000				
SCALE2	0.000000	1.000000	-0.000000			0.000000				
SCALE3	0.000000	0.000000	1.000000			0.000000				
HETATM	1	Fe1	UNK	0	1	-0.017	0.002	-0.017	1.00	0.00
HETATM	2	N2	UNK	0	1	0.749	1.912	-0.313	1.00	0.00
HETATM	3	N3	UNK	0	1	1.914	-0.771	-0.265	1.00	0.00
HETATM	4	N4	UNK	0	1	-0.780	-1.904	-0.383	1.00	0.00
HETATM	5	N5	UNK	0	1	-1.946	0.775	-0.318	1.00	0.00
HETATM	6	C18	UNK	0	1	3.168	1.359	-0.464	1.00	0.00
HETATM	7	C19	UNK	0	1	1.350	-3.183	-0.318	1.00	0.00
HETATM	8	C20	UNK	0	1	-3.207	-1.351	-0.446	1.00	0.00
HETATM	9	C21	UNK	0	1	-1.385	3.184	-0.305	1.00	0.00
HETATM	10	C22	UNK	0	1	0.024	3.080	-0.286	1.00	0.00
HETATM	11	C23	UNK	0	1	2.079	2.259	-0.379	1.00	0.00
HETATM	12	C24	UNK	0	1	3.068	-0.048	-0.453	1.00	0.00
HETATM	13	C25	UNK	0	1	2.251	-2.099	-0.365	1.00	0.00
HETATM	14	C26	UNK	0	1	-0.061	-3.074	-0.305	1.00	0.00
HETATM	15	C27	UNK	0	1	-2.113	-2.247	-0.379	1.00	0.00
HETATM	16	C28	UNK	0	1	-3.110	0.056	-0.446	1.00	0.00
HETATM	17	C29	UNK	0	1	-2.287	2.104	-0.369	1.00	0.00
HETATM	18	C30	UNK	0	1	0.930	4.205	-0.311	1.00	0.00
HETATM	19	H31	UNK	0	1	0.637	5.245	-0.301	1.00	0.00
HETATM	20	C32	UNK	0	1	2.196	3.700	-0.362	1.00	0.00
HETATM	21	H33	UNK	0	1	3.123	4.254	-0.392	1.00	0.00
HETATM	22	C34	UNK	0	1	4.179	-0.958	-0.667	1.00	0.00
HETATM	23	H35	UNK	0	1	5.199	-0.664	-0.868	1.00	0.00
HETATM	24	C36	UNK	0	1	3.677	-2.220	-0.607	1.00	0.00
HETATM	25	H37	UNK	0	1	4.210	-3.148	-0.754	1.00	0.00
HETATM	26	C38	UNK	0	1	-0.973	-4.192	-0.222	1.00	0.00
HETATM	27	H39	UNK	0	1	-0.687	-5.229	-0.126	1.00	0.00
HETATM	28	C40	UNK	0	1	-2.237	-3.683	-0.272	1.00	0.00
HETATM	29	H41	UNK	0	1	-3.167	-4.230	-0.226	1.00	0.00
HETATM	30	C42	UNK	0	1	-4.231	0.970	-0.581	1.00	0.00
HETATM	31	H43	UNK	0	1	-5.263	0.681	-0.719	1.00	0.00
HETATM	32	C44	UNK	0	1	-3.726	2.231	-0.516	1.00	0.00
HETATM	33	H45	UNK	0	1	-4.269	3.162	-0.582	1.00	0.00
HETATM	34	C46	UNK	0	1	4.537	1.950	-0.615	1.00	0.00
HETATM	35	C47	UNK	0	1	5.510	1.784	0.384	1.00	0.00
HETATM	36	H48	UNK	0	1	5.259	1.222	1.279	1.00	0.00
HETATM	37	C49	UNK	0	1	6.786	2.332	0.242	1.00	0.00
HETATM	38	H50	UNK	0	1	7.522	2.195	1.030	1.00	0.00
HETATM	39	C51	UNK	0	1	7.115	3.058	-0.905	1.00	0.00
HETATM	40	H52	UNK	0	1	8.108	3.485	-1.016	1.00	0.00
HETATM	41	C53	UNK	0	1	6.159	3.229	-1.908	1.00	0.00
HETATM	42	H54	UNK	0	1	6.406	3.786	-2.808	1.00	0.00
HETATM	43	C55	UNK	0	1	4.883	2.680	-1.764	1.00	0.00
HETATM	44	H56	UNK	0	1	4.145	2.809	-2.551	1.00	0.00
HETATM	45	C57	UNK	0	1	1.937	-4.561	-0.328	1.00	0.00
HETATM	46	C58	UNK	0	1	2.745	-5.003	0.733	1.00	0.00
HETATM	47	H59	UNK	0	1	2.930	-4.335	1.570	1.00	0.00
HETATM	48	C60	UNK	0	1	3.301	-6.283	0.727	1.00	0.00
HETATM	49	H61	UNK	0	1	3.918	-6.607	1.560	1.00	0.00
HETATM	50	C62	UNK	0	1	3.060	-7.147	-0.344	1.00	0.00
HETATM	51	H63	UNK	0	1	3.493	-8.144	-0.350	1.00	0.00
HETATM	52	C64	UNK	0	1	2.261	-6.720	-1.407	1.00	0.00

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CONNECT	74	75	76
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CONNECT	76	77	
CONNECT	77		

