Supporting Information

Atomic Charges in Molecules Defined by Molecular Real Space Partition into Atomic Subspaces

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1. Dependence on the basis sets

1.1 HF molecule

Table S1. The H atomic charges (e) of HF molecule by PAEMQCT, QTAIM, Hirshfeld, Mulliken, NPA, APT, CHELPG, and MK population methods obtained from the CISD method with 19 different basis sets.

Basis sets	PAEMQCT	QTAIM	Hirshfeld	NPA	MK	CHELPG	APT	Mulliken
6-31G	0.319	0.601	0.230	0.527	0.502	0.499	0.392	0.453
6-311G	0.330	0.597	0.228	0.512	0.509	0.506	0.392	0.462
6-31G(d)	0.327	0.690	0.230	0.540	0.442	0.435	0.388	0.494
6-311G(d)	0.338	0.649	0.236	0.516	0.485	0.480	0.396	0.487
6-31+G(d)	0.332	0.656	0.217	0.566	0.467	0.462	0.424	0.551
6-311+G(d)	0.345	0.656	0.227	0.532	0.497	0.492	0.415	0.423
6-31 G(d,p)	0.315	0.711	0.225	0.541	0.432	0.426	0.376	0.373
6-311G(d,p)	0.319	0.701	0.222	0.518	0.439	0.434	0.393	0.299
6-31+G(d,p)	0.325	0.724	0.212	0.568	0.457	0.452	0.414	0.401
6-311+G(d,p)	0.322	0.707	0.212	0.534	0.451	0.447	0.417	0.278
6-311++G(d,p)	0.321	0.708	0.211	0.532	0.451	0.447	0.417	0.283
6-311+G(2d,2p)	0.326	0.736	0.210	0.539	0.434	0.428	0.400	0.344
6-311+G(2df,2pd)	0.328	0.752	0.211	0.539	0.431	0.425	0.401	0.279
6-31++G(3df,3pd)	0.330	0.742	0.210	0.533	0.421	0.414	0.390	0.510
6-311++G(3df,3pd)	0.328	0.752	0.210	0.536	0.427	0.421	0.393	0.357
cc-pVDZ	0.309	0.723	0.221	0.517	0.423	0.418	0.388	0.215
cc-pVTZ	0.333	0.743	0.217	0.531	0.423	0.417	0.389	0.323
aug-cc-pVDZ	0.326	0.720	0.201	0.552	0.419	0.413	0.385	0.273
aug-cc-pVTZ	0.329	0.753	0.208	0.540	0.420	0.414	0.390	0.348
Average	0.3264	0.7011	0.2178	0.5354	0.4489	0.4437	0.3979	0.3765

1.2. H_2O molecule

Table S2. The H atomic charges (e) of H_2O molecule by PAEMQCT, QTAIM, Hirshfeld, Mulliken, NPA, APT, CHELPG, and MK population methods obtained from the CISD method with 19 different basis sets.

Basis sets	PAEMQCT	QTAIM	Hirshfeld	NPA	MK	CHELPG	APT	Mulliken
6-31G	0.218	0.472	0.168	0.368	0.458	0.264	0.456	0.450
6-311G	0.235	0.453	0.168	0.371	0.423	0.258	0.457	0.451
6-31G(d)	0.221	0.560	0.170	0.413	0.466	0.272	0.396	0.386
6-311G(d)	0.241	0.525	0.174	0.405	0.427	0.263	0.422	0.413

