

Packing of tetrahedral EX_4 molecules with $E = \text{C, Si, Ge, Sn, Pb}$ and $X = \text{F, Cl, Br, I}$

Alexandra Kerstin Wolf, Jürgen Glinnemann, Martin Ulrich Schmidt*

Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe-Universität, Max-von-Laue-Str. 7, D-60438 Frankfurt am Main, Germany.

* m.schmidt@chemie.uni-frankfurt.de

1 Bond-length Terms

Table 1: Bond-length terms

EX_4	value /Å
CF ₄	1.3290
CCl ₄	1.7500
CBr ₄	1.9125
CI ₄	2.1540
SiF ₄	1.5850
SiCl ₄	2.0080
SiBr ₄	2.2500
SiI ₄	2.4300
GeF ₄	1.7330
GeCl ₄	2.0950
GeBr ₄	2.2670
GeI ₄	2.5700
SnF ₄	1.8500
SnCl ₄	2.2800
SnBr ₄	2.4100
SnI ₄	2.6500
PbF ₄	1.9500
PbCl ₄	2.3620
PbBr ₄	2.5300
PbI ₄	2.7700

2 Calculated polymorphs for all EX₄ compounds

Table 2: Calculated polymorphs for CF₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-23.225	8.711	4.316	8.323	90	117.82	90
<i>I</i> $\bar{4}2m$	2	$\bar{4}2m$	-23.160	4.341	4.341	7.436	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-22.882	7.572	4.899	7.643	90	101.38	90
<i>Pa</i> $\bar{3}$	8	3	-22.480	8.229	8.229	8.229	90	90	90
<i>C2/c</i>	32	all on 1	-22.128	16.659	9.106	16.365	90	113.66	90
<i>P</i> $\bar{4}3m$	1	$\bar{4}3m$	-19.116	4.267	4.267	4.267	90	90	90

Table 3: Calculated polymorphs for CCl₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>Pa</i> $\bar{3}$	8	3	-51.508	9.875	9.875	9.875	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-51.468	9.065	5.988	9.084	90	102.29	90
<i>C2/c</i>	4	2	-51.059	10.664	5.122	10.015	90	118	90
<i>I</i> $\bar{4}2m$	2	$\bar{4}2m$	-50.402	5.123	5.123	9.287	90	90	90
<i>P4</i> ₂ / <i>nmc</i>	2	$\bar{4}2m$	-49.596	6.907	6.907	5.122	90	90	90
<i>C2/c</i>	32	all on 1	-49.004	20.262	10.978	19.664	90	114.71	90
<i>P</i> $\bar{4}3m$	1	$\bar{4}3m$	-45.384	5.044	5.044	5.044	90	90	90

Table 4: Calculated polymorphs for CBr₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>Pa</i> $\bar{3}$	8	3	-60.760	10.138	10.138	10.138	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-60.596	9.284	6.181	9.289	90	101.95	90
<i>C2</i> / <i>c</i>	4	2	-60.188	11.080	5.196	10.210	90	117.35	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-59.584	5.190	5.190	9.745	90	90	90
<i>P</i> $\bar{1}$	2	1	-59.580	6.150	6.194	7.236	90	105.01	90
<i>P4</i> ₂ / <i>nmc</i>	2	$\bar{4}$ 2 <i>m</i>	-59.300	7.098	7.098	5.200	90	90	90
<i>C2</i> / <i>c</i>	32	all on 1	-57.004	20.929	11.285	20.256	90	115.25	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-56.128	5.119	5.119	5.119	90	90	90

Table 5: Calculated polymorphs for Cl₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2</i> / <i>c</i>	4	2	-78.068	11.948	5.526	10.880	90	116.92	90
<i>P2</i> ₁ / <i>c</i>	4	1	-77.669	9.935	6.616	9.962	90	101.57	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-77.392	5.518	5.518	10.553	90	90	90
<i>P4</i> ₂ / <i>nmc</i>	2	$\bar{4}$ 2 <i>m</i>	-77.348	7.605	7.605	5.545	90	90	90
<i>Pa</i> $\bar{3}$	8	3	-76.896	10.869	10.869	10.869	90	90	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-74.060	5.448	5.448	5.448	90	90	90
<i>P</i> $\bar{1}$	2	1	-72.926	6.633	7.269	7.803	75.28	89.78	63.99
<i>C2</i> / <i>c</i>	32	all on 1	-72.396	22.449	12.078	21.811	90	225.45	90

