

Inorganic Chemistry

including bioinorganic chemistry

Inorg. Chem., 1996, 35(26), 7671-7678, DOI:[10.1021/ic960546f](https://doi.org/10.1021/ic960546f)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1996 American Chemical Society

Table A1. Ground State Millimeter-Wave Transitions (MHz) of PH₂F

upper			lower			V _{obs}	V _{obs-calc}	weight
J	K _a	K _c	J	K _a	K _c			
04	01	03	03	00	03	236963.802	0.059	1000.0
05	00	05	04	00	04	150411.973	0.005	1000.0
05	01	05	04	01	04	149995.807	-0.019	1000.0
05	01	04	04	01	03	150828.672	0.009	1000.0
05	02	04	04	02	03	150405.038	-0.032	1000.0
05	02	03	04	02	02	150408.541	-0.052	1000.0
05	03	02	04	03	01	150393.295	-0.100	1000.0
05	04	01	04	04	00	150375.346	-0.114	1000.0
06	01	05	05	00	05	298034.868	0.053	1000.0
08	03	05	09	02	07	308062.819	0.028	1000.0
08	03	06	09	02	08	308120.870	0.038	1000.0
09	00	09	08	01	07	151874.443	-0.058	1000.0
10	00	10	09	00	09	300736.829	0.036	1000.0
10	01	10	09	01	09	299922.142	0.028	1000.0
10	01	09	09	01	08	301586.235	0.038	1000.0
10	02	08	09	02	07	300770.920	0.015	1000.0
10	02	09	09	02	08	300741.896	0.015	1000.0
10	03	07	09	03	06	300724.804	-0.053	1000.0
10	04	06	09	04	05	300687.552	-0.038	1000.0
10	05	05	09	05	04	300641.198	-0.051	1000.0
10	06	04	09	06	03	300585.100	-0.066	1000.0
10	07	03	09	07	02	300519.112	-0.053	1000.0
10	08	02	09	08	01	300443.195	0.003	1000.0
10	09	01	09	09	00	300357.322	0.084	1000.0
12	00	12	11	01	10	239464.886	-0.004	1000.0
14	00	14	13	01	12	297363.900	0.081	1000.0
16	04	12	17	03	14	298794.966	-0.135	1000.0
16	04	13	17	03	15	298799.268	-0.138	1000.0
17	01	17	16	02	15	151037.165	0.066	1000.0
18	04	14	19	03	16	238649.282	0.141	1000.0
18	04	15	19	03	17	238657.530	0.116	1000.0
19	01	18	18	02	16	238706.875	0.144	1000.0
20	01	20	19	02	18	236310.408	-0.025	1000.0
21	01	20	20	02	18	301632.855	-0.081	1000.0
30	02	29	30	01	29	308811.578	-0.001	1000.0

Table A2. Ground State Millimeter-Wave Transitions (MHz) of PH₂³⁵Cl

upper			lower			V _{obs}	V _{obs-calc}	weight
J	K _a	K _c	J	K _a	K _c			
08	01	07	07	00	07	231852.304	0.111	1000.0
13	01	12	12	00	12	299913.710	0.099	500.0
15	02	13	16	01	15	154101.027	-0.005	1000.0
15	02	14	16	01	16	158613.200	-0.280	250.0
17	00	17	16	00	16	228319.438	0.148	250.0
17	01	16	16	01	15	228603.659	-0.007	1000.0
17	01	17	16	01	16	228038.320	-0.006	1000.0
17	02	16	16	02	15	228314.271	-0.035	1000.0
17	02	15	16	02	14	228319.438	-0.171	250.0
17	03	14	16	03	13	228303.711	-0.035	1000.0
17	04	13	16	04	12	228286.447	-0.076	1000.0
17	05	13	16	05	12	228264.549	-0.114	500.0
17	06	11	16	06	10	228237.930	-0.116	500.0
21	00	21	20	01	19	154699.260	0.009	500.0
23	00	23	22	00	22	308787.281	0.003	1000.0
23	01	23	22	01	22	308412.438	-0.009	1000.0
23	01	22	22	01	21	309175.936	0.017	1000.0
23	02	22	22	02	21	308785.683	-0.044	1000.0
23	02	21	22	02	20	308798.889	0.046	1000.0
23	03	20	22	03	19	308773.105	-0.018	1000.0
23	04	19	22	04	18	308749.411	-0.005	1000.0
23	05	18	22	05	17	308719.675	0.030	1000.0
23	06	17	22	06	16	308683.569	0.067	1000.0
27	00	27	26	01	25	232715.405	-0.005	1000.0
28	01	27	27	01	26	376243.995	0.007	1000.0
28	03	25	29	02	27	229154.823	0.018	1000.0
28	03	26	29	02	28	229358.023	-0.003	1000.0