6-31+G(d)	0.231	0.569	0.165	0.473	0.485	0.297	0.419	0.410
6-311+G(d)	0.239	0.534	0.169	0.372	0.440	0.281	0.438	0.430
6-31G(d,p)	0.219	0.574	0.167	0.319	0.467	0.259	0.382	0.373
6-311G(d,p)	0.229	0.548	0.166	0.233	0.427	0.251	0.377	0.368
6-31+G(d,p)	0.226	0.585	0.162	0.350	0.486	0.286	0.405	0.396
6-311+G(d,p)	0.226	0.560	0.160	0.247	0.442	0.274	0.392	0.384
6-311++G(d,p)	0.228	0.560	0.160	0.245	0.441	0.273	0.392	0.383
6-311+G(2d,2p)	0.228	0.571	0.157	0.224	0.454	0.264	0.362	0.351
6-311+G(2df,2pd)	0.229	0.598	0.159	0.169	0.456	0.267	0.360	0.349
6-31++G(3df,3pd)	0.229	0.600	0.157	0.458	0.455	0.260	0.348	0.335
6-311++G(3df,3pd)	0.229	0.596	0.158	0.449	0.455	0.258	0.352	0.340
cc-pVDZ	0.215	0.593	0.165	0.138	0.437	0.246	0.357	0.348
cc-pVTZ	0.234	0.589	0.164	0.232	0.448	0.254	0.355	0.343
aug-cc-pVDZ	0.221	0.593	0.153	0.113	0.472	0.252	0.347	0.335
aug-cc-pVTZ	0.225	0.601	0.159	0.211	0.457	0.258	0.347	0.334
Average	0.228	0.562	0.163	0.305	0.452	0.265	0.388	0.378

2. The linear correlation plots between D_{pb} for PAEMQCT and electron density at bond critical point for QTAIM

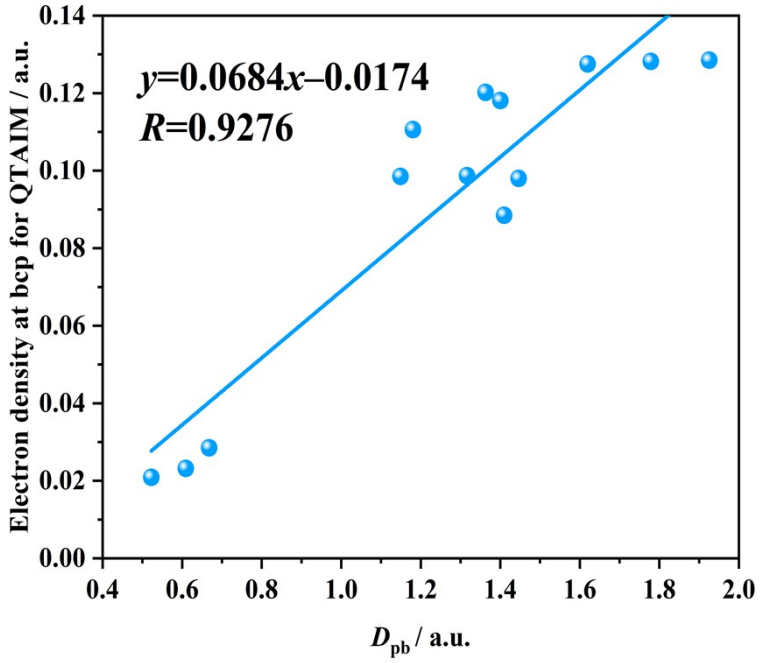


Figure S1. Linear correlation plot between D_{pb} for PAEMQCT and electron density at bcp for QTAIM for the molecules containing Si atom, all units are a.u.