Table 6: Calculated polymorphs for SiF₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-51.359	8.871	4.392	8.301	90	116.14	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-51.180	4.487	4.487	7.385	90	90	90
<i>I</i> $\bar{4}$ 3 <i>m</i>	2	$\bar{4}$ 3 <i>m</i>	-50.492	5.530	5.530	5.530	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-46.884	7.659	4.872	8.141	90	97.69	90
<i>C2/c</i>	32	all on 1	-43.852	16.801	9.478	16.635	90	110.03	90
<i>Pa</i> $\bar{3}$	8	3	-42.588	8.418	8.418	8.418	90	90	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-38.484	4.311	4.311	4.311	90	90	90

Table 7: Calculated polymorphs for SiCl₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-73.429	10.989	5.168	10.066	90	116.78	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-72.346	5.177	5.177	9.587	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-70.583	9.244	6.066	9.355	90	100.64	90
<i>Pa</i> $\bar{3}$	8	3	-68.120	10.099	10.099	10.099	90	90	90
<i>R3c</i>	6	1	-66.336	9.168	9.168	11.665	90	90	120
<i>C2/c</i>	32	all on 1	-65.760	20.733	11.194	20.390	90	114.75	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-65.236	5.078	5.078	5.078	90	90	90
<i>P</i> $\bar{1}$	2	1	-59.908	6.087	6.198	7.390	90.14	105.82	98.58

Table 8: Calculated polymorphs for SiBr₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-81.204	11.523	5.294	10.423	90	116.66	90
$\bar{I}4_2m$	2	$\bar{4}2m$	-79.904	5.289	5.289	10.199	90	90	90
<i>P2₁/c</i>	4	1	-78.716	9.563	6.317	9.656	90	100.72	90
<i>Pa$\bar{3}$</i>	8	3	-76.512	10.456	10.456	10.456	90	90	90
$\bar{P}4_3m$	1	$\bar{4}3m$	-74.280	5.248	5.248	5.248	90	90	90
<i>R3c</i>	6	1	-74.136	9.322	9.322	12.199	90	90	120
<i>Pban</i>	2	222	-73.896	10.328	5.272	5.272	90	90	90
<i>C2/c</i>	32	all on 1	-72.364	21.710	11.527	21.356	90	116.13	90

Table 9: Calculated polymorphs for SiI₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-89.247	12.499	5.574	11.165	90	116.53	90
<i>C2/m</i>	4	m	-85.200	13.696	7.903	6.845	90	109.43	90
$\bar{P}4_3m$	1	$\bar{4}3m$	-85.032	5.589	5.589	5.589	90	90	90
<i>Pa$\bar{3}$</i>	8	3	-85.012	11.170	11.170	11.170	90	90	90
$\bar{I}4_2m$	2	$\bar{4}2m$	-84.960	5.582	5.582	11.187	90	90	90
<i>P4₂/nmc</i>	2	$\bar{4}2m$	-84.956	7.910	7.910	5.570	90	90	90
<i>P2₁/c</i>	4	1	-84.392	10.225	6.841	10.200	90	101.20	90
<i>C2/c</i>	32	all on 1	-77.480	23.402	12.366	22.728	90	117.11	90

Table 10: Calculated polymorphs for GeF₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>I</i> $\bar{4}3m$	2	$\bar{4}3m$	-86.860	5.697	5.697	5.697	90	90	90
<i>C</i> 2/ <i>c</i>	4	2	-79.880	9.019	4.499	8.452	90	116.77	90
<i>P</i> 2 ₁ / <i>c</i>	4	1	-73.568	7.686	4.937	8.637	90	96.60	90
<i>P</i> $\bar{1}$	16	1	-68.324	9.664	9.676	16.575	85.26	82	68.06
<i>C</i> 2/ <i>c</i>	32	all on 1	-67.412	17.332	9.727	17.264	90	107.56	90
<i>P</i> a $\bar{3}$	8	3	-65.504	8.537	8.537	8.537	90	90	90
<i>P</i> $\bar{4}3m$	1	$\bar{4}3m$	-49.152	4.394	4.394	4.394	90	90	90