Table A3. Ground State Millimeter-Wave Transitions (MHz) of PH₂³⁷Cl

upper			lower			v _{obs}	v _{obs-calc}	weight
J	K _a	K _c	J	K _a	K _c			
08	01	07	07	00	07	229080.776	-0.252	500.0
12	00	12	11	00	11	157092.516	0.023	1000.0
12	01	11	11	01	10	157281.852	0.059	1000.0
17	00	17	16	00	16	222498.793	-0.081	1000.0
17	01	16	16	01	15	222768.713	0.063	1000.0
17	01	17	16	01	16	222231.900	-0.030	1000.0
17	03	14	16	03	13	222483.721	-0.047	1000.0
18	00	18	17	00	17	235574.601	0.035	1000.0
18	01	18	17	01	17	235292.411	-0.048	1000.0
18	01	17	17	01	16	235860.697	0.079	1000.0
18	02	16	17	02	15	235575.537	0.035	1000.0
23	00	23	22	00	22	300918.610	0.035	1000.0
23	01	22	22	01	21	301287.169	0.041	1000.0
23	01	23	22	01	22	300562.132	-0.011	1000.0
23	02	21	22	02	20	300928.412	0.067	1000.0
23	02	22	22	02	21	300916.476	-0.044	1000.0
23	03	20	22	03	19	300904.293	-0.044	1000.0
23	04	19	22	04	18	300881.775	-0.044	1000.0
23	05	18	22	05	17	300853.452	-0.052	1000.0
23	06	18	22	06	17	300819.057	-0.060	1000.0
23	07	16	22	07	15	300778.680	0.098	1000.0
29	00	29	28	00	28	379239.992	0.047	1000.0
29	01	29	28	01	28	378798.266	0.012	1000.0
29	01	28	28	01	27	379710.369	-0.060	1000.0

Table A4. $v_4 = 1$ Millimeter-Wave Transitions (MHz) of PH₂F

upper			lower			ν_{obs}	$\nu_{\text{obs-calc}}$	weight
J	K_a	K_c	J	K_a	K_c			
05	00	05	04	00	04	149057.552	-0.107	1000.0
05	01	04	04	01	03	149477.835	0.193	1000.0
05	01	05	04	01	04	148637.145	-0.296	1000.0
05	02	04	04	02	03	149049.249	0.219	1000.0
05	02	03	04	02	02	149052.727	0.070	1000.0
05	03	02	04	03	01	149035.597	0.411	1000.0
05	04	01	04	04	00	149014.808	0.656	1000.0
08	00	08	07	00	07	238456.171	-0.379	1000.0
08	01	08	07	01	07	237790.747	-0.745	1000.0
08	01	07	07	01	06	239135.225	-0.257	1000.0
08	02	06	07	02	05	238465.777	-0.148	1000.0
08	02	07	07	02	06	238450.978	0.283	1000.0
08	03	05	07	03	04	238431.721	0.430	1000.0
08	04	04	07	04	03	238397.912	0.846	1000.0
08	05	03	07	05	02	238355.034	1.170	1000.0
08	06	02	07	06	01	238302.493	1.155	1000.0
08	07	02	07	07	01	238239.319	-0.070	1000.0
10	00	10	09	00	09	298028.823	-0.676	1000.0
10	01	09	09	01	08	298885.569	-0.604	1000.0
10	01	10	09	01	09	297206.084	-0.509	1000.0
10	02	09	09	02	08	298031.671	0.323	1000.0
10	02	08	09	02	07	298060.665	-0.589	1000.0
10	03	07	09	03	06	298010.629	0.356	1000.0
10	04	06	09	04	05	297967.816	0.996	1000.0
10	05	05	09	05	04	297913.904	1.365	1000.0
10	06	04	09	06	03	297848.033	1.300	1000.0
10	07	04	09	07	03	297769.412	0.207	1000.0

