Recommended DOSDs and pseudospectra

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Supplementary information for an article entitled
**Dipole properties of PH_3 , PF_3 , PF_5 , PCl_3 , SiCl_4 ,
 GeCl_4 , and SnCl_4**
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1 PH₃

Photoabsorption data used for the recommended PH ₃ DOSD.		
Energy range (eV)	Intervals	Source
5.09–10.0	2	Robin [1]
10.0–11.7	1	Xia et al. [2]
11.7–88.7	6	Carravetta and Cacelli [3]
88.7–130	3	Zarate et al. [4], low resolution
130–139	1	Friedrich et al. [5]
139–220	3	Zarate et al. [4], low resolution
220–30,000	12	Henke et al. [6]
30,000–100,000	1	Chantler [7, 8]
100,000– ∞	1	Eq. (7)

The constraints used were the KRT sum rule and the CCSD(T)/q static dipole polarizability from this work.

Pseudospectrum for PH ₃ .	
E_i	f_i
1.930206E-01	3.123885E-04
2.371340E-01	1.858287E-02
2.730327E-01	2.256790E-01
3.540094E-01	9.483740E-01
4.631507E-01	2.589992E+00
6.597845E-01	2.591859E+00
1.171344E+00	9.962772E-01
5.655883E+00	4.533239E+00
2.336128E+01	5.710148E+00
5.922369E+02	3.855359E-01

2 PF_3

Photoabsorption data used for the recommended PF_3 DOSD.

Energy range (eV)	Intervals	Source
5–133	14	Au et al. [9], low resolution
133–278	5	Ishiguro et al. [10]
278–300	1	Au et al. [9], low resolution
300–30,000	10	Henke et al. [6]
30,000–100,000	1	Chantler [7, 8]
100,000– ∞	1	Eq. (7)

The constraints used were the KRT sum rule and the CCSD(T)/q static dipole polarizability from this work.

Pseudospectrum for PF_3 .

E_i	f_i
1.884424E-01	1.357346E-03
2.095666E-01	3.171241E-03
2.762324E-01	2.108261E-01
3.368645E-01	4.217837E-01
5.000586E-01	1.470908E+00
7.761556E-01	5.075774E+00
1.430911E+00	8.041138E+00
3.861763E+00	1.203012E+01
2.238221E+01	1.394399E+01
4.771655E+02	8.009300E-01

3 PF_5

Photoabsorption data used for the recommended PF_5 DOSD.

Energy range (eV)	Intervals	Source
10–133	19	Au and Brion [11], low resolution
133–153	1	Au and Brion [11], high resolution
153–301	3	Au and Brion [11], low resolution
301–30,000	11	Henke et al. [6]
30,000–100,000	1	Chantler [7, 8]
100,000– ∞	1	Eq. (7)

The constraints used were the KRT sum rule and the CCSD(T)/q static dipole polarizability from this work.

Pseudospectrum for PF_5 .

E_i	f_i
3.845309E-01	9.546964E-03
4.348989E-01	1.940867E-01
5.121328E-01	8.113886E-01
6.505672E-01	2.456409E+00
8.858718E-01	6.386473E+00
1.337836E+00	9.292146E+00
2.438856E+00	1.180487E+01
6.228404E+00	1.420156E+01
3.542609E+01	1.420069E+01
5.654233E+02	6.428261E-01

4 PCl_3

Photoabsorption data used for the recommended PCl_3 DOSD.

Energy range (eV)	Intervals	Source
4.5–5.16	1	Au and Brion [12], low resolution
5.16–6.71	1	Halmann [13]
6.71–350	31	Au and Brion [12], low resolution
350–30,000	11	Henke et al. [6]
30,000–100,000	1	Chantler [7, 8]
100,000– ∞	1	Eq. (7)

The constraints used were the KRT sum rule and the CCSD(T)/q static dipole polarizability from this work.

Pseudospectrum for PCl_3 .

E_i	f_i
1.689230E-01	2.480725E-03
1.986643E-01	3.354268E-02
2.335342E-01	1.301737E-01
3.117112E-01	9.380820E-01
4.298132E-01	4.393405E+00
6.289846E-01	9.826531E+00
1.013025E+00	7.091912E+00
5.011679E+00	1.047398E+01
2.208886E+01	3.129471E+01
6.737146E+02	1.815174E+00

5 SiCl₄

Photoabsorption data used for the recommended SiCl₄ DOSD.

Energy range (eV)	Intervals	Source
6.13–7.72	1	Ibuki et al. [14]
7.72–10.90	1	Causley and Russell [15]
10.90–30.92	9	Ibuki et al. [14]
30.92–1840	21	Henke et al. [6]
1840–1899	1	Ferrer et al. [16]
1899–2816	2	Henke et al. [6]
2816–2880	1	Ferrer et al. [16]
2880–30,000	4	Henke et al. [6]
30,000–100,000	1	Chantler [7, 8]
100,000– ∞	1	Eq. (7)

The constraints used were the KRT sum rule and the refractivity at 680 nm measured by Holemann and Goldschmidt [17].

Pseudospectrum for SiCl₄.

E_i	f_i
2.300657E-01	1.043238E-02
2.535270E-01	1.978190E-02
3.286200E-01	7.350290E-01
4.118290E-01	3.477915E+00
5.429246E-01	8.300935E+00
8.028597E-01	1.086023E+01
1.373899E+00	4.199857E+00
6.222681E+00	2.070454E+01
2.617836E+01	3.176044E+01
7.182769E+02	1.930847E+00

6 GeCl₄

Photoabsorption data used for the recommended GeCl₄ DOSD.

Energy range (eV)	Intervals	Source
6.17–10.94	2	Causley and Russell [15]
10.94–15.50	3	Ali [18]
15.50–30.56	5	Ibuki and Kamamoto [19]
30.56–500	19	Henke et al. [6]
500–1000	4	Chantler [7, 8]
1000–30,000	9	Henke et al. [6]
30,000–100,000	1	Chantler [7, 8]
100,000– ∞	1	Eq. (7)

The constraints used were the KRT sum rule and the CCSD(T)/q static dipole polarizability from this work.

Pseudospectrum for GeCl ₄ .	
E_i	f_i
2.393793E-01	5.131218E-02
2.592011E-01	2.675776E-01
3.350137E-01	8.767252E-01
3.966992E-01	3.794082E+00
5.417827E-01	7.774298E+00
8.113302E-01	1.088293E+01
1.545899E+00	5.434999E+00
5.898561E+00	2.646996E+01
2.997847E+01	4.256370E+01
1.424128E+03	1.884414E+00

7 SnCl_4

Photoabsorption data used for the recommended SnCl_4 DOSD.

Energy range (eV)	Intervals	Source
5.52–6.17	1	Fernandez et al. [20]
6.17–31.05	9	Tokue and Ibuki [21]
31.05–30,000	39	Henke et al. [6]
30,000–100,000	1	Chantler [7, 8]
100,000– ∞	1	Eq. (7)

The constraints used were the KRT sum rule and the refractivity at 500 nm measured by Holemann and Goldschmidt [17].

Pseudospectrum for SnCl_4 .	
E_i	f_i
2.104191E-01	4.897338E-02
2.291506E-01	2.745961E-01
2.793514E-01	4.242414E-01
3.595845E-01	3.250903E+00
4.905739E-01	6.991478E+00
7.502645E-01	1.181557E+01
1.465226E+00	9.519297E+00
4.484648E+00	2.387364E+01
3.143497E+01	5.997931E+01
2.945780E+03	1.821990E+00

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