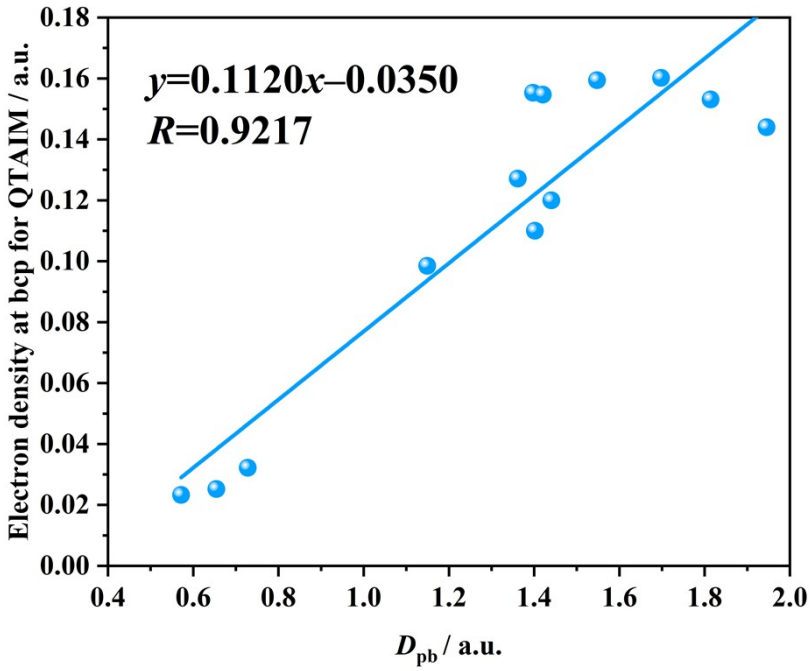


Figure S2. Linear correlation plot between D_{pb} for PAEMQCT and electron density at bcp for QTAIM for the molecules containing P atom, all units are a.u.

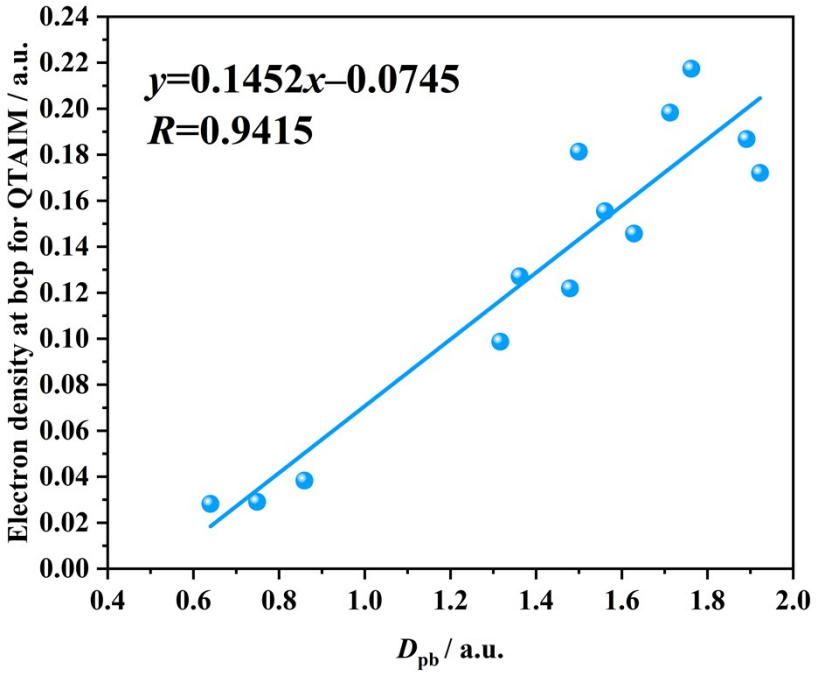
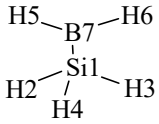
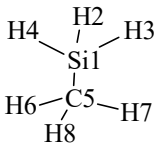
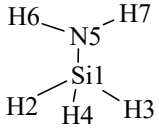
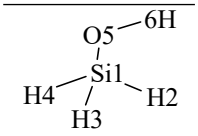
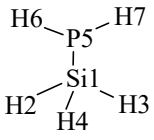
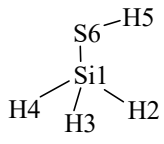


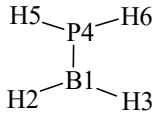
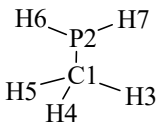
Figure S3. Linear correlation plot between D_{pb} for PAEMQCT and electron density at bcp for QTAIM for the molecules containing S atom, all units are a.u.

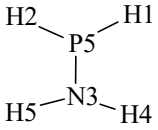
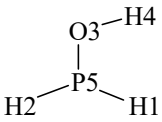
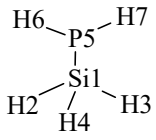
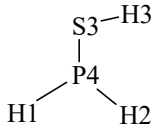
3. Polyatomic molecules

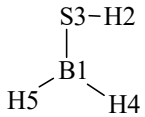
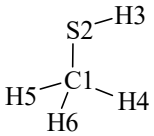
Table S3. Atomic charges (e) of polyatomic molecules containing Si, P, and S atoms obtained by PAEMQCT, QTAIM, Hirshfeld, Mulliken, NPA, APT, CHELPG, and MK population methods at the CISD/6-311++G(d,p) level of theory.