Table A5. Ground State Millimeter-Wave Transitions (MHz) of PD₂F

upper			lower			v _{obs}	v _{obs-calc}	weight
J	K _a	K _c	J	K _a	K _c			
11	00	11	10	00	10	302191.257	0.200	1000.0
11	01	10	10	01	09	304586.135	0.182	1000.0
11	01	11	10	01	10	300436.668	0.153	1000.0
11	02	09	10	02	08	302966.672	0.202	1000.0
11	02	10	10	02	09	302538.671	0.031	1000.0
11	03	08	10	03	07	302647.524	0.105	1000.0
11	03	09	10	03	08	302639.416	0.109	1000.0
11	04	07	10	04	06	302589.758	0.072	1000.0
11	05	06	10	05	05	302542.642	0.077	1000.0
11	06	05	10	06	04	302492.636	-0.045	1000.0
11	07	04	10	07	03	302437.036	-0.117	1000.0
11	08	04	10	08	03	302374.663	-0.205	1000.0
11	09	03	10	09	02	302305.028	-0.299	1000.0
11	10	02	10	10	01	302227.879	-0.405	1000.0
13	00	13	12	00	12	356896.973	0.067	1000.0
13	01	12	12	01	11	359866.890	0.040	1000.0
13	01	13	12	01	12	354974.487	0.041	1000.0
13	02	11	12	02	10	358172.024	0.107	1000.0
13	02	12	12	02	11	357470.681	-0.089	1000.0
13	03	10	12	03	09	357663.277	0.015	1000.0
13	03	11	12	03	10	357644.372	0.002	1000.0
13	05	08	12	05	07	357517.449	-0.010	1000.0
13	06	07	12	06	06	357455.742	-0.035	1000.0
13	07	06	12	07	05	357388.456	-0.058	1000.0
13	08	06	12	08	05	357313.760	-0.069	1000.0
13	09	05	12	09	04	357230.840	-0.045	1000.0
13	10	04	12	10	03	357139.160	-0.107	1000.0
14	00	14	13	00	13	384209.185	0.031	1000.0
14	01	13	13	01	12	387488.521	-0.064	1000.0
14	01	14	13	01	13	382228.215	-0.043	1000.0
14	02	12	13	02	11	385793.897	0.030	1000.0
14	02	13	13	02	12	384922.975	-0.209	1000.0
14	03	11	13	03	10	385169.876	-0.058	1000.0
14	03	12	13	03	11	385142.423	-0.066	1000.0
14	05	09	13	05	08	384998.861	-0.042	1000.0
14	06	08	13	06	07	384930.808	-0.015	1000.0
14	07	07	13	07	06	384857.398	0.003	1000.0
14	08	06	13	08	05	384776.265	-0.048	1000.0
14	12	02	13	12	01	384361.079	0.223	1000.0
14	13	01	13	13	00	384233.320	0.340	1000.0

