Supporting Information

****
**** Cartesian Coordinates for Fe(P)F_2 (Å)******
****

Fe(IV), S=1

Center	Label	x	y	z
1	FE	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.757870
3	F	0.000000	0.000000	-1.757870
4	N1	2.068519	0.000000	0.000000
5	N1	-2.068519	0.000000	0.000000
6	N2	0.000000	2.068519	0.000000
7	N2	0.000000	-2.068519	0.000000
8	C11	4.247515	0.680184	0.000000
9	C11	-4.247515	0.680184	0.000000
10	C11	4.247515	-0.680184	0.000000
11	C11	-4.247515	-0.680184	0.000000
12	C21	2.869318	1.107266	0.000000
13	C21	-2.869318	1.107266	0.000000
14	C21	2.869318	-1.107266	0.000000
15	C21	-2.869318	-1.107266	0.000000
16	C3	2.428009	2.428009	0.000000
17	C3	-2.428009	2.428009	0.000000
18	C3	2.428009	-2.428009	0.000000
19	C3	-2.428009	-2.428009	0.000000
20	C22	1.107266	2.869318	0.000000
21	C22	-1.107266	2.869318	0.000000
22	C22	1.107266	-2.869318	0.000000
23	C22	-1.107266	-2.869318	0.000000
24	C12	0.680184	4.247515	0.000000
25	C12	-0.680184	4.247515	0.000000
26	C12	0.680184	-4.247515	0.000000
27	C12	-0.680184	-4.247515	0.000000
28	H11	5.098329	1.344342	0.000000
29	H11	-5.098329	1.344342	0.000000
30	H11	5.098329	-1.344342	0.000000
31	H11	-5.098329	-1.344342	0.000000
32	H22	1.344342	5.098329	0.000000
33	H22	-1.344342	5.098329	0.000000
34	H22	1.344342	-5.098329	0.000000
35	H22	-1.344342	-5.098329	0.000000
36	H3	3.193758	3.193758	0.000000
37	H3	-3.193758	3.193758	0.000000
38	H3	3.193758	-3.193758	0.000000
39	H3	-3.193758	-3.193758	0.000000

Fe(IV), S=2, $^5B_{1g}$

Center	Label	x	y	z
1	FE	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.757870
3	F	0.000000	0.000000	-1.757870
4	N1	2.068519	0.000000	0.000000
5	N1	-2.068519	0.000000	0.000000
6	N2	0.000000	2.068519	0.000000
7	N2	0.000000	-2.068519	0.000000
8	C11	4.247515	0.680184	0.000000
9	C11	-4.247515	0.680184	0.000000
10	C11	4.247515	-0.680184	0.000000
11	C11	-4.247515	-0.680184	0.000000
12	C21	2.869318	1.107266	0.000000
13	C21	-2.869318	1.107266	0.000000
14	C21	2.869318	-1.107266	0.000000
15	C21	-2.869318	-1.107266	0.000000
16	C3	2.428009	2.428009	0.000000
17	C3	-2.428009	2.428009	0.000000
18	C3	2.428009	-2.428009	0.000000
19	C3	-2.428009	-2.428009	0.000000
20	C22	1.107266	2.869318	0.000000
21	C22	-1.107266	2.869318	0.000000
22	C22	1.107266	-2.869318	0.000000
23	C22	-1.107266	-2.869318	0.000000
24	C12	0.680184	4.247515	0.000000
25	C12	-0.680184	4.247515	0.000000
26	C12	0.680184	-4.247515	0.000000
27	C12	-0.680184	-4.247515	0.000000
28	H11	5.098329	1.344342	0.000000
29	H11	-5.098329	1.344342	0.000000
30	H11	5.098329	-1.344342	0.000000
31	H11	-5.098329	-1.344342	0.000000
32	H22	1.344342	5.098329	0.000000
33	H22	-1.344342	5.098329	0.000000
34	H22	1.344342	-5.098329	0.000000
35	H22	-1.344342	-5.098329	0.000000
36	H3	3.193758	3.193758	0.000000
37	H3	-3.193758	3.193758	0.000000
38	H3	3.193758	-3.193758	0.000000
39	H3	-3.193758	-3.193758	0.000000