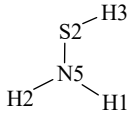
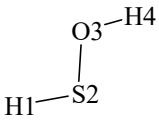
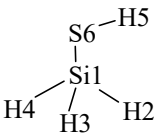
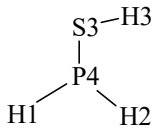
Molecule	Atom	PAEMQCT	QTAIM	Hirshfeld	Mulliken	NPA	APT	CHELPG	MK
SiH_4	Si1	0.564	2.853	0.336	0.705	0.751	1.098	0.687	0.791
	H2	-0.141	-0.713	-0.084	-0.176	-0.188	-0.274	-0.172	-0.198
	H3	-0.141	-0.713	-0.084	-0.176	-0.188	-0.274	-0.172	-0.197
	H4	-0.141	-0.713	-0.084	-0.176	-0.188	-0.274	-0.172	-0.197
	H5	-0.141	-0.713	-0.084	-0.176	-0.188	-0.274	-0.172	-0.198
BH_2SiH_3	Si1	0.492	2.756	0.264	0.671	0.587	0.872	0.276	0.352
	H2	-0.151	-0.720	-0.088	-0.174	-0.178	-0.277	-0.117	-0.133
	H3	-0.151	-0.720	-0.088	-0.174	-0.178	-0.277	-0.117	-0.133
	H4	-0.147	-0.705	-0.082	-0.175	-0.168	-0.264	-0.113	-0.124
	H5	-0.111	-0.657	-0.074	-0.036	-0.106	-0.173	-0.196	-0.167
	H6	-0.111	-0.657	-0.074	-0.036	-0.106	-0.173	-0.196	-0.167
	B7	0.179	0.704	0.142	-0.077	0.149	0.290	0.463	0.371
CH_3SiH_3	Si1	0.633	2.903	0.360	0.811	1.004	1.202	0.769	0.892
	H2	-0.160	-0.730	-0.094	-0.178	-0.206	-0.304	-0.207	-0.234
	H3	-0.160	-0.730	-0.094	-0.178	-0.206	-0.304	-0.207	-0.233
	H4	-0.160	-0.730	-0.094	-0.178	-0.206	-0.304	-0.207	-0.234
	C5	-0.162	-0.710	-0.197	-0.753	-1.014	-0.302	-0.369	-0.494
	H6	0.003	-0.001	0.040	0.159	0.210	0.004	0.074	0.100
	H7	0.003	-0.001	0.040	0.159	0.210	0.004	0.074	0.101
	H8	0.003	-0.001	0.040	0.159	0.210	0.004	0.074	0.102
NH_2SiH_3	Si1	0.738	2.989	0.406	0.761	1.202	1.451	1.071	1.139
	H2	-0.156	-0.728	-0.093	-0.158	-0.223	-0.298	-0.229	-0.241
	H3	-0.156	-0.728	-0.093	-0.158	-0.223	-0.298	-0.229	-0.241
	H4	-0.171	-0.742	-0.107	-0.175	-0.244	-0.348	-0.270	-0.290
	N5	-0.501	-1.530	-0.338	-0.784	-1.261	-0.881	-1.099	-1.143
	H6	0.123	0.369	0.113	0.257	0.374	0.187	0.377	0.388
	H7	0.123	0.369	0.113	0.257	0.374	0.187	0.377	0.388
SiH_3OH	Si1	0.823	3.009	0.440	0.771	1.310	1.553	1.045	1.142