Table 11: Calculated polymorphs for GeCl₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C</i> 2/ <i>c</i>	4	2	-82.033	11.048	5.199	10.114	90	116.77	90
<i>I</i> $\bar{4}2m$	2	$\bar{4}2m$	-80.388	5.211	5.211	9.624	90	90	90
<i>P</i> 2 ₁ / <i>c</i>	4	1	-78.184	9.289	6.077	9.465	90	100.41	90
<i>R</i> 3 <i>c</i>	6	1	-77.412	9.211	9.211	11.715	90	90	120
<i>P</i> a $\bar{3}$	8	3	-74.652	10.157	10.157	10.157	90	90	90
<i>C</i> 2/ <i>c</i>	32	all on 1	-72.344	20.849	11.255	20.571	90	114.54	90
<i>P</i> $\bar{4}3m$	1	$\bar{4}3m$	-70.872	5.108	5.108	5.108	90	90	90

Table 12: Calculated polymorphs for GeBr₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-89.530	11.463	15.300	10.401	90	116.71	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-87.712	5.299	5.299	10.106	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-86.411	9.540	6.281	9.674	90	100.57	90
<i>R3c</i>	6	1	-83.873	9.304	9.304	12.139	90	90	120
<i>Pa</i> $\bar{3}$	8	3	-83.428	10.432	10.432	10.432	90	90	90
<i>Pban</i>	2	222	-80.208	10.276	5.279	5.279	90	90	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-79.596	5.249	5.249	5.249	90	90	90
<i>C2/c</i>	32	all on 1	-79.380	21.624	11.493	21.329	90	115.86	90

Table 13: Calculated polymorphs for GeI₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-88.072	12.694	5.645	11.325	90	116.40	90
<i>P2</i> ₁ / <i>c</i>	4	1	-87.284	10.361	6.906	10.363	90	100.94	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-87.280	5.691	5.691	11.310	90	90	90
<i>Pa</i> $\bar{3}$	8	3	-87.232	11.317	11.317	11.317	90	90	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-85.036	5.711	5.711	5.711	90	90	90
<i>C2/m</i>	4	m	-81.919	14.013	8.098	6.937	90	109.31	90
<i>C2/c</i>	32	all on 1	-79.976	23.801	12.397	23.348	90	117.99	90
<i>Cc</i>	4	1	-78.696	10.416	10.166	7.271	90	96.29	90

Table 14: Calculated polymorphs for SnF₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-58.461	9.552	4.561	8.746	90	116.25	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-56.540	4.565	4.565	8.325	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-53.622	8.111	5.234	8.385	90	98.28	90
<i>R3c</i>	6	1	-53.233	7.880	7.880	10.444	90	90	120
<i>Pa</i> $\bar{3}$	8	3	-50.288	8.878	8.878	8.878	90	90	90
<i>C2/c</i>	32	all on 1	-49.218	18.380	9.738	18.143	90	114.65	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-46.380	4.487	4.487	4.487	90	90	90

Table 15: Calculated polymorphs for SnCl₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-73.525	11.636	5.242	10.423	90	116.55	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-73.068	5.241	5.241	5.241	90	90	90
<i>P4</i> ₂ <i>n</i> <i>mc</i>	2	$\bar{4}$ 2 <i>m</i>	-73.020	7.375	7.375	5.245	90	90	90
<i>Pa</i> $\bar{3}$	8	3	-71.672	10.455	10.455	10.455	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-71.575	9.604	6.366	9.581	90	100.59	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-71.244	5.236	5.236	5.236	90	90	90
<i>P</i> $\bar{1}$	2	1	-68.724	6.381	6.407	7.480	89.96	106.87	99.50
<i>C2/c</i>	32	all on 1	-65.620	21.938	11.522	21.505	90	117.31	90

Table 16: Calculated polymorphs for SnBr₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-81.706	11.971	5.310	10.671	90	116.41	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-81.292	5.344	5.344	5.344	90	90	90
<i>Pa</i> $\bar{3}$	8	3	-81.156	10.667	10.667	10.667	90	90	90
<i>P4</i> ₂ <i>n</i> <i>mc</i>	2	$\bar{4}$ 2 <i>m</i>	-81.078	7.593	7.593	5.280	90	90	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-80.104	5.366	5.366	5.366	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-80.104	9.806	6.517	9.756	90	100.62	90
<i>C2/c</i>	32	all on 1	-73.248	22.515	11.742	22.018	90	118.07	90