Fe(IV), S=2, $^5A_{1g}$

Center	Label		x	y	z
1	FE		0.000000	0.000000	0.000000
2	F		0.000000	0.000000	1.880703
3	F		0.000000	0.000000	-1.880703
4	N1		2.040941	0.000000	0.000000
5	N1		-2.040941	0.000000	0.000000
6	N2		0.000000	2.040941	0.000000
7	N2		0.000000	-2.040941	0.000000
8	C11		4.221256	0.678914	0.000000
9	C11		-4.221256	0.678914	0.000000
10	C11		4.221256	-0.678914	0.000000
11	C11		-4.221256	-0.678914	0.000000
12	C21		2.845550	1.104472	0.000000
13	C21		-2.845550	1.104472	0.000000
14	C21		2.845550	-1.104472	0.000000
15	C21		-2.845550	-1.104472	0.000000
16	C3		2.422895	2.422895	0.000000
17	C3		-2.422895	2.422895	0.000000
18	C3		2.422895	-2.422895	0.000000
19	C3		-2.422895	-2.422895	0.000000
20	C22		1.104472	2.845550	0.000000
21	C22		-1.104472	2.845550	0.000000
22	C22		1.104472	-2.845550	0.000000
23	C22		-1.104472	-2.845550	0.000000
24	C12		0.678914	4.221256	0.000000
25	C12		-0.678914	4.221256	0.000000
26	C12		0.678914	-4.221256	0.000000
27	C12		-0.678914	-4.221256	0.000000
28	H11		5.067262	1.348791	0.000000
29	H11		-5.067262	1.348791	0.000000
30	H11		5.067262	-1.348791	0.000000
31	H11		-5.067262	-1.348791	0.000000
32	H22		3.187973	3.187973	0.000000
33	H22		-3.187973	3.187973	0.000000
34	H22		3.187973	-3.187973	0.000000
35	H22		-3.187973	-3.187973	0.000000
36	H3		1.348791	5.067262	0.000000
37	H3		-1.348791	5.067262	0.000000
38	H3		1.348791	-5.067262	0.000000
39	H3		-1.348791	-5.067262	0.000000

Fe(III) S=5/2, a1u hole, ferro

Center	Label	x	y	z
1	FE	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.893490
3	F	0.000000	0.000000	-1.893490
4	N1	2.090638	0.000000	0.000000
5	N1	-2.090638	0.000000	0.000000
6	N2	0.000000	2.090638	0.000000
7	N2	0.000000	-2.090638	0.000000
8	C11	4.283430	0.674531	0.000000
9	C11	-4.283430	0.674531	0.000000
10	C11	4.283430	-0.674531	0.000000
11	C11	-4.283430	-0.674531	0.000000
12	C21	2.877926	1.101128	0.000000
13	C21	-2.877926	1.101128	0.000000
14	C21	2.877926	-1.101128	0.000000
15	C21	-2.877926	-1.101128	0.000000
16	C3	2.427813	2.427813	0.000000
17	C3	-2.427813	2.427813	0.000000
18	C3	2.427813	-2.427813	0.000000
19	C3	-2.427813	-2.427813	0.000000
20	C22	1.101128	2.877926	0.000000
21	C22	-1.101128	2.877926	0.000000
22	C22	1.101128	-2.877926	0.000000
23	C22	-1.101128	-2.877926	0.000000
24	C12	0.674531	4.283430	0.000000
25	C12	-0.674531	4.283430	0.000000
26	C12	0.674531	-4.283430	0.000000
27	C12	-0.674531	-4.283430	0.000000
28	H11	5.133499	1.339627	0.000000
29	H11	-5.133499	1.339627	0.000000
30	H11	5.133499	-1.339627	0.000000
31	H11	-5.133499	-1.339627	0.000000
32	H22	3.193664	3.193664	0.000000
33	H22	-3.193664	3.193664	0.000000
34	H22	3.193664	-3.193664	0.000000
35	H22	-3.193664	-3.193664	0.000000
36	H3	1.339627	5.133499	0.000000
37	H3	-1.339627	5.133499	0.000000
38	H3	1.339627	-5.133499	0.000000
39	H3	-1.339627	-5.133499	0.000000