	H2	-0.158	-0.733	-0.096	-0.173	-0.248	-0.324	-0.242	-0.269
	H3	-0.141	-0.720	-0.084	-0.148	-0.229	-0.284	-0.200	-0.220
	H4	-0.158	-0.733	-0.096	-0.173	-0.248	-0.324	-0.242	-0.269
	O5	-0.597	-1.413	-0.342	-0.556	-1.057	-0.942	-0.793	-0.812
	H6	0.231	0.590	0.178	0.279	0.473	0.320	0.431	0.427
SiH_3F	Si1	0.913	3.017	0.478	0.823	1.379	1.613	1.003	1.140
	F2	-0.508	-0.862	-0.228	-0.335	-0.644	-0.731	-0.391	-0.421
	H3	-0.135	-0.719	-0.084	-0.163	-0.245	-0.294	-0.204	-0.240
	H4	-0.135	-0.719	-0.084	-0.163	-0.245	-0.294	-0.204	-0.240
	H5	-0.135	-0.719	-0.084	-0.163	-0.245	-0.294	-0.204	-0.240
SiH_3PH_2	Si1	0.528	2.713	0.280	0.550	0.684	1.039	0.769	0.875
	H2	-0.146	-0.721	-0.081	-0.158	-0.188	-0.285	-0.191	-0.214
	H3	-0.146	-0.721	-0.081	-0.158	-0.188	-0.285	-0.191	-0.214
	H4	-0.147	-0.724	-0.083	-0.163	-0.189	-0.318	-0.210	-0.248
	P5	0.035	0.596	0.037	0.083	-0.044	0.092	-0.335	-0.357
	H6	-0.062	-0.572	-0.036	-0.077	-0.038	-0.122	0.079	0.079
	H7	-0.062	-0.572	-0.036	-0.077	-0.038	-0.122	0.079	0.079
SiH_3SH	Si1	0.622	2.839	0.344	0.593	0.848	1.251	0.722	0.811
	H2	-0.140	-0.722	-0.086	-0.158	-0.200	-0.308	-0.182	-0.204
	H3	-0.134	-0.714	-0.080	-0.136	-0.191	-0.272	-0.134	-0.153
	H4	-0.140	-0.722	-0.086	-0.158	-0.200	-0.308	-0.182	-0.204
	H5	0.040	-0.133	0.059	0.011	0.111	0.027	0.184	0.188
	S6	-0.248	-0.546	-0.152	-0.152	-0.369	-0.390	-0.408	-0.437
SiH_3Cl	Si1	0.734	2.900	0.419	0.566	0.973	1.443	0.747	0.746
	Cl2	-0.353	-0.757	-0.183	-0.191	-0.373	-0.569	-0.281	-0.291
	H3	-0.127	-0.714	-0.079	-0.125	-0.200	-0.291	-0.155	-0.151
	H4	-0.127	-0.714	-0.079	-0.125	-0.200	-0.291	-0.155	-0.153
	H5	-0.127	-0.714	-0.079	-0.125	-0.200	-0.291	-0.155	-0.153
SiH_3Br	Si1	0.670	2.858	0.428	0.740	0.889	1.364	0.644	0.844
	H2	-0.118	-0.713	-0.072	-0.155	-0.193	-0.292	-0.133	-0.182
	H3	-0.118	-0.713	-0.072	-0.155	-0.193	-0.292	-0.133	-0.181
	H4	-0.118	-0.713	-0.072	-0.155	-0.193	-0.292	-0.133	-0.182