HEADER	CSD ENTRY [Fe(TPP)(1,2-DiMeIm0] Tsblr S5									
CRYST1	1.0000	1.0000	1.0000	90.00	90.00	90.00	Unknown			
SCALE1	1.000000	-0.000000	-0.000000			0.000000				
SCALE2	0.000000	1.000000	-0.000000			0.000000				
SCALE3	0.000000	0.000000	1.000000			0.000000				
HETATM	1	Fe1	UNK	0	1	-0.024	0.011	-0.125	1.00	0.00
HETATM	2	N2	UNK	0	1	-1.738	1.175	-0.379	1.00	0.00
HETATM	3	N3	UNK	0	1	1.127	1.734	-0.412	1.00	0.00
HETATM	4	N4	UNK	0	1	1.677	-1.145	-0.485	1.00	0.00
HETATM	5	N5	UNK	0	1	-1.179	-1.708	-0.433	1.00	0.00
HETATM	6	C21	UNK	0	1	-0.687	3.422	-0.392	1.00	0.00
HETATM	7	C22	UNK	0	1	3.364	0.676	-0.614	1.00	0.00
HETATM	8	C23	UNK	0	1	0.633	-3.395	-0.417	1.00	0.00
HETATM	9	C24	UNK	0	1	-3.417	-0.646	-0.576	1.00	0.00
HETATM	10	C25	UNK	0	1	-3.025	0.711	-0.517	1.00	0.00
HETATM	11	C26	UNK	0	1	-1.796	2.546	-0.410	1.00	0.00
HETATM	12	C27	UNK	0	1	0.667	3.028	-0.433	1.00	0.00
HETATM	13	C28	UNK	0	1	2.494	1.787	-0.556	1.00	0.00
HETATM	14	C29	UNK	0	1	2.970	-0.681	-0.561	1.00	0.00
HETATM	15	C30	UNK	0	1	1.740	-2.518	-0.450	1.00	0.00
HETATM	16	C31	UNK	0	1	-0.723	-3.001	-0.445	1.00	0.00
HETATM	17	C32	UNK	0	1	-2.548	-1.759	-0.543	1.00	0.00
HETATM	18	C33	UNK	0	1	-3.930	1.836	-0.633	1.00	0.00
HETATM	19	H34	UNK	0	1	-4.999	1.768	-0.777	1.00	0.00
HETATM	20	C35	UNK	0	1	-3.173	2.966	-0.560	1.00	0.00
HETATM	21	H36	UNK	0	1	-3.511	3.989	-0.633	1.00	0.00
HETATM	22	C37	UNK	0	1	1.791	3.935	-0.554	1.00	0.00
HETATM	23	H38	UNK	0	1	1.726	5.013	-0.582	1.00	0.00
HETATM	24	C39	UNK	0	1	2.913	3.172	-0.651	1.00	0.00
HETATM	25	H40	UNK	0	1	3.930	3.512	-0.786	1.00	0.00
HETATM	26	C41	UNK	0	1	3.884	-1.804	-0.543	1.00	0.00
HETATM	27	H42	UNK	0	1	4.961	-1.736	-0.574	1.00	0.00
HETATM	28	C43	UNK	0	1	3.126	-2.934	-0.466	1.00	0.00
HETATM	29	H44	UNK	0	1	3.475	-3.955	-0.422	1.00	0.00
HETATM	30	C45	UNK	0	1	-1.848	-3.908	-0.555	1.00	0.00
HETATM	31	H46	UNK	0	1	-1.783	-4.986	-0.601	1.00	0.00
HETATM	32	C47	UNK	0	1	-2.973	-3.144	-0.608	1.00	0.00
HETATM	33	H48	UNK	0	1	-3.995	-3.483	-0.692	1.00	0.00
HETATM	34	C49	UNK	0	1	-0.985	4.891	-0.392	1.00	0.00
HETATM	35	C50	UNK	0	1	-1.527	5.507	0.748	1.00	0.00
HETATM	36	H51	UNK	0	1	-1.720	4.905	1.632	1.00	0.00
HETATM	37	C52	UNK	0	1	-1.813	6.873	0.757	1.00	0.00
HETATM	38	H53	UNK	0	1	-2.229	7.331	1.651	1.00	0.00
HETATM	39	C54	UNK	0	1	-1.563	7.649	-0.377	1.00	0.00
HETATM	40	H55	UNK	0	1	-1.786	8.713	-0.371	1.00	0.00
HETATM	41	C56	UNK	0	1	-1.028	7.050	-1.518	1.00	0.00
HETATM	42	H57	UNK	0	1	-0.837	7.644	-2.408	1.00	0.00
HETATM	43	C58	UNK	0	1	-0.743	5.683	-1.526	1.00	0.00
HETATM	44	H59	UNK	0	1	-0.336	5.217	-2.418	1.00	0.00
HETATM	45	C60	UNK	0	1	4.830	0.956	-0.760	1.00	0.00
HETATM	46	C61	UNK	0	1	5.559	1.575	0.269	1.00	0.00
HETATM	47	H62	UNK	0	1	5.047	1.852	1.186	1.00	0.00
HETATM	48	C63	UNK	0	1	6.923	1.832	0.128	1.00	0.00
HETATM	49	H64	UNK	0	1	7.468	2.309	0.939	1.00	0.00
HETATM	50	C65	UNK	0	1	7.588	1.474	-1.047	1.00	0.00
HETATM	51	H66	UNK	0	1	8.650	1.674	-1.157	1.00	0.00
HETATM	52	C67	UNK	0	1	6.877	0.858	-2.079	1.00	0.00

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