Fe(III) S=5/2, a1u hole, antiferro

Center	Label	x	y	z
1	FE	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.892418
3	F	0.000000	0.000000	-1.892418
4	N1	2.091281	0.000000	0.000000
5	N1	-2.091281	0.000000	0.000000
6	N2	0.000000	2.091281	0.000000
7	N2	0.000000	-2.091281	0.000000
8	C11	4.283780	0.674550	0.000000
9	C11	-4.283780	0.674550	0.000000
10	C11	4.283780	-0.674550	0.000000
11	C11	-4.283780	-0.674550	0.000000
12	C21	2.878314	1.101263	0.000000
13	C21	-2.878314	1.101263	0.000000
14	C21	2.878314	-1.101263	0.000000
15	C21	-2.878314	-1.101263	0.000000
16	C3	2.427970	2.427970	0.000000
17	C3	-2.427970	2.427970	0.000000
18	C3	2.427970	-2.427970	0.000000
19	C3	-2.427970	-2.427970	0.000000
20	C22	1.101263	2.878314	0.000000
21	C22	-1.101263	2.878314	0.000000
22	C22	1.101263	-2.878314	0.000000
23	C22	-1.101263	-2.878314	0.000000
24	C12	0.674550	4.283780	0.000000
25	C12	-0.674550	4.283780	0.000000
26	C12	0.674550	-4.283780	0.000000
27	C12	-0.674550	-4.283780	0.000000
28	H11	5.133933	1.339552	0.000000
29	H11	-5.133933	1.339552	0.000000
30	H11	5.133933	-1.339552	0.000000
31	H11	-5.133933	-1.339552	0.000000
32	H22	3.193811	3.193811	0.000000
33	H22	-3.193811	3.193811	0.000000
34	H22	3.193811	-3.193811	0.000000
35	H22	-3.193811	-3.193811	0.000000
36	H3	1.339552	5.133933	0.000000
37	H3	-1.339552	5.133933	0.000000
38	H3	1.339552	-5.133933	0.000000
39	H3	-1.339552	-5.133933	0.000000

Fe(III) S=5/2, a2u hole, ferro

Center	Label	x	y	z
1	FE	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.889632
3	F	0.000000	0.000000	-1.889632
4	N1	2.100013	0.000000	0.000000
5	N1	-2.100013	0.000000	0.000000
6	N2	0.000000	2.100013	0.000000
7	N2	0.000000	-2.100013	0.000000
8	C11	4.280778	0.680517	0.000000
9	C11	-4.280778	0.680517	0.000000
10	C11	4.280778	-0.680517	0.000000
11	C11	-4.280778	-0.680517	0.000000
12	C21	2.893554	1.099302	0.000000
13	C21	-2.893554	1.099302	0.000000
14	C21	2.893554	-1.099302	0.000000
15	C21	-2.893554	-1.099302	0.000000
16	C3	2.423578	2.423578	0.000000
17	C3	-2.423578	2.423578	0.000000
18	C3	2.423578	-2.423578	0.000000
19	C3	-2.423578	-2.423578	0.000000
20	C22	1.099302	2.893554	0.000000
21	C22	-1.099302	2.893554	0.000000
22	C22	1.099302	-2.893554	0.000000
23	C22	-1.099302	-2.893554	0.000000
24	C12	0.680517	4.280778	0.000000
25	C12	-0.680517	4.280778	0.000000
26	C12	0.680517	-4.280778	0.000000
27	C12	-0.680517	-4.280778	0.000000
28	H11	5.133765	1.341807	0.000000
29	H11	-5.133765	1.341807	0.000000
30	H11	5.133765	-1.341807	0.000000
31	H11	-5.133765	-1.341807	0.000000
32	H22	3.190537	3.190537	0.000000
33	H22	-3.190537	3.190537	0.000000
34	H22	3.190537	-3.190537	0.000000
35	H22	-3.190537	-3.190537	0.000000
36	H3	1.341807	5.133765	0.000000
37	H3	-1.341807	5.133765	0.000000
38	H3	1.341807	-5.133765	0.000000
39	H3	-1.341807	-5.133765	0.000000