	Br5	-0.316	-0.719	-0.210	-0.274	-0.309	-0.489	-0.244	-0.298
SiH_3Li	Si1	0.158	1.323	-0.099	0.429	-0.127	0.379	-0.770	-0.423
	H2	-0.201	-0.737	-0.121	-0.231	-0.190	-0.311	0.039	-0.042
	H3	-0.201	-0.737	-0.121	-0.231	-0.190	-0.311	0.039	-0.041
	H4	-0.201	-0.737	-0.121	-0.231	-0.190	-0.311	0.039	-0.048
	Li5	0.445	0.888	0.461	0.263	0.698	0.553	0.654	0.553
SiH_3Na	Si1	0.152	1.469	-0.107	0.292	-0.090	0.449	-0.600	-0.175
	H2	-0.203	-0.741	-0.125	-0.223	-0.198	-0.351	-0.008	-0.109
	H3	-0.203	-0.741	-0.125	-0.223	-0.198	-0.351	-0.008	-0.108
	H4	-0.203	-0.741	-0.125	-0.223	-0.198	-0.351	-0.008	-0.111
	Na5	0.457	0.754	0.482	0.378	0.686	0.603	0.624	0.502
SiH_3K	Si1	0.063	1.472	-0.151	0.058	-0.175	0.387	-0.329	-0.479
	H2	-0.215	-0.756	-0.136	-0.229	-0.209	-0.372	-0.110	-0.056
	H3	-0.215	-0.756	-0.136	-0.229	-0.209	-0.372	-0.110	-0.057
	H4	-0.215	-0.756	-0.136	-0.229	-0.209	-0.372	-0.110	-0.058
	K5	0.582	0.797	0.559	0.629	0.800	0.728	0.658	0.650
PH_3	P1	0.153	1.689	0.119	0.227	0.149	0.390	-0.185	-0.189
	H2	-0.051	-0.563	-0.040	-0.076	-0.050	-0.130	0.062	0.064
	H3	-0.051	-0.563	-0.040	-0.076	-0.050	-0.130	0.062	0.063
	H4	-0.051	-0.563	-0.040	-0.076	-0.050	-0.130	0.062	0.063
BH_2PH_2	B1	0.237	1.633	0.097	-0.093	0.117	0.467	0.441	0.318
	H2	-0.117	-0.658	-0.066	-0.025	-0.085	-0.156	-0.164	-0.114
	H3	-0.117	-0.658	-0.066	-0.025	-0.085	-0.156	-0.164	-0.114
	P4	0.087	0.821	0.081	0.245	0.086	-0.025	-0.276	-0.267
	H5	-0.045	-0.569	-0.023	-0.051	-0.017	-0.065	0.082	0.088
	H6	-0.045	-0.569	-0.023	-0.051	-0.017	-0.065	0.081	0.088
CH_3PH_2	C1	-0.073	-0.528	-0.166	-0.595	-0.834	-0.092	0.236	0.875
	P2	0.178	1.722	0.135	0.332	0.388	0.440	-0.321	-0.214
	H3	0.007	0.000	0.041	0.145	0.195	-0.034	-0.057	-0.214
	H4	0.008	0.001	0.043	0.149	0.197	0.001	-0.018	-0.248
	H5	0.008	0.001	0.043	0.149	0.197	0.001	-0.018	-0.357
	H6	-0.064	-0.598	-0.048	-0.090	-0.071	-0.159	0.088	0.079

	H7	-0.064	-0.598	-0.048	-0.090	-0.071	-0.159	0.088	0.079
NH_2PH_2	H1	-0.068	-0.609	-0.050	-0.008	-0.092	-0.171	0.086	0.106
	H2	-0.084	-0.620	-0.063	-0.034	-0.112	-0.218	0.083	0.075
	N3	-0.420	-1.438	-0.316	-0.557	-1.130	-0.729	-0.691	-0.746
	H4	0.125	0.368	0.117	0.257	0.363	0.165	0.321	0.332
	H5	0.126	0.372	0.116	0.258	0.366	0.184	0.327	0.357
	P6	0.321	1.927	0.195	0.085	0.605	0.770	-0.125	-0.124
PH_2OH	H1	-0.059	-0.604	-0.045	-0.031	-0.102	-0.168	0.102	0.119
	H2	-0.059	-0.604	-0.045	-0.031	-0.102	-0.167	0.102	0.120
	O3	-0.526	-1.312	-0.317	-0.413	-0.949	-0.790	-0.526	-0.569
	H4	0.228	0.583	0.174	0.283	0.462	0.301	0.415	0.454
	P5	0.416	1.936	0.234	0.192	0.690	0.824	-0.093	-0.124
PH_2F	P1	0.544	1.983	0.297	0.359	0.812	0.975	0.032	0.033
	F2	-0.450	-0.789	-0.216	-0.252	-0.581	-0.653	-0.198	-0.196
	H3	-0.047	-0.597	-0.041	-0.053	-0.116	-0.161	0.083	0.081
	H4	-0.047	-0.597	-0.041	-0.053	-0.116	-0.161	0.083	0.081
SiH_3PH_2	Si1	0.528	2.713	0.280	0.550	0.684	1.039	0.769	0.875
	H2	-0.146	-0.721	-0.081	-0.158	-0.188	-0.285	-0.191	-0.214
	H3	-0.146	-0.721	-0.081	-0.158	-0.188	-0.285	-0.191	-0.214
	H4	-0.147	-0.724	-0.083	-0.163	-0.189	-0.318	-0.210	-0.248
	P5	0.035	0.596	0.037	0.083	-0.044	0.092	-0.335	-0.357
	H6	-0.062	-0.572	-0.036	-0.077	-0.038	-0.122	0.079	0.079
	H7	-0.062	-0.572	-0.036	-0.077	-0.038	-0.122	0.079	0.079
PH_2SH	H1	-0.050	-0.589	-0.039	-0.059	-0.061	-0.138	0.108	0.124
	H2	-0.050	-0.589	-0.039	-0.059	-0.061	-0.138	0.108	0.124
	H3	0.046	-0.123	0.059	0.022	0.104	0.033	0.181	0.211
	P4	0.231	1.475	0.140	0.226	0.276	0.509	-0.148	-0.179
	S5	-0.177	-0.174	-0.121	-0.130	-0.257	-0.266	-0.249	-0.279
PH_2Cl	P1	0.337	1.698	0.241	0.182	0.445	0.748	-0.018	-0.015
	Cl2	-0.270	-0.529	-0.177	-0.132	-0.302	-0.466	-0.164	-0.166
	H3	-0.033	-0.584	-0.032	-0.025	-0.071	-0.141	0.091	0.090
	H4	-0.033	-0.584	-0.032	-0.025	-0.071	-0.141	0.091	0.091