Table 17: Calculated polymorphs for SnI₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>Pa</i> $\bar{3}$	8	3	-93.484	11.398	11.398	11.398	90	90	90
<i>I2</i> ₁ / <i>a</i>	4	2	-92.956	11.427	5.655	12.885	90	116.46	90
<i>P2</i> ₁ / <i>c</i>	4	1	-92.175	10.462	6.969	10.423	90	100.71	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-91.990	5.741	5.741	11.448	90	90	90
<i>P2</i> ₁ / <i>m</i>	2	m	-91.360	6.948	8.115	6.683	90	90	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-90.128	5.777	5.777	5.777	90	90	90
<i>C2/c</i>	32	all on 1	-84.456	24.110	12.445	23.701	90	118.87	90
<i>R3c</i>	6	1	-81.680	10.030	10.030	13.552	90	90	120

Table 18: Calculated polymorphs for PbF₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-50.197	9.850	4.600	9.937	90	126.31	90
<i>I</i> $\bar{4}$ 2 <i>m</i>	2	$\bar{4}$ 2 <i>m</i>	-48.745	4.589	4.589	8.696	90	90	90
<i>P2</i> ₁ / <i>c</i>	4	1	-46.691	8.301	5.388	8.419	90	98.93	90
<i>Pa</i> $\bar{3}$	8	3	-44.671	9.048	9.048	9.048	90	90	90
<i>C2/c</i>	32	all on 1	-42.731	18.864	9.894	18.672	90	116.04	90
<i>P</i> $\bar{4}$ 3 <i>m</i>	1	$\bar{4}$ 3 <i>m</i>	-42.704	4.545	4.545	4.545	90	90	90

Table 19: Calculated polymorphs for PbCl₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>C2/c</i>	4	2	-69.976	11.830	5.273	10.563	90	116.46	90
<i>P42_nmc</i>	2	$\bar{4}2m$	-69.609	7.500	7.500	5.256	90	90	90
<i>I$\bar{4}2m$</i>	2	$\bar{4}2m$	-69.606	5.294	5.294	10.566	90	90	90
<i>Pa$\bar{3}$</i>	8	3	-68.973	10.570	10.570	10.570	90	90	90
<i>P2₁/c</i>	4	1	-68.337	9.718	6.450	9.673	90	100.57	90
<i>P$\bar{4}3m$</i>	1	$\bar{4}3m$	-68.301	5.308	5.308	5.308	90	90	90
<i>C2/c</i>	32	all on 1	-62.481	22.286	11.634	21.829	90	117.89	90

Table 20: Calculated polymorphs for PbBr₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>Pa$\bar{3}$</i>	8	3	-77.768	10.826	10.826	10.826	90	90	90
<i>C2/c</i>	4	2	-77.625	12.213	5.369	10.851	90	116.27	90
<i>P42_nmc</i>	2	$\bar{4}2m$	-77.354	7.779	7.779	5.286	90	90	90
<i>I$\bar{4}2m$</i>	2	$\bar{4}2m$	-76.713	5.453	5.453	10.875	90	90	90
<i>P2₁/c</i>	4	1	-76.452	9.960	6.615	9.903	90	100.48	90
<i>P$\bar{1}$</i>	2	1	-76.316	6.620	6.659	7.746	106.77	90.03	99.62
<i>P$\bar{4}3m$</i>	1	$\bar{4}3m$	-74.794	5.489	5.489	5.489	90	90	90
<i>C2/c</i>	32	all on 1	-69.862	23.003	11.825	22.601	90	119.10	90

Table 21: Calculated polymorphs for PbI₄

Space group	Z	Site sym.	E/(kJ/mol)	a/Å	b/Å	c/Å	α/°	β/°	γ/°
<i>Pa</i> $\bar{3}$	8	3	-90.733	11.551	11.551	11.551	90	90	90
<i>C2/c</i>	4	2	-89.752	13.057	5.736	11.590	90	115.94	90
<i>P2₁/c</i>	4	1	-89.616	10.600	7.048	10.578	90	100.52	90
<i>P4_{2n}mc</i>	2	$\bar{4}2m$	-89.458	8.383	8.383	5.557	90	90	90
<i>P21/m</i>	2	m	-87.629	7.019	8.295	6.774	90	90	90
<i>I</i> $\bar{4}2m$	2	$\bar{4}2m$	-87.212	5.872	5.872	11.553	90	90	90
<i>P</i> $\bar{4}3m$	1	$\bar{4}3m$	-83.979	5.911	5.911	5.911	90	90	90
<i>C2/c</i>	32	all on 1	-82.338	24.600	12.469	24.330	90	119.90	90