Fe(III) S=5/2, a2u hole, antiferro

Center	Label	x	y	z
1	FE	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.889279
3	F	0.000000	0.000000	-1.889279
4	N1	2.100019	0.000000	0.000000
5	N1	-2.100019	0.000000	0.000000
6	N2	0.000000	2.100019	0.000000
7	N2	0.000000	-2.100019	0.000000
8	C11	4.280770	0.680666	0.000000
9	C11	-4.280770	0.680666	0.000000
10	C11	4.280770	-0.680666	0.000000
11	C11	-4.280770	-0.680666	0.000000
12	C21	2.893536	1.098832	0.000000
13	C21	-2.893536	1.098832	0.000000
14	C21	2.893536	-1.098832	0.000000
15	C21	-2.893536	-1.098832	0.000000
16	C3	2.423748	2.423748	0.000000
17	C3	-2.423748	2.423748	0.000000
18	C3	2.423748	-2.423748	0.000000
19	C3	-2.423748	-2.423748	0.000000
20	C22	1.098832	2.893536	0.000000
21	C22	-1.098832	2.893536	0.000000
22	C22	1.098832	-2.893536	0.000000
23	C22	-1.098832	-2.893536	0.000000
24	C12	0.680666	4.280770	0.000000
25	C12	-0.680666	4.280770	0.000000
26	C12	0.680666	-4.280770	0.000000
27	C12	-0.680666	-4.280770	0.000000
28	H11	5.133903	1.341779	0.000000
29	H11	-5.133903	1.341779	0.000000
30	H11	5.133903	-1.341779	0.000000
31	H11	-5.133903	-1.341779	0.000000
32	H22	3.190685	3.190685	0.000000
33	H22	-3.190685	3.190685	0.000000
34	H22	3.190685	-3.190685	0.000000
35	H22	-3.190685	-3.190685	0.000000
36	H3	1.341779	5.133903	0.000000
37	H3	-1.341779	5.133903	0.000000
38	H3	1.341779	-5.133903	0.000000
39	H3	-1.341779	-5.133903	0.000000

****
**** Cartesian Coordinates for Mn(P)F_2 (Å)******
****

Mn(IV) S=3/2

Center	Label		x	y	z
1	MN		0.000000	0.000000	0.000000
2	F		0.000000	0.000000	1.794572
3	F		0.000000	0.000000	-1.794572
4	N1		2.031281	0.000000	0.000000
5	N1		-2.031281	0.000000	0.000000
6	N2		0.000000	2.031281	0.000000
7	N2		0.000000	-2.031281	0.000000
8	C11		4.218642	0.678693	0.000000
9	C11		-4.218642	0.678693	0.000000
10	C11		4.218642	-0.678693	0.000000
11	C11		-4.218642	-0.678693	0.000000
12	C21		2.842783	1.101891	0.000000
13	C21		-2.842783	1.101891	0.000000
14	C21		2.842783	-1.101891	0.000000
15	C21		-2.842783	-1.101891	0.000000
16	C3		2.420632	2.420632	0.000000
17	C3		-2.420632	2.420632	0.000000
18	C3		2.420632	-2.420632	0.000000
19	C3		-2.420632	-2.420632	0.000000
20	C22		1.101891	2.842783	0.000000
21	C22		-1.101891	2.842783	0.000000
22	C22		1.101891	-2.842783	0.000000
23	C22		-1.101891	-2.842783	0.000000
24	C12		0.678693	4.218642	0.000000
25	C12		-0.678693	4.218642	0.000000
26	C12		0.678693	-4.218642	0.000000
27	C12		-0.678693	-4.218642	0.000000
28	H11		5.064463	1.348784	0.000000
29	H11		-5.064463	1.348784	0.000000
30	H11		5.064463	-1.348784	0.000000
31	H11		-5.064463	-1.348784	0.000000
32	H22		1.348784	5.064463	0.000000
33	H22		-1.348784	5.064463	0.000000
34	H22		1.348784	-5.064463	0.000000
35	H22		-1.348784	-5.064463	0.000000
36	H3		3.185828	3.185828	0.000000
37	H3		-3.185828	3.185828	0.000000
38	H3		3.185828	-3.185828	0.000000
39	H3		-3.185828	-3.185828	0.000000