PH_2Br	H1	-0.028	-0.580	-0.023	-0.084	-0.065	-0.138	0.087	0.092
	H2	-0.028	-0.580	-0.023	-0.084	-0.065	-0.138	0.087	0.092
	P3	0.266	1.542	0.260	0.432	0.361	0.659	-0.031	-0.032
	Br4	-0.210	-0.383	-0.215	-0.265	-0.232	-0.383	-0.144	-0.152
$LiPH_2$	H1	-0.122	-0.600	-0.079	-0.154	-0.053	-0.158	0.018	0.023
	H2	-0.122	-0.600	-0.079	-0.154	-0.053	-0.158	0.018	0.023
	Li3	0.514	0.895	0.468	0.271	0.749	0.599	0.635	0.632
	P4	-0.270	0.305	-0.311	0.037	-0.642	-0.283	-0.672	-0.678
$NaPH_2$	H1	-0.128	-0.614	-0.087	-0.166	-0.068	-0.169	0.022	0.025
	H2	-0.128	-0.614	-0.087	-0.166	-0.068	-0.169	0.022	0.025
	P3	-0.255	0.465	-0.327	-0.074	-0.597	-0.286	-0.681	-0.677
	Na4	0.511	0.765	0.502	0.407	0.733	0.624	0.638	0.628
KPH_2	H1	-0.133	-0.633	-0.099	-0.175	-0.080	-0.190	0.025	0.033
	H2	-0.133	-0.633	-0.099	-0.175	-0.080	-0.190	0.025	0.033
	P3	-0.361	0.468	-0.376	-0.369	-0.672	-0.353	-0.784	-0.784
	K4	0.627	0.800	0.575	0.719	0.832	0.733	0.735	0.717
H_2S	S1	-0.102	0.226	-0.108	-0.049	-0.205	-0.064	-0.283	-0.315
	H2	0.051	-0.113	0.054	0.025	0.102	0.032	0.142	0.158
	H3	0.051	-0.113	0.054	0.025	0.102	0.032	0.142	0.158
BH_2SH	B1	0.306	1.919	0.130	-0.094	0.168	0.571	0.381	0.276
	H2	0.055	-0.120	0.066	0.025	0.106	0.022	0.176	0.178
	S3	-0.133	-0.478	-0.050	0.108	-0.107	-0.275	-0.274	-0.259
	H4	-0.115	-0.662	-0.073	-0.028	-0.084	-0.158	-0.161	-0.121
	H5	-0.113	-0.660	-0.073	-0.012	-0.083	-0.160	-0.121	-0.075
CH_3SH	C1	0.012	-0.066	-0.087	-0.504	-0.654	0.142	0.049	0.811
	S2	-0.118	0.277	-0.089	0.055	-0.009	-0.090	-0.369	-0.204
	H3	0.044	-0.288	0.047	0.005	0.086	0.000	0.202	-0.153
	H4	0.017	0.020	0.039	0.142	0.188	-0.032	0.016	-0.204
	H5	0.028	0.038	0.051	0.159	0.202	0.012	0.086	0.188
	H6	0.017	0.019	0.039	0.142	0.188	-0.032	0.016	-0.437
NH_2SH	H1	0.132	0.367	0.109	0.254	0.351	0.157	0.371	0.397
	H2	0.132	0.367	0.109	0.254	0.351	0.157	0.371	0.397