Table A6. Ground State Millimeter-Wave Transitions (MHz) of PD₂³⁵Cl

upper			lower			V _{obs}	V _{obs-calc}	weight
J	K _a	K _c	J	K _a	K _c			
28	06	22	27	06	21	352734.177	-0.055	1000.0
28	07	21	27	07	20	352692.303	-0.087	1000.0
28	08	20	27	08	19	352645.076	-0.097	1000.0
28	09	20	27	09	19	352592.180	-0.089	1000.0
28	10	19	27	10	18	352533.513	-0.004	1000.0
28	11	17	27	11	16	352468.884	0.054	1000.0
28	12	17	27	12	16	352398.367	0.209	1000.0
29	00	29	28	00	28	365120.013	0.056	1000.0
29	01	28	28	01	27	366446.914	0.076	1000.0
29	01	29	28	01	28	364221.399	0.067	1000.0
29	02	27	28	02	26	365639.470	0.089	1000.0
29	02	28	28	02	27	365350.445	0.050	500.0
29	03	26	28	03	25	365423.274	0.037	1000.0
29	03	27	28	03	26	365416.179	0.039	1000.0
29	04	25	28	04	24	365380.212	-0.021	1000.0
29	05	24	28	05	23	365344.243	-0.023	1000.0
29	06	23	28	06	22	365305.463	-0.055	1000.0
29	07	22	28	07	21	365261.948	-0.071	1000.0
29	08	21	28	08	20	365212.944	-0.064	1000.0
29	09	20	28	09	19	365158.099	-0.038	1000.0
29	10	19	28	10	18	365097.261	0.033	1000.0
30	00	30	29	00	29	377661.169	0.002	1000.0
30	01	29	29	01	28	379047.889	0.029	1000.0
30	01	30	29	01	29	376747.482	0.039	1000.0
30	02	28	29	02	27	378235.553	0.052	1000.0
30	02	29	29	02	28	377916.362	-0.022	500.0
30	03	27	29	03	26	377998.449	0.027	1000.0
30	03	28	29	03	27	377990.033	0.015	1000.0
30	04	26	29	04	25	377952.094	-0.059	1000.0
30	05	25	29	05	24	377914.371	-0.028	1000.0
30	06	24	29	06	23	377873.967	-0.061	1000.0
30	07	23	29	07	22	377828.803	-0.053	1000.0
30	08	22	29	08	21	377777.992	-0.048	1000.0
30	09	21	29	09	20	377721.218	0.025	1000.0

Table A7. Harmonic contributions α in MHz.

	α^A	α^B	α^C
PH ₃		-1512.67	-1136.12
PD ₃		-565.04	-397.22
PH ₂ F	-900.9 ^a	-33.82	-37.77
PD ₂ F	-387.7 ^b	-29.71	-36.03
PHF ₂	-112.8 ^a	-24.28	-6.87
PDF ₂	-89.7 ^b	-22.27	-7.34
PH ₂ ³⁵ Cl	-779.1 ^a	-10.19	-11.00
PH ₂ ³⁷ Cl	-776.5 ^a	-9.80	-10.55
PD ₂ ³⁵ Cl	-320.5 ^c	-9.32	-10.70
P ³⁵ Cl ₃		-4.0	
P ³⁷ Cl ₃		-3.73	

^a) Accuracy: 10 MHz. ^b) Accuracy: 20 MHz. ^c) Accuracy: 50 MHz.

Table A8. Isotopic differences $r_z(\text{isotopic species}) - r_z(\text{parent species})$, in Å.

Parent species	PH ₂ ³⁵ Cl		PH ₂ F	PHF ₂
Isotopic species	PH ₂ ³⁷ Cl	PD ₂ ³⁵ Cl	PD ₂ F	PDF ₂
$r(\text{P-H})$	-8.10 ⁻⁶	-0.003	-0.003	-0.002
$r(\text{P-X}^a)$	-6.10 ⁻⁵	-4.10 ⁻⁵	-1.10 ⁻⁴	-6.10 ⁻⁵

^aX = F or Cl.