Mn(III) S=2, a1u, ferro

Center	Label	x	y	z
1	MN	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.819066
3	F	0.000000	0.000000	-1.819066
4	N1	2.099240	0.000000	0.000000
5	N1	-2.099240	0.000000	0.000000
6	N2	0.000000	2.099240	0.000000
7	N2	0.000000	-2.099240	0.000000
8	C11	4.291172	0.674834	0.000000
9	C11	-4.291172	0.674834	0.000000
10	C11	4.291172	-0.674834	0.000000
11	C11	-4.291172	-0.674834	0.000000
12	C21	2.884194	1.101868	0.000000
13	C21	-2.884194	1.101868	0.000000
14	C21	2.884194	-1.101868	0.000000
15	C21	-2.884194	-1.101868	0.000000
16	C3	2.429426	2.429426	0.000000
17	C3	-2.429426	2.429426	0.000000
18	C3	2.429426	-2.429426	0.000000
19	C3	-2.429426	-2.429426	0.000000
20	C22	1.101868	2.884194	0.000000
21	C22	-1.101868	2.884194	0.000000
22	C22	1.101868	-2.884194	0.000000
23	C22	-1.101868	-2.884194	0.000000
24	C12	0.674834	4.291172	0.000000
25	C12	-0.674834	4.291172	0.000000
26	C12	0.674834	-4.291172	0.000000
27	C12	-0.674834	-4.291172	0.000000
28	H11	5.142346	1.338715	0.000000
29	H11	-5.142346	1.338715	0.000000
30	H11	5.142346	-1.338715	0.000000
31	H11	-5.142346	-1.338715	0.000000
32	H22	1.338715	5.142346	0.000000
33	H22	-1.338715	5.142346	0.000000
34	H22	1.338715	-5.142346	0.000000
35	H22	-1.338715	-5.142346	0.000000
36	H3	3.195447	3.195447	0.000000
37	H3	-3.195447	3.195447	0.000000
38	H3	3.195447	-3.195447	0.000000
39	H3	-3.195447	-3.195447	0.000000

Mn(IV) S=2, a1u, antiferro

Center	Label	x	y	z
1	MN	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.817943
3	F	0.000000	0.000000	-1.817943
4	N1	2.100350	0.000000	0.000000
5	N1	-2.100350	0.000000	0.000000
6	N2	0.000000	2.100350	0.000000
7	N2	0.000000	-2.100350	0.000000
8	C11	4.291836	0.674802	0.000000
9	C11	-4.291836	0.674802	0.000000
10	C11	4.291836	-0.674802	0.000000
11	C11	-4.291836	-0.674802	0.000000
12	C21	2.884642	1.101996	0.000000
13	C21	-2.884642	1.101996	0.000000
14	C21	2.884642	-1.101996	0.000000
15	C21	-2.884642	-1.101996	0.000000
16	C3	2.429507	2.429507	0.000000
17	C3	-2.429507	2.429507	0.000000
18	C3	2.429507	-2.429507	0.000000
19	C3	-2.429507	-2.429507	0.000000
20	C22	1.101996	2.884642	0.000000
21	C22	-1.101996	2.884642	0.000000
22	C22	1.101996	-2.884642	0.000000
23	C22	-1.101996	-2.884642	0.000000
24	C12	0.674802	4.291836	0.000000
25	C12	-0.674802	4.291836	0.000000
26	C12	0.674802	-4.291836	0.000000
27	C12	-0.674802	-4.291836	0.000000
28	H11	5.143109	1.338536	0.000000
29	H11	-5.143109	1.338536	0.000000
30	H11	5.143109	-1.338536	0.000000
31	H11	-5.143109	-1.338536	0.000000
32	H22	1.338536	5.143109	0.000000
33	H22	-1.338536	5.143109	0.000000
34	H22	1.338536	-5.143109	0.000000
35	H22	-1.338536	-5.143109	0.000000
36	H3	3.195532	3.195532	0.000000
37	H3	-3.195532	3.195532	0.000000
38	H3	3.195532	-3.195532	0.000000
39	H3	-3.195532	-3.195532	0.000000