	H3	0.046	-0.121	0.045	0.042	0.075	-0.003	0.177	0.207
	S4	0.026	0.523	-0.017	-0.011	0.174	0.147	-0.131	-0.155
	N5	-0.336	-1.135	-0.247	-0.538	-0.951	-0.458	-0.788	-0.844
SHOH	H1	0.046	-0.108	0.048	0.029	0.056	-0.013	0.152	0.164
	S2	0.168	0.622	0.041	0.068	0.305	0.316	-0.060	-0.074
	O3	-0.457	-1.092	-0.256	-0.369	-0.814	-0.576	-0.467	-0.480
	H4	0.243	0.578	0.168	0.272	0.454	0.273	0.375	0.390
HSF	H1	0.063	-0.066	0.064	0.041	0.060	0.028	0.163	0.181
	S2	0.296	0.684	0.100	0.174	0.417	0.472	0.037	0.008
	F3	-0.359	-0.618	-0.165	-0.215	-0.477	-0.499	-0.200	-0.188
SiH_3SH	Si1	0.622	2.839	0.344	0.593	0.848	1.251	0.722	0.811
	H2	-0.140	-0.722	-0.086	-0.158	-0.200	-0.308	-0.182	-0.204
	H3	-0.134	-0.714	-0.080	-0.136	-0.191	-0.272	-0.134	-0.153
	H4	-0.140	-0.722	-0.086	-0.158	-0.200	-0.308	-0.182	-0.204
	H5	0.040	-0.133	0.059	0.011	0.111	0.027	0.184	0.188
	S6	-0.248	-0.546	-0.152	-0.152	-0.369	-0.390	-0.408	-0.437
PH_2SH	H1	-0.050	-0.589	-0.039	-0.059	-0.061	-0.138	0.108	0.124
	H2	-0.050	-0.589	-0.039	-0.059	-0.061	-0.138	0.108	0.124
	H3	0.046	-0.123	0.059	0.022	0.104	0.033	0.181	0.211
	P4	0.231	1.475	0.140	0.226	0.276	0.509	-0.148	-0.179
	S5	-0.177	-0.174	-0.121	-0.130	-0.257	-0.266	-0.249	-0.279
HSCl	H1	0.078	-0.064	0.065	0.026	0.093	0.025	0.162	0.180
	S2	0.056	0.292	0.041	0.034	0.061	0.221	-0.070	-0.089
	Cl3	-0.134	-0.228	-0.106	-0.061	-0.154	-0.246	-0.092	-0.092
HSBr	H1	0.076	-0.064	0.074	0.024	0.099	0.027	0.159	0.181
	S2	0.007	0.169	0.060	0.115	-0.032	0.125	-0.100	-0.115
	Br3	-0.083	-0.105	-0.134	-0.140	-0.068	-0.152	-0.059	-0.066
LiSH	H1	-0.025	-0.251	0.009	-0.027	0.090	-0.024	0.088	0.117
	Li2	0.594	0.916	0.488	0.373	0.814	0.717	0.697	0.703
	S3	-0.569	-0.665	-0.497	-0.346	-0.904	-0.693	-0.785	-0.819
NaSH	H1	-0.031	-0.278	-0.007	-0.042	0.076	-0.044	0.084	0.115
	S2	-0.580	-0.584	-0.552	-0.496	-0.938	-0.720	-0.841	-0.869

	Na3	0.611	0.862	0.560	0.538	0.862	0.763	0.757	0.754
KSH	H1	-0.049	-0.316	-0.015	-0.042	0.071	-0.044	0.090	0.126
	S2	-0.665	-0.554	-0.582	-0.721	-0.989	-0.804	-0.908	-0.933
	K3	0.714	0.870	0.597	0.763	0.918	0.848	0.818	0.807