Mn(III) S=2, a2u, ferro

Center	Label	x	y	z
1	MN	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.816212
3	F	0.000000	0.000000	-1.816212
4	N1	2.109101	0.000000	0.000000
5	N1	-2.109101	0.000000	0.000000
6	N2	0.000000	2.109101	0.000000
7	N2	0.000000	-2.109101	0.000000
8	C11	4.288894	0.680779	0.000000
9	C11	-4.288894	0.680779	0.000000
10	C11	4.288894	-0.680779	0.000000
11	C11	-4.288894	-0.680779	0.000000
12	C21	2.899989	1.099818	0.000000
13	C21	-2.899989	1.099818	0.000000
14	C21	2.899989	-1.099818	0.000000
15	C21	-2.899989	-1.099818	0.000000
16	C3	2.425051	2.425051	0.000000
17	C3	-2.425051	2.425051	0.000000
18	C3	2.425051	-2.425051	0.000000
19	C3	-2.425051	-2.425051	0.000000
20	C22	1.099818	2.899989	0.000000
21	C22	-1.099818	2.899989	0.000000
22	C22	1.099818	-2.899989	0.000000
23	C22	-1.099818	-2.899989	0.000000
24	C12	0.680779	4.288894	0.000000
25	C12	-0.680779	4.288894	0.000000
26	C12	0.680779	-4.288894	0.000000
27	C12	-0.680779	-4.288894	0.000000
28	H11	5.142751	1.341143	0.000000
29	H11	-5.142751	1.341143	0.000000
30	H11	5.142751	-1.341143	0.000000
31	H11	-5.142751	-1.341143	0.000000
32	H22	1.341143	5.142751	0.000000
33	H22	-1.341143	5.142751	0.000000
34	H22	1.341143	-5.142751	0.000000
35	H22	-1.341143	-5.142751	0.000000
36	H3	3.192205	3.192205	0.000000
37	H3	-3.192205	3.192205	0.000000
38	H3	3.192205	-3.192205	0.000000
39	H3	-3.192205	-3.192205	0.000000

Mn(III) S=2, a2u, antiferro

Center	Label	x	y	z
1	MN	0.000000	0.000000	0.000000
2	F	0.000000	0.000000	1.816908
3	F	0.000000	0.000000	-1.816908
4	N1	2.108716	0.000000	0.000000
5	N1	-2.108716	0.000000	0.000000
6	N2	0.000000	2.108716	0.000000
7	N2	0.000000	-2.108716	0.000000
8	C11	4.288613	0.680806	0.000000
9	C11	-4.288613	0.680806	0.000000
10	C11	4.288613	-0.680806	0.000000
11	C11	-4.288613	-0.680806	0.000000
12	C21	2.899747	1.099754	0.000000
13	C21	-2.899747	1.099754	0.000000
14	C21	2.899747	-1.099754	0.000000
15	C21	-2.899747	-1.099754	0.000000
16	C3	2.425097	2.425097	0.000000
17	C3	-2.425097	2.425097	0.000000
18	C3	2.425097	-2.425097	0.000000
19	C3	-2.425097	-2.425097	0.000000
20	C22	1.099754	2.899747	0.000000
21	C22	-1.099754	2.899747	0.000000
22	C22	1.099754	-2.899747	0.000000
23	C22	-1.099754	-2.899747	0.000000
24	C12	0.680806	4.288613	0.000000
25	C12	-0.680806	4.288613	0.000000
26	C12	0.680806	-4.288613	0.000000
27	C12	-0.680806	-4.288613	0.000000
28	H11	5.142798	1.340748	0.000000
29	H11	-5.142798	1.340748	0.000000
30	H11	5.142798	-1.340748	0.000000
31	H11	-5.142798	-1.340748	0.000000
32	H22	1.340748	5.142798	0.000000
33	H22	-1.340748	5.142798	0.000000
34	H22	1.340748	-5.142798	0.000000
35	H22	-1.340748	-5.142798	0.000000
36	H3	3.192227	3.192227	0.000000
37	H3	-3.192227	3.192227	0.000000
38	H3	3.192227	-3.192227	0.000000
39	H3	-3.192227	-3.192227